EUMETSAT AC SAF ATMOSPHERIC COMPOSITION MONITORING

ALGORITHM THEORETICAL BASIS DOCUMENT

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PRODUCT USER MANUAL

GOME-2 NO_2, H_2O, O_3, SO_2, HCHO and BrO Level 3 daily gridded products

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Products:

Identifier	Name	Acronym
O3M-303	Level 3 daily averaged total ozone	MxG-O-O3-daily
O3M-340	Level 3 dailly averaged total NO_2	MxG-O-NO2-daily
O3M-343	Level 3 daily averaged tropospheric NO_2	MxG-O-NO2Tr-daily
O3M-318	Level 3 daily averaged BrO	MxG-O-BrO-daily
O3M-387	Level 3 daily averaged H_2O	MxG-O-H2O-daily
O3M-346	Level 3 daily averaged HCHO	MxG-O-HCHO-daily
O3M-376	Level 3 daily averaged SO_2	MxG-O-SO2-daily

Reporting period:

GOME-2/Metop-A Jan 2007 – June 2020

GOME-2/Metop-B Jan 2013 – June 2020

GOME-2/Metop-C Feb 2019 – June 2020

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GOME-2A Level 2GDP 4.8

GOME-2B Level 2 GDP 4.8

GOME-2C Level 2 GDP 4.9

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

Background

The monitoring of atmospheric chemistry is essential due to several human caused changes in the atmosphere, like global warming, loss of stratospheric ozone, increasing UV radiation, and pollution.
Furthermore, the monitoring is used to react to the threats caused by the natural hazards as well as follow the effects of the international protocols.
Therefore, monitoring the chemical composition and radiation of the atmosphere is a very important duty for EUMETSAT and the target is to provide information for policy makers, scientists, and general public.

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, OClO, CO, NH_3), 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 and IASI instruments onboard Metop satellites. Another important task besides the near real-time (NRT) and offline data dissemination is the provision of long-term, high-quality atmospheric composition products resulting from reprocessing activities.

Product categories, timeliness and dissemination

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 (total and tropospheric O_3 and NO_2, total SO_2, total HCHO, CO) and ozone profiles
- Near real-time absorbing aerosol height and absorbing aerosol index from polarization measurement detectors
- Near real-time UV indexes, clear-sky and cloud-corrected

Offline products are available within two weeks after measurement and disseminated via dedicated web services.

- Offline trace gas columns (total and tropospheric O_3 and NO_2, total SO_2, total BrO, total HCHO, total H_2O) and ozone profiles
- Offline absorbing aerosol height and absorbing aerosol index from polarization measurement detectors
- Offline surface UV, daily doses and daily maximum values with several weighting functions

Data records are available after reprocessing activities from the AC SAF archives.

- Data records generated in reprocessing
- Lambertian-equivalent reflectivity
- Total OClO
- Total CHOCHO
- Tropospheric BrO

Users can access the AC SAF offline products and data records (free of charge) by registering at the AC SAF web site.

More information about the AC SAF project, products and services: http://acsaf.org/

AC SAF Helpdesk: helpdesk@acsaf.org

Twitter: https://twitter.com/Atmospheric_SAF

CONTENTS

ACRONYMS AND ABBREVIATIONS

AC SAF	SAF on Atmospheric Chemistry Monitoring
AMF	Air Mass Factor
BRDF	Bidirectional Reflectance Distribution Function
DLR	German Aerospace Centre
DOAS	Differential Optical Absorption Spectroscopy
ECV	Essential Climate Variable
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FDCR	Fundamental Climate Data Record
FMI	Finnish Meteorological Institute
GCOS	Global Climate Observing System
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
H2O	Water Vapour
IMF	Remote Sensing Technology Institute
ITCZ	Intertropical Convergence Zone
LOS	Line Of Sight
NIR	Near-infrared
NO2	Nitrogen Dioxide
OCRA	Optical Cloud Recognition Algorithm
REMSS	Remote Sensing System
RMSE	Root Mean Square Error
ROCINN	Retrieval of Cloud Information using Neural Networks
SAD	Scan Angle Dependency
SCD	Slant Column Density
SSD	Service Specification Document
SSMIS	Special Sensor Microwave Imager Sounder
SZA	Solar Zenith Angle
TCDR	Thematic Climate Data Record
TCWV	Total Column Water Vapour
UPAS	Universal Processor for UV/VIS Atmospheric Spectrometers
VIS	Visible
VCD	Vertical Column Density

1. INTRODUCTION

1.1 Purpose and scope

The purpose of this document is to present the theoretical basis and the user manual of the GOME-2 Level 3 daily gridded products. These products contain global daily mean total and tropospheric nitrogen dioxide (NO_2), water vapour (H_2O), ozone (O_3), formaldehyde (HCHO), sulphur dioxide (SO_2) and bromine oxide (BrO). The "Level" terminology is used to denote broad categories of GOME-2 data products: Level 0 (L0) denotes raw spectral channel counts, Level 1B (L1B) denotes calibrated and geo-located radiances, Level 2 (L2) denotes orbital-swath science products, and finally Level 3 (L3) denotes global-gridded science products.

1.2 GOME-2 Level 3 daily gridded products

Satellite instruments provide essential means of obtaining observations of the Earth's atmosphere from a near-global perspective. Therefore the future of the global atmospheric chemistry and air quality observing system depends critically upon a major satellite component. A key requirement for the monitoring of atmospheric chemistry and air quality is consistency and stability which can be best achieved in stable operational environments such as provided by the AC SAF. Satellite data contributing to the determination of long-term records must be part of a system implemented and operated so as to ensure that these data are accurate and adequately homogeneous.

Atmospheric water vapour is the most important natural greenhouse gas in the troposphere, accounting for more than 60 % of the greenhouse effect (Clough and Iacono, 1995; Kiehl and Trenberth, 1997). The knowledge of the effective distribution of the total column water vapour (TCWV) is fundamental for weather monitoring as well as for the evaluation of climate models. Advancing in understanding of variability and changes in water vapour is vital, especially considering that, in contrast to most other greenhouse gases, the H_2O distribution is highly variable.

Ozone (O_3) is an important trace gas of the Earth's atmosphere. In the stratosphere, ozone absorbs ultraviolet radiation from the sun, thus protecting the biosphere from harmful radiation (Eleftheratos et al., 2013; Hegglin et al., 2015). In the lower atmosphere and near the surface, natural ozone has an equally important beneficial role, because it initiates the chemical removal of air pollutants from the atmosphere such as carbon monoxide, nitrogen oxides, and methane. However, ozone at high concentration can also be harmful to humans, plants, and animals. In addition, ozone is a greenhouse gas, warming the Earth's surface. In both the stratosphere and the troposphere, ozone absorbs infrared radiation emitted from Earth's surface, trapping heat in the atmosphere. As a result, increases or decreases in stratospheric or tropospheric ozone induce a climate forcing (Hegglin et al., 2015).

Nitrogen dioxide (NO_2) plays a key role in air quality and atmospheric chemistry. It is an air pollutant affecting human health and ecosystems. In addition, it is an important ozone precursor. NO_2 is catalysis in ozone depletion processes in the stratosphere and it is important for climate change studies, due to its indirect effect on the global climate (Shindell et al., 2009).

Sulphur dioxide (SO_2) is an important trace species playing key role in atmospheric chemistry at both local and global scales through the formation of sulphate aerosols and sulphuric acid. The impacts of SO_2 range from short-term pollution to climate forcing. SO_2 emits to the atmosphere via both natural and anthropogenic processes. About one-third of the global sulphur emissions originate from natural sources (volcanoes and biogenic dimethyl sulphide), the main contributor to the total budget is from anthropogenic emissions mainly from the combustion of fossil fuels (coal and oil) and from smelting.

Formaldehyde (HCHO) is an intermediate product of the oxidation of almost all volatile organic compounds (VOCs). Therefore, it is widely used as an indicator of non-methane volatile organic compounds (NMVOCs) (Fried et al., 2011). VOCs also have significant impacts on the abundance of hydroxyl (OH) radicals in the atmosphere, which is the major oxidant in the troposphere. Major HCHO sources over the continents include the oxidation of VOCs emitted from plants, biomass burning, traffic and industrial emissions. Oxidation of methane (CH_4) emitted from the ocean is the main source of HCHO over water.

Bromine monoxide (BrO) in the lower stratosphere is involved in chain reactions that deplete ozone (Wennberg et al., 1994), while in the troposphere BrO changes the oxidizing capacity through the destruction of ozone. In particular, large amounts of BrO are often observed in the polar boundary layer during spring-time, known as “bromine explosion”, and lead to severe tropospheric ozone depletion by autocatalytic reactions. In addition to polar sea ice regions, enhanced BrO concentrations were also detected over salt lakes/marshes, in the marine boundary layer, and in volcanic plumes.

The daily gridded L3 water vapor, ozone, NO_2, SO_2, HCHO and BrO column products from GOME-2 are generated with consolidated algorithms applied in a consistent way to a homogeneous (reprocessed) Level-2 data-set, as described in this document. A validation/verification of the GOME-2 Level 3 daily gridded products has been carried out in the framework of an AC SAF AS project and is described in [VAL].

1.3 Product Description

The algorithm used for the generation of the L3 daily gridded products takes as input the Level 2 reprocessed data generated by DLR using the GOME Data Processor (GDP) version 4.8 [ATBD, PUM] for GOME-2/Metop-A and GOME-2/Metop-B and GOME Data Processor (GDP) version 4.9 [ATBD, PUM] for GOME-2/ Metop-C. GOME-2/Metop-A data are available over the time period from January 2007 onwards, GOME-2/Metop-B data from January 2013 onwards, and GOME-2/Metop-C data from February 2019 onwards.

All L3 GOME-2 atmospheric products data are organized into user-friendly and self-describing NetCDF-4 (Network Common Data Form) files, based upon the platform (Metop-A, Metop-B or Metop-C) and the temporal period of collection (Daily data set). The L3 daily gridded data products are stored in separate files.

The logical file name convention is:

SENSOR_GAS_LV_YYYYMMDD_SAT_DLR_RV.TYPE

The meaning of the different subset of character string is given below:

- SENSOR denotes the instrument, i.e. GOME
- GAS is the name of the trace gas included in the product, i.e. H2O, O3, NO2, SO2, HCHO, BrO
- LV is the product level, i.e. L3
- DD, MM and YYYY are the day, month and year of the processed products
- SAT is the platform (METOPA/B/C)
- RV is the two digit product review
- TYPE denotes the product format used, i.e. NetCDF-4 (.nc)

Global and group attributes for the files common to all products are listed in the following table:

Table 1-1: List of Global and Group attributes with typical values and a short description.

Global Attributes	typical values	Description
Description	Level 3 Water Vapour data Level 3 O_3 data Level 3 NO_2 data Level 3 SO_2 data Level 3 HCHO data Level 3 BrO data	short description of the file content
Conventions	CF-1.7	Climate and Forecast convention for variable names, units and dates
Filename	GOME_NO2_L3_YYYYMMDD_METOPA_DLR_RV.nc GOME_H2O_L3_YYYYMMDD_METOPB_DLR_RV.nc	The file name starts with the sensor name, followed by the content (NO_2, H_2O, O_3, SO_2, HCHO, BrO), the coverage, the year and the month, the platform and

	GOME_O3_L3_YYYYMMDD_METOPC_DLR_RV.nc	ends with the version number and type

Group Attributes	**typical values**	**Description**
composite_type	1_day	Gridded daily data set
institution	DLR Deutsches Zentrum für Luft und Raumfahrt	Name of the institution responsible for the data
reference	https://acsaf.org/	
creator_name	Pieter Valks	Name of the person responsible for the data
creator_email	Pieter.Valks@dlr.de	contact address
processing_time	YYYY-MM-DDTHH:mm:ssZ	date and time (UTC) when this file was created
base_product	Level2 GDP	Basis of this data product
base_product_version	v 4.8 v 4.9	version of the underlying data
product_algorithm_name	G2_L3_O3	Algorithm name
product_algorithm_version	v 1.0	Version of this data product
product_content	O3,Cloud_Parameters, Surface_Properties	Content of product (main parameters)
product_format_type	netCDF	File type
product_format_version	4	type version
projects	EUMETSAT AC SAF	
geospatial_latitude_min	-90	minimum latitude (degree)
geospatial_latitude_max	90	maximum latitude (degree)
geospatial_latitude_resolution	0.25	Lat. resolution (degree)
geospatial_lat_units	degrees North	
geospatial_longitude_min	-180	minimum longitude (degree)
geospatial_longitude_max	180	maximum longitude (degree)
geospatial_longitude_resolution	0.25	Lon. resolution (degree)
geospatial_long_units	degrees East	
sensor	GOME_2	sensor name
platform	MetOp-A/B/C	Satellite
time_coverage_start	YYYYMMddTHH:mm:ssZ	beginning of the measurement period
time_coverage_end	YYYYMMddTHH:mm:ssZ	end of the measurement period
product_ID	O3M-303 – O3M-376	

The GOME-2 L3 gridded data fields are grouped in the NetCDF file as follows (see also Chap. 3):

PRODUCT group:

- Trace gas columns
- Errors associated to the trace gas columns
- Statistical information
- SUPPORT DATA/DETAILED_RESULTS/ sub-group:
  - CLOUD_PARAMETERS:

- Cloud Fraction
- Cloud Height
- Cloud Albedo

- SURFACE_PROPERTIES:
  - Surface Albedo
  - Surface Height
  - Surface Flag

Each L3 product is produced at a spatial resolution of 0.25°×0.25°, from the complete set of L2 orbit files that span a particular day. The latitude/longitude grid defines the dimensions of the data set (see Table 1.2). A number of statistical summaries are computed for each of these L3 products, depending on the parameters being considered (e.g. standard deviations, fraction of pixels which satisfy some condition for the surface flag).

Table 1.2: Overview of the dimension in the data file.

Dimension			
Dimension name	**Unit**	**Size**	**Description**
latitude	Degree north (-90, 90)	720	0.25° latitudinal resolution
longitude	Degree east (-180, 180	1440	0.25° longitudinal resolution

1.4 Structure of the document

Section 2 gives an overview of the GOME-2 instruments together with a brief description of the level 1-to-2 algorithm used for the retrieval of the H_2O, O_3, NO_2, SO_2, HCHO, and BrO columns. We also introduce the GOME-2 cloud parameters (which are included in the support data provided in the L3 NetCDF-4 files).

In Section 3, the sampling and gridding approaches and the L3 products are described. Topics covered in this section include the computational approaches and the derived statistics associated to each of the L3 daily mean products.

2. INSTRUMENT AND LEVEL-2 RETRIEVAL OVERVIEW

2.1 The GOME-2 instruments

The GOME-2 sensor (Callies et al., 2000) is the follow up of the Global Monitoring Experiment (GOME), launched in 1995 on ERS-2 (Burrows et al., 1999), and the SCIAMACHY sensor, launched in 2002 on ENVISAT (Bovensmann et al., 1999). GOME-2 is a nadir viewing scanning spectrometer which covers the same spectral range as GOME, i.e. from 240 to 790 nm, with a spectral resolution of about 0.54 nm in the visible spectral region. Additionally, two polarization components are measured with polarization measurement devices (PMDs) using 30 broadband channels covering the full spectral range at higher spatial resolution. The German Aerospace Centre (DLR) plays a major role in the design, implementation and operation of the GOME-2 ground segment for trace gas products (including TCWV), as well as cloud properties in the framework of the EUMETSAT's AC SAF project.

The first GOME-2 instrument was mounted on the Metop-A satellite (GOME-2A), which follows a sun-synchronous orbit with a mean altitude of 817 km. The overpass local time at the equator is 09:30 Local Time (LT) with a repeat cycle of 29 days. Metop-A was launched on the 19 October 2006 and operational GOME-2 products are available from January 2007 onwards. A second GOME-2 type sensor on board of the Metop-B satellite (GOME-2B) was launched on the 17 September 2012 and has been fully operational since December 2012. GOME-2 tandem operations started on 15 July 2013. In the tandem mode, GOME-2A operates on a reduced swath width of 960 km, thereby increasing its spatial resolution (40 by 40 km), while GOME-2B continues to operate on a nominal wide swath of 1920 km. This configuration allows the use of the higher spatial resolution data to further study the consistency of the two products in the overlap regions of the GOME-2A and GOME-2B orbits. Finally, the third satellite of the EUMETSAT Polar System series, GOME-2/Metop-C, was launched on 7 November 2018 and provide operational data since January 2019. We can identify important differences between the GOME-type instruments (summarized in Table 2.1), in particular with respect to spatial resolution, default swath width and equator crossing time.

Table 2-1: Summary of the GOME-type instrument characteristics, illustrating the main improvement of GOME-2 compared to its predecessors.

Sensor Satellite	**GOME ERS-2**	**SCIAMACHY ENVISAT**	**GOME-2 Metop-A**	**GOME-2 Metop-B**	**GOME-2 Metop-C**
Data period	06/1995 - 07/2011	08/2002 - 04/2012	01/2007 - present	12/2012 - present	01/2019 - present
Spectral coverage	240 - 790 nm	240-2380 nm	240 - 790 nm	240 - 790 nm	240 - 790 nm
Ground pixel size	320x40 km^2	60 x 30 km^2	80 x 40 km^2 – 40 x 40 km^2 (*)	80 x 40 km^2	80 x 40 km^2
Swath width	960 km	960 km	1920 km - 960 km (*)	1920 km	1920 km
Equator crossing time	10:30 a.m. LT	10:00 a.m. LT	9:30 a.m. LT	9:30 a.m. LT	9:30 a.m. LT
Global coverage	3 days(**)	6 days	1.5 days	1.5 days	1.5 days

(*) GOME-2A tandem operation since 15 July 2013. (**) GOME global coverage was lost in June 2003.

2.2 Level 2 retrieval algorithms

As input for the creation of the L3 gridded products, the GOME-2 L2 columns from GOME-2/Metop-A and GOME-2/Metop-B processed by GDP 4.8 [ATBD] and GOME-2/Metop-C processed by GDP 4.9 [ATBD] are used. A summary of the level 2 retrieval algorithms for each product is given below.

2.2.1 Total Column Water Vapour

Various retrieval methods of the TCWV from space-born spectrometers operating in the visible region have been developed (AMC-DOAS: Noël et al., 1999, Lichtenberg et al., 2010; ERA: Casadio et al., 2000; OCM: Maurellis et al., 2000; IGAM: Lang et al. 2003, 2007; Classical DOAS: Wagner et al. 2003). In contrast to most other methods, the GDP algorithm for the retrieval of water vapour is directly based on a classical DOAS approach, performed in the wavelength interval 614-683 nm, and does not include explicit numerical modelling of the atmospheric radiative transfer. One specific advantage of the DOAS method is that it is only sensitive to differential absorptions, which makes the retrievals less sensitive to instrument changes or instrument degradation. The algorithm consists of three basic steps (described in detail by Wagner et al., 2003, 2006): (1) DOAS fitting, (2) non-linearity absorption correction and (3) Vertical Column Density (VCD) calculation.

In the first step, the spectral DOAS fitting is carried out, taking into account the cross sections of O_2 and O_4, in addition to that of water vapour. To improve the broadband filtering, 3 types of vegetation spectra are included in the fit, together with a synthetic Ring spectrum and, finally, an inverse solar spectrum to correct for possible offsets, e.g. caused by instrumental stray light. In the second step, the water vapour slant column density (SCD) is corrected for the non-linearities arising from the fact that the fine structure water vapour absorption lines are not spectrally resolved by the GOME instrument. In the last step, the water vapour SCD is divided by a "measured" Air Mass Factor (AMF) which is derived from the simultaneously retrieved O_2 and it is defined as the ratio between the measured SCD of O_2 and the known VCD of O_2 for a standard atmosphere. This simple approach has the advantage that it corrects in first order for the effect of varying albedo, aerosol load and cloud cover without the use of additional independent information. It is also important to remark that, in contrast to most other algorithms, the water vapour product from GOME-2 does not rely on additional information, except for the use of an albedo database for the AMF correction. The surface albedo used for the correction is taken from monthly varying albedo maps, which are composite of albedo derived from GOME observations (Koelemeijer et al., 2003) for high latitude (>50°), and SCIAMACHY observations (Grzegorski, 2009) at mid and low latitudes (<40°). For the transition between 40° and 50°, both products are interpolated linearly. This serves the aim to derive a climatologically relevant time series of Total Column Water Vapour (TCWV) measurements (Wagner et al., 2006; Lang et al., 2007; Noël et al., 2008). Currently, the effect of elevated surface terrain is not taken into account in the AMF correction, i.e. over high mountain areas (> 1000 m), the retrieval error in H_2O column is significantly higher.

Compared to GOME/ERS-2 and SCIAMACHY, the observations of GOME-2 have a much wider swath (1920 km scan width). While this broader swath results in a largely improved coverage, also some modification to the H_2O retrieval becomes necessary. In particular, we observe that water vapour total column present a significant Scan Angle Dependency (SAD). There is a bias up to 10

kg/m^2 between the H_2O product for the west and east part of the swath and the central ground pixels. The effect is particularly strong over ocean areas, while the land surface is less affected.

In GDP 4.8, we use the empirical correction for the scan angle dependency introduced in the previous version of the algorithm (Grossi et al., 2015). The correction is based on the GOME-2A full time series and is computed separately over land and ocean surfaces, to take into account the diverse reflectivity properties of the surface. It is computed as follows. Multi-annual monthly mean H_2O total columns are created and employed to select the latitudinal binned regions which contain a sufficient large number of measurements to avoid that the correction is affected by natural variability in the H_2O total columns. Scan angle read-outs toward the nadir scan angle (scan pixel numbers 9-10-11) are then used as reference values to normalize the H_2O total column for every forward angle position and derive a self-consistent correction. Finally, a polynomial is fitted to the normalized measurements in order to remove outliers and obtain a smooth correction function. With this procedure, residuals are of the order of few percent and the bias between the east and west part of the scan is reduced to negligible values.

The water vapour retrieval algorithm uses two cloud indicators to identify and flag cloudy pixels. This is necessary to remove potential systematic effects due to the different altitude profiles of H_2O and O_2 which might still appear in the water vapour product.

The first H_2O cloud flag is set if the retrieved O_2 slant column is below 80% of the maximum O_2 SCD for the respective solar zenith angle (roughly when about 20% from the column to ground is missing). Especially for low and medium high clouds, the relative fraction of the VCD from the ground which is shielded by clouds for O_2 and H_2O can be quite different. Therefore, we require that the main part of the O_2 column is present.

The second cloud flag is set if the product of the GOME-2 cloud fraction and cloud top albedo (see below) exceeds 0.6 (anomalously high cloud top reflection). In this case, the H_2O total column is also set to ‘invalid’ as the pixel might be considered fully clouded.

2.2.2 Total Ozone Column

The retrieval of ozone slant column is based on the DOAS method. Ozone slant columns are retrieved from GOME-2 (ir)radiance within the wavelength window from 325 to 335 nm. Ozone absorption features are prominent in this wavelength range, and GOME-2 measurements have high signal-to-noise and manageable interference effects from other species. The DOAS fits includes two ozone cross sections at 318 K and 343 K in addition an NO_2 cross section and the ring effect are included. Detailed description of the DOAS fit settings can be found in the [ATBD, PUM].

The retrieved ozone slant columns are converted to vertical columns using air mass factors. Vertical distribution profiles are essential a priori information to the calculation of the air mass factor. The air mass factor calculation for ozone vertical column retrieval follows an iterative approach. The algorithm uses a standard ozone profile to retrieve an initial ozone vertical column. Based on the retrieval initial ozone vertical column, the algorithm selects the most appropriate a priori profile from the climatology database (Bhartia, 2003 - TOMS version 8). The radiative transfer model, LIDORT (Spur, 2003), is called online for the radiative transfer calculation of air mass factor with respective a priori ozone profile and cloud information. This iterative retrieval procedure is described in detail in Hao et al. 2014. The iterations end when the change in the retrieved VCDs is less than 0.1% or if a maximum number of iterations are performed. For GOME-2 ozone VCD retrieval, the number of iterations is in most cases smaller than 4.

The cloud parameters are retrieved from GOME-2 measurements using the OCRA and ROCINN algorithms (see Sect. 2.3) and the ozone absorption inside and below the cloud is treated by the intra cloud correction term, which is a function of the SZA and the cloud albedo (Loyola et al., 2011).

2.2.3 Total and tropospheric NO_2 column

The Differential Optical Absorption Spectroscopy (DOAS) method is used to determine NO_2 slant column densities from calibrated GOME-2 (ir)radiance data in the wavelength interval 425–450 nm (Valks et al., 2011) for GOME-2/Metop-A and GOME-2/Metop-B(GDP 4.8). NO_2 absorption features are prominent in this wavelength range, and GOME-2 measurements have high signal-to-noise and manageable interference effects. For GOME-2/Metop-C (GDP 4.9), an alternative fitting-window 430.2-465 nm is used, as there are systematic structures in the DOAS fitting residual for GOME-2C for wavelengths < 430 nm. A single NO_2 cross-section reference spectrum at 240 K (Vandaele et al. 2002) is used, and the interfering species ozone, O_2-O_2 and H_2O are included in the DOAS fit, as well as an additive Fraunhofer Ring spectrum. The NO_2 absorption cross-section has a marked temperature dependence, which has to be taken into account to improve the accuracy of the retrieved columns. In the GDP, an a posteriori correction for the difference between the atmospheric temperature and the 240 K cross-sections temperature is performed on the air mass factor level.

The initial total VCD is computed under the assumption that the troposphere is not polluted. Therefore, the air mass factor is based on stratospheric NO_2 profiles only, whereas the tropospheric NO_2 amount is assumed to be negligible. This approach is valid over large parts of the Earth, but in areas with significant tropospheric NO_2, the total column densities are underestimated and need to be corrected, as described below. The air mass factors are calculated with the LIDORT radiative transfer model for the window mid-point (437.5 nm), since NO_2 is an optically thin absorber in this wavelength region. To incorporate the seasonal and latitudinal variation in stratospheric NO_2 in the air mass factor calculations, a harmonic climatology of stratospheric NO_2 profiles is used (Lambert and Granville, 2004).

Tropospheric NO_2 columns are obtained from the initial total columns by estimating the stratospheric content and removing it from the total amount. Several methods exist for the stratosphere estimation, e.g. see Boersma et al. (2007) and Beirle et al. (2010). In the GDP 4.8, a spatial filtering approach (Wenig et al., 2004) is used by masking potentially polluted areas and then applying a low-pass filter in the zonal direction. This method has been shown to be an improvement on the Pacific reference sector method, which rests on the assumption of a longitudinally homogeneous stratospheric NO_2 layer.

After the stratosphere-troposphere separation, the tropospheric VCD can be determined using a tropospheric air mass factor. For the tropospheric air mass factor computation, monthly average NO_2 profiles from the MOZART-2 CTM are used, determined for the satellite overpass time. GOME-2 derived cloud properties, determined with the OCRA and ROCINN algorithms are used to calculate the air mass factors for scenarios in the presence of clouds (see also Sect. 2.3). The calculation of the tropospheric VCD is complicated in case of (partly) cloudy conditions. For many measurements over cloudy scenes, the cloud-top is well above the NO_2 pollution in the boundary layer, and when the clouds are optical thick, the enhanced tropospheric NO_2 concentrations cannot be detected by GOME-2. Therefore, the tropospheric VCDs calculated for observations with cloud fraction > 20% are flagged in the GOME-2 L2 product.

2.2.4 Total SO_2 Column

The DOAS algorithm for SO_2 (Rix et al., 2009, 2012) is based on the DOAS algorithm developed for ozone retrieval with adjustments to optimize for SO_2 retrieval. The DOAS retrieval of SO_2 slant column is performed in the UV wavelength range of 315-326 nm for GOME-2/Metop-A and -B (GDP 4.8) and 312-325nm for GOME-2/Metop-C (GDP 4.9). Detailed description of the DOAS fit settings can be found in the [ATBD].

The atmospheric background level of SO_2 is in general very low. In order to account for any systematic bias in the retrieved SO_2 column and to ensure a geophysical consistency of the results, a background correction is applied to the data to avoid non-zero columns over regions known to have very low SO_2 and at high solar zenith angles. Therefore, a background correction scheme based on latitude and surface height is used. This offset is calculated on a daily basis for latitude binned within 2 degree width. Furthermore, the offset values are separately calculated for 5 different surface altitude bins. In order to minimize the effect of outliers or missing data in the daily dataset, a median offset value based on the offset values calculated for the last two weeks before the day of interest is finally calculated. This latitude and altitude dependent value is finally subtracted from the SO_2 slant column densities.

Corrected SO_2 slant columns are then converted to vertical columns by using AMFs. The main challenge of the SO_2 retrieval is the unknown height of the SO_2 layer in the atmosphere which can range from the ground up to the stratosphere, depending on the type of emission. To keep it simple and avoid confusion, we assume that most of the atmospheric SO_2 is emitted from volcanic related activities. The SO_2 plume is assumed to follow a Gaussian profile shape with central plume height of 6 km a.s.l. (at about 500 hPa) in the calculation of AMF. The AMF is calculated with the radiative transfer model LIDORT at 320 nm (GOME-2A and GOME-2B) and 313 nm (GOME-2C). For scenarios in the presence of clouds, GOME-2 cloud properties determined with the OCRA and ROCINN algorithms are used to calculate the air mass factors. When the clouds are optically thick, they can strongly affect the detection of SO_2. Therefore, the SO_2 VCDs calculated for observations with cloud radiance fraction >50% are not used in the calculation of Level 3 product.

2.2.5 Total HCHO Column

The total HCHO column algorithm follows a two step approach with DOAS retrieval of HCHO slant columns and subsequently converts the slant columns to vertical columns by using AMFs. To reduce the interference between HCHO and BrO absorption features, a two-step DOAS retrieval of HCHO slant columns is used (De Smedt et al., 2012). The first step is to determine BrO slant columns with a larger fitting window of 332-359 nm which includes five BrO absorption peaks and effectively minimize the cross-correlation between BrO and HCHO. The retrieved BrO slant columns are then used fixed in the subsequent DOAS retrieval of HCHO slant columns in the spectral band of 328.5-346 nm. Detailed description of the DOAS fit settings can be found in the [ATBD, PUM].

Although the DOAS fit settings are optimized to minimize interference from other factors, there are still unresolved spectral interferences between HCHO and BrO absorption features and results in obvious zonally and seasonally dependency. In order to reduce the impact of the artefacts, an absolute normalisation is applied to HCHO slant columns on a daily basis using the reference sector method (Khokhar et al., 2005). The reference sector is chosen over the Pacific Ocean (Longitude: 140°-160° W), where the only source of HCHO is the oxidation of CH_4which can be reproduced by model simulation quite well. The mean HCHO slant column density in the reference sector is

determined by a polynomial fit, which is then subtracted from the retrieved slant columns on this day, and replaced by a HCHO background value taken from IMAGESv2 model simulation.

Corrected HCHO slant columns are then converted to vertical columns by using AMFs. In the GDP, HCHO AMFs are calculated at 335 nm using the radiative transfer model LIDORT. The a priori HCHO profiles are monthly averaged profiles taken from chemistry transport model (CTM) IMAGES version 2 (Müller and Stavrakou, 2005) simulation in 2007. The model data has a horizontal resolution of 2.0° (latitude) x 2.5° (longitude), with 40 vertical layers extending from the surface up to ~44 hPa. For scenarios in the presence of clouds, GOME-2 cloud properties determined with the OCRA and ROCINN algorithms are used to calculate the air mass factors. For cloudy scene measurements, clouds are usually above the boundary layer where the major part of HCHO is located. If the clouds are optically thick, HCHO below cloud cannot be detected by the satellite. Therefore, the HCHO VCDs calculated for observations with cloud radiance fraction >50% are not used in the calculation of Level 3 product.

2.2.6 Total BrO Column

The total BrO column algorithm also follows a two step approach with DOAS retrieval of BrO slant columns and subsequently converts the slant columns to vertical columns by using AMFs. The DOAS retrieval of BrO slant columns is applied to the spectral range of 332-359 nm which covers five BrO absorption peaks and minimizes the interference from other trace gases, especially formaldehyde (Theys et al., 2011). This fitting window can also minimize other artefacts due to instrument noise, viewing angle dependency and interference from incomplete ring effect correction. Detailed description of the DOAS fit settings can be found in the [ATBD, PUM].

The instrumental degradation of GOME-2A has negative influences on the DOAS fit residuals, the noise level in the BrO columns, and the average slant columns values. Therefore, an equatorial offset correction is applied on a daily basis to the BrO data (Richter and Burrows, 2002). This correction enables to correct – to some extend – for the effect of the instrumental degradation on the total BrO column data time series. Averaged BrO slant columns in the tropical latitudinal band between ±5° are calculated on a daily basis, assuming small equatorial BrO columns with no significant seasonal variations. These averaged slant columns are then subtracted from all slant columns and a constant equatorial slant column offset of 7.5×10^{13} molec/cm² is added.

Corrected BrO slant columns are then converted to vertical columns by using AMFs. In the GDP, BrO AMFs are calculated at 344 nm (mid-point of spectral fitting window) using the radiative transfer model LIDORT. Monthly climatology BrO profiles (Bruns et al., 2003) are used in the AMF calculations. These climatology BrO profiles are taken from the chemistry transport model SLIMCAT simulations. For scenarios in the presence of clouds, GOME-2 cloud properties determined with the OCRA and ROCINN algorithms are used to calculate the air mass factors. As BrO has major contribution from the stratosphere which is usually above clouds, therefore, all measurements (cloudy and clear sky) are used in the Level 3 product.

2.3 Cloud parameters

The presence of clouds significantly affects the retrieval of tropospheric trace gases in the visible spectral range and it is very important to derive information on cloud properties from the GOME-2 observations to study the indirect effects of residual cloud contamination in the Level 2 product. In

most cases the predominant effect of clouds is to shield the absorption below the cloud. However, there can also be an enhancement in the absorption due to multiple scattering events within the cloud. In the retrieval of the trace gases the computation of the VCD assumes the independent pixel approximation (IPA) for cloud treatment. For water vapour, especially in the case of low clouds and large cloud fractions, very large errors can occur because of the differential shielding of the O_2 and H_2O profiles and cloudy cases are flagged.

In the GDP, the OCRA and ROCINN algorithms (Loyola et al., 2007) are used for obtaining GOME-2 cloud information. Clouds are regarded as reflecting Lambertian surfaces and cloud information is reduced to the specification of three parameters: cloud fraction, cloud-top albedo and cloud-top pressure. While OCRA provides the radiometric cloud fraction using the broad-band polarization UVN measurements, ROCINN provides effective cloud pressure and cloud albedo from measurements in and adjacent to the oxygen A-band around 760 nm.

The basic idea in OCRA (Optical Cloud Recognition Algorithm (Loyola and Ruppert, 1998; Lutz et al., 2016) is to break down each optical sensor measurement into two components: a cloud-free background and a residual contribution expressing the influence of clouds. The key to the algorithm is the construction of a cloud-free composite that is invariant with respect to atmosphere, to topography and to solar and viewing angles. The effective cloud fraction is determined by examining the separation between the reflectance measured by the PMDs of GOME-2 and their cloud-free composite values. Note that being sensitive to light scattered by clouds, OCRA is also sensitive to scattering by aerosols present in a given GOME-2 scene, so that both effects are subsumed in the retrieved cloud fraction. Moreover, an important upgrade for GOME-2 is the ability to distinguish clouds in measurements affected by ocean surface sun-glint, a phenomenon that is common at the edges of the GOME-2 swath. OCRA discriminates clouds in the region affected by sun-glint by analysing the broad-band polarization measurements (Loyola et al., 2011; Lutz et al., 2016).

The cloud fraction derived from the OCRA algorithm is taken as fixed input to the ROCINN algorithm (Loyola, 2004), which delivers cloud-top height and cloud albedo using measurements inside the O_2-A absorption band. In the simulations, attenuation through oxygen absorption of the direct solar beam and its reflection from ground or cloud-top is considered and surfaces are assumed to be Lambertian reflectors. The surface albedo is an important input parameter for the simulations and in ROCINN version 3, the MERIS black-sky albedo climatology is used. In ROCINN v3, the radiative transfer simulations include also Rayleigh scattering and polarization. High-resolution reflectances computed with VLIDORT (Spurr, 2006) are used to create a complete data set of simulated reflectance for all viewing geometries and geophysical scenarios, and for various combinations of cloud fraction, cloud-top height and cloud-top albedo. The inversion is performed using neural network techniques. Finally, the cloud-top pressure for GOME-2 scenes is derived from the cloud-top height provided by ROCINN and an appropriated pressure profile (U.S. Standard Atmosphere).

3. LEVEL 3 DATA

3.1 Theoretical description: sampling and gridding

GOME Level 3 data products are developed with the aim of providing the scientific community with easily translatable data, to both facilitate scientific progress (e.g. on climate trend analysis and low-frequency climate variability) and satisfy public interest.

The creation of GOME-2 L3 data involves the selection of a global, 2- dimensional spatial grid for binning the equivalent L2 data into the grid cell. A latitude longitude grid of 0.25º×0.25º was used for translating the spatial information expressed in the GOME-2 ground pixels into a regular latitude longitude grid system. Analyses using various different resolutions (i.e. 0.1º×0.1º, 0.25º×0.25º and 0.5º×0.5º) showed that the spatial resolution of 0.25º × 0.25º is a balance to preserve the satellite resolution (40 km×40 km and 40 km×80 km) while capturing the strong spatial variations in most of the tropospheric gases, i.e., water vapour, NO_2, SO_2 and HCHO.

The binning process for the data set included taking the arithmetic mean and standard deviation of all L2 data points falling into the grid cell in a given month, with possible trimming of low quality measurements due to large spectral fit residual and cloud contamination for tropospheric species, i.e., water vapour, tropospheric NO_2, SO_2 and HCHO. For all species, only forward-scan pixels are used in the gridding process. In case of cloudy measurements, most of the tropospheric gases, i.e., water vapour, tropospheric NO_2, SO_2 and HCHO, are mainly situated below the clouds, while satellite observations could not measure the part below cloud and result in large uncertainties. Therefore, these measurements are not used in the gridding. For these tropospheric species, measurements with cloud radiance fraction larger than 0.5 are not used, while no cloud filtering is applied for stratospheric species, i.e., total NO_2, O_3 and BrO.

Because of the relatively large GOME-2 pixel size, a significant grid effect would be induced by assigning each GOME-2 measurement to a single grid point based on the center coordinates of the GOME-2 ground pixel, without taking into account the pixel geometry and extension. Therefore, the regridding process considers the overlapping area of GOME-2 ground pixel and latitude longitude grid. For grid cells partially overlapping with the satellite pixel, the percentage of overlap (satellite pixel fully cover the entire grid cell is considered as 100% overlap) is calculated and used as weighting for the calculation of mean value. Because of the large dimension of the data set, the weighted mean and variance are calculated in a single pass, using a stable online algorithm (Knuth, 1998). To compute the variance we update the sum of squares of differences from the current mean (below denoted as $M_{2,n}$), as:

$$s_n^2 = \frac{M_{2,n}}{n-1},\ M_{2,n} = M_{2,n-1} + (x_n - \bar{x}_{n-1}) * (x_n - \bar{x}_n) \quad (1)$$

where:

$$\bar{x}_n = \bar{x}_{n-1} + \frac{(x_n - \bar{x}_{n-1})}{n} \quad (2)$$

is the sample mean of the first n measurements. This algorithm is much less prone to catastrophic cancellation and can be extended to handle the area weights by replacing the simple counter “n” in Eq. 1 and 2 with the sum of weights in the grid cell (West, 1979).

3.2 Level 3 mapped H_2O parameters

The daily averaged GOME-2 TCWV for each grid cell is given in the PRODUCT group. The temporal resolution of the product is daily. Grid maps coordinates range from -180.0° to +180.0° in longitude and from -90.0° to 90.0° in latitude. Both the mean errors associated to the L2 measurements and the standard deviations associated to the observed values are computed. An area weighted tessellation technique is used to compute the TCWV and the associated standard deviation, as described in Sect. 3.1

Table 3.1: List of Level 3 mapped H_2O products

Variable name	Unit	Size	Description
latitude	Degree north	720 / 0.25°	Centre of the gridded data Latitudinal resolution
longitude	Degree east	1440 / 0.25°	Centre of the gridded data Longitudinal resolution
group: PRODUCT			
tcwv	kg m^{-2}	720 × 1440	averaged total column water vapour
tcwv_err	kg m^{-2}	720 × 1440	averaged error associated to the total column water vapour retrieval
tcwv_stddev	kg m^{-2}	720 × 1440	standard deviation associated to the total column water vapour grid cells
nobs	-	720 × 1440	number of individual observations in the grid cell
group: SUPPORT_DATA			
group: DETAILED_RESULTS			
CLOUD_PARAMETERS		Table 3.7	
SURFACE_PROPERTIES		Table 3.8	

Figure 3.1 shows an example of the daily gridded total column water vapour (parameter *tcwv* in PRODUCT group) derived from GOME-2/Metop-A measurements on 1 February 2018. The Level-2 data retrieval is performed in the visible/near-infrared spectral range and it is very sensitive to water vapour in the lower troposphere, which contributes the major fraction of the total atmospheric column. The spatial patterns in the humidity distribution show high values in the tropics and low humidity at higher latitudes.

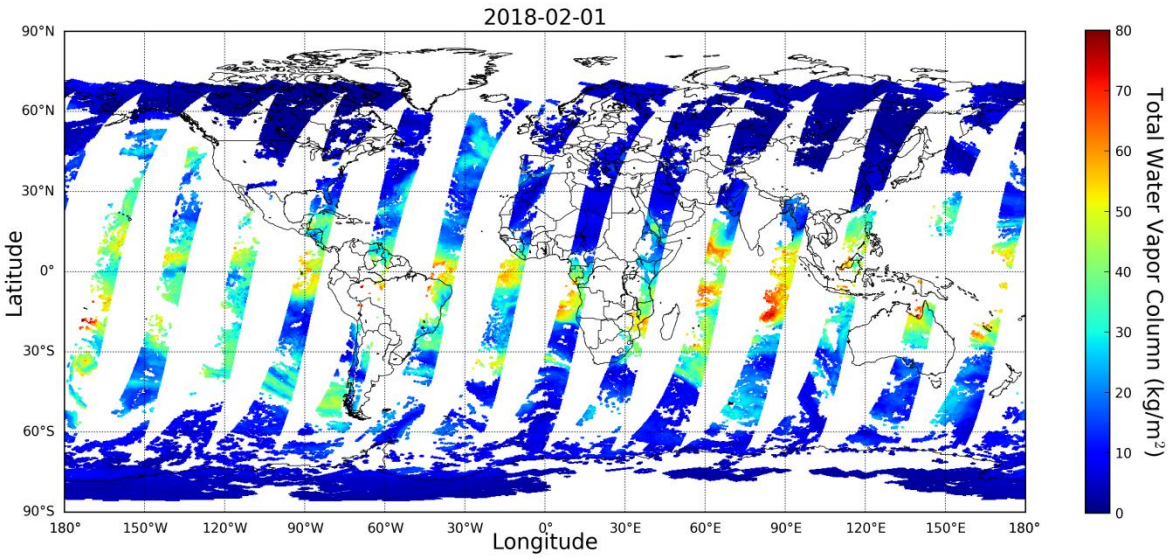

Figure 3.1: Geographical distribution of vertical column of water vapour derived from GOME-2/Metop-A measurements on 1 February 2018. Missing data is due to cloud filtering.

3.3 Level 3 mapped O_3 parameters

The daily averaged GOME-2 total ozone column for each grid cell is given in the PRODUCT group. The temporal resolution of the product is daily. Grid maps coordinates range from -180.0° to +180.0° in longitude and from -90.0° to 90.0° in latitude. Both the mean errors associated to the L2 measurements and the standard deviations associated to the observed values are computed. An area weighted tessellation technique is used to compute the total ozone column and the associated standard deviation, as described in Sect. 3.1.

Table 3.2: List of Level 3 mapped O_3 products

Variable name	**Unit**	**Size**	**Description**
latitude	Degree north	720 / 0.25°	Centre of the gridded data Latitudinal resolution
longitude	Degree east	1440 / 0.25°	Centre of the gridded data Longitudinal resolution
group: PRODUCT			
o3	DU	720 × 1440	averaged total O_3 column
o3_err	DU	720 × 1440	averaged error associated to the total O_3 column
o3_stddev	DU	720 × 1440	total O_3 column standard deviation
o3_nobs	-	720 × 1440	number of individual observations in the grid cell
group: SUPPORT_DATA			
group: DETAILED_RESULTS			
CLOUD_PARAMETERS		Table 3.7	
SURFACE_PROPERTIES		Table 3.8	

Figure 3.2 shows an example of the daily gridded total ozone column (parameter *O3* in PRODUCT group) derived from GOME-2/Metop-A measurements in February 2018. Enhanced ozone column can be observed over high latitudes in the northern hemisphere, while lower ozone levels are expected over the tropics.

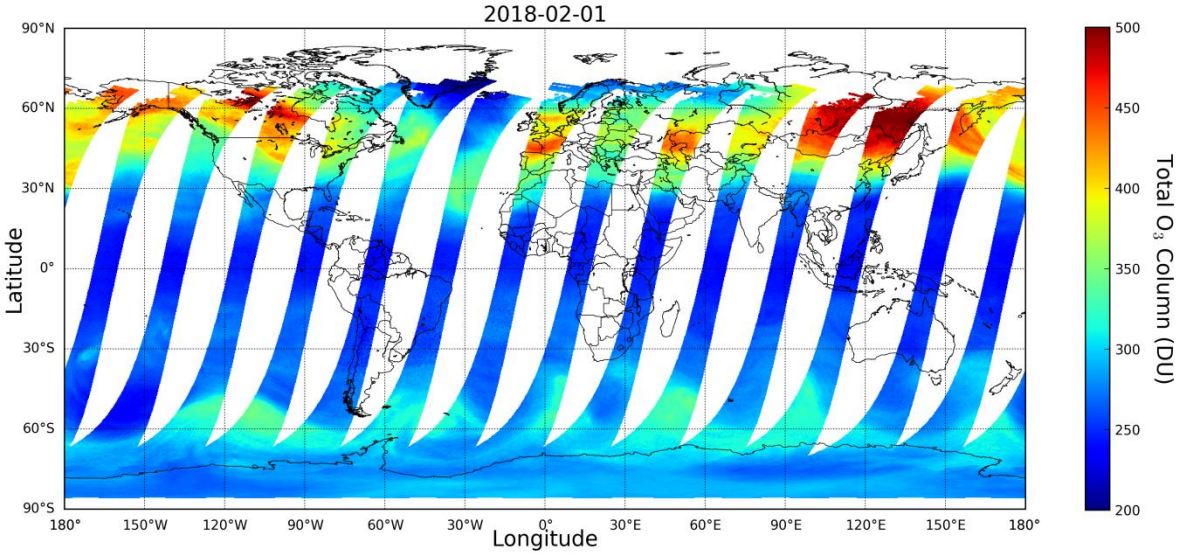

Figure 3.2: Geographical distribution of total ozone columns derived from GOME-2/Metop-A measurements on 1 February 2018.

3.4 Level 3 mapped NO_2 parameters

The daily averaged GOME-2 total and tropospheric NO_2 column for each grid cell is given in the PRODUCT group. The temporal resolution of the product is daily. Grid maps coordinates range from -180.0° to +180.0° in longitude and from -90.0° to 90.0° in latitude. Both the mean errors associated to the L2 retrieval and the standard deviations associated to the variation of the individual (gridded) measurements in each grid-cell are computed. An area weighted tessellation technique is used to compute the NO_2 columns and the associated standard deviations, as described in Sect. 3.1.

Table 3.3: List of Level 3 mapped NO_2 products.

Variable name	Unit	Size	Description
latitude	Degree north	720 / 0.25°	Centre of the gridded data Latitudinal resolution
longitude	Degree east	1440 / 0.25°	Centre of the gridded data Longitudinal resolution
group: PRODUCT			
no2total	molec cm^{-2}	720 × 1440	averaged total NO_2 column
no2total_err	molec cm^{-2}	720 × 1440	averaged error associated to the total NO_2 column
no2total_stddev	molec cm^{-2}	720 × 1440	total NO_2 column standard deviation
no2total_nobs	-	720 × 1440	number of individual total NO_2 observations in the grid cell
no2trop	molec cm^{-2}	720 × 1440	averaged troposphericNO_2 column
no2trop_err	molec cm^{-2}	720 × 1440	averaged error associated to the troposphericNO_2 column retrieval
no2trop_stddev	molec cm^{-2}	720 × 1440	standard deviation associated to the tropospheric NO_2 column grid cells
no2trop_nobs	-	720 × 1440	number of individual tropospheric NO_2 observations in the grid cell
group: SUPPORT_DATA			
group: DETAILED_RESULTS			
CLOUD_PARAMETERS		Table 3.7	
SURFACE_PROPERTIES		Table 3.8	

As an example, the daily gridded tropospheric NO_2 column (parameter *NO2trop* in PRODUCT group) derived from GOME-2/Metop-A measurements using area weighted tessellation is shown in Fig. 3.3 for February 2018. Clearly visible are the high tropospheric NO_2 concentrations above large urban and industrial areas in Asia.

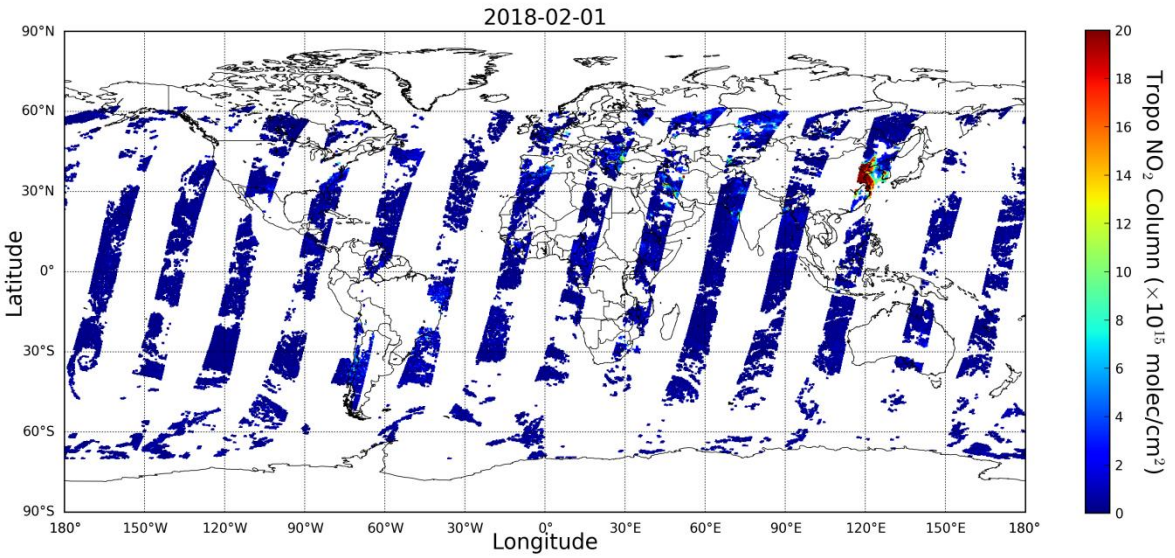

Figure 3.3: Geographical distribution of tropospheric NO_2 column derived from GOME-2/Metop-A measurements on 1 February 2018. Missing data is due to cloud filtering.

3.5 Level 3 mapped SO_2 parameters

The daily averaged GOME-2 total SO_2 column for each grid cell is given in the PRODUCT group. The temporal resolution of the product is daily. Grid maps coordinates range from -180.0° to +180.0° in longitude and from -90.0° to 90.0° in latitude. Both the mean errors associated to the L2 measurements and the standard deviations associated to the observed values are computed. An area weighted tessellation technique is used to compute the SO_2 column and the associated standard deviation, as described in Sect. 3.1

Table 3.4: List of Level 3 mapped SO_2 products

Variable name	Unit	Size	Description
latitude	Degree north	720 / 0.25°	Centre of the gridded data Latitudinal resolution
longitude	Degree east	1440 / 0.25°	Centre of the gridded data Longitudinal resolution
group: PRODUCT			
so2	DU	720 × 1440	averaged total SO_2 column
so2_err	DU	720 × 1440	averaged error associated to the total SO_2 column
so2_stddev	DU	720 × 1440	total SO_2 column standard deviation
so2_nobs	-	720 × 1440	number of individual observations in the grid cell
group: SUPPORT_DATA			
group: DETAILED_RESULTS			
CLOUD_PARAMETERS		Table 3.7	
SURFACE_PROPERTIES		Table 3.8	

Figure 3.4 shows an example of the daily gridded total SO_2 column (parameter *SO2* in PRODUCT group) derived from GOME-2/Metop-A measurements in Feb. 2018. The SO_2 levels are in general very low (below 1DU).

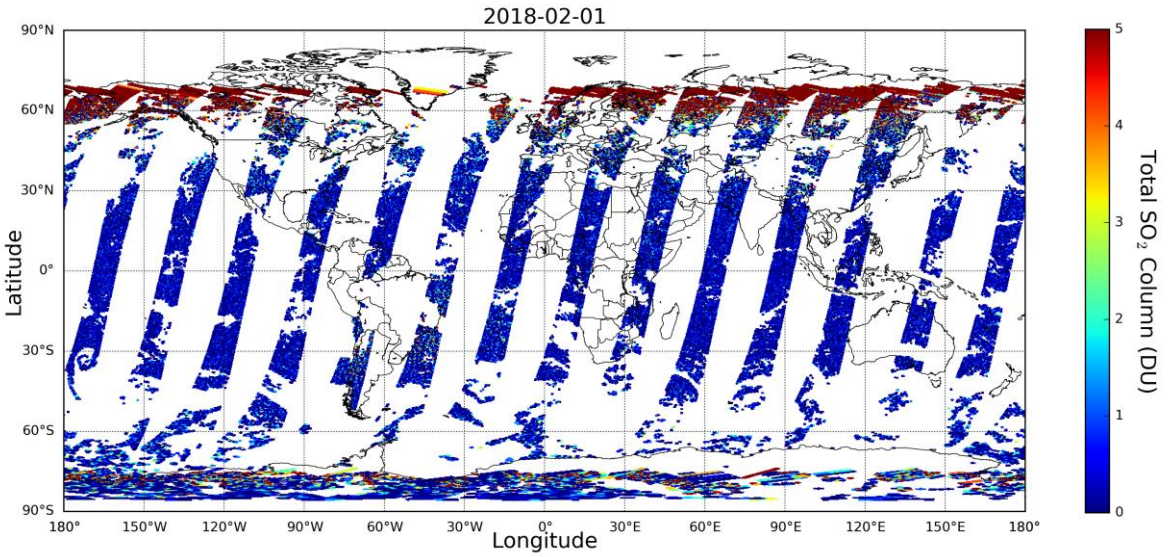

Figure 3.4: Geographical distribution of total SO_2 columns derived from GOME-2/Metop-A measurements 1 February 2018. Missing data is due to cloud filtering.

3.6 Level 3 mapped HCHO parameters

The daily averaged GOME-2 total HCHO column for each grid cell is given in the PRODUCT group. The temporal resolution of the product is daily. Grid maps coordinates range from -180.0° to +180.0° in longitude and from -90.0° to 90.0° in latitude. Both the mean errors associated to the L2 measurements and the standard deviations associated to the observed values are computed. An area weighted tessellation technique is used to compute the HCHO column and the associated standard deviation, as described in Sect. 3.1

Table 3.5: List of Level 3 mapped HCHO products

Variable name	Unit	Size	Description
latitude	Degree north	720 / 0.25°	Centre of the gridded data Latitudinal resolution
longitude	Degree east	1440 / 0.25°	Centre of the gridded data Longitudinal resolution
group: PRODUCT			
hcho	molec cm^{-2}	720 × 1440	averaged total HCHO column
hcho_err	molec cm^{-2}	720 × 1440	averaged error associated to the total HCHO column
hcho_stddev	molec cm^{-2}	720 × 1440	total HCHO column standard deviation
hcho_nobs	-	720 × 1440	number of individual observations in the grid cell
group: SUPPORT_DATA			
group: DETAILED_RESULTS			
CLOUD_PARAMETERS		Table 3.7	
SURFACE_PROPERTIES		Table 3.8	

Figure 3.5 shows an example of the daily gridded total HCHO column (parameter *HCHO* in PRODUCT group) derived from GOME-2/Metop-A measurements on 1 February 2018. Elevated HCHO column can be observed over Central Africa, India, Indochina Peninsula and Indonesia which is related to enhanced agriculture related biomass burning activities during spring time.

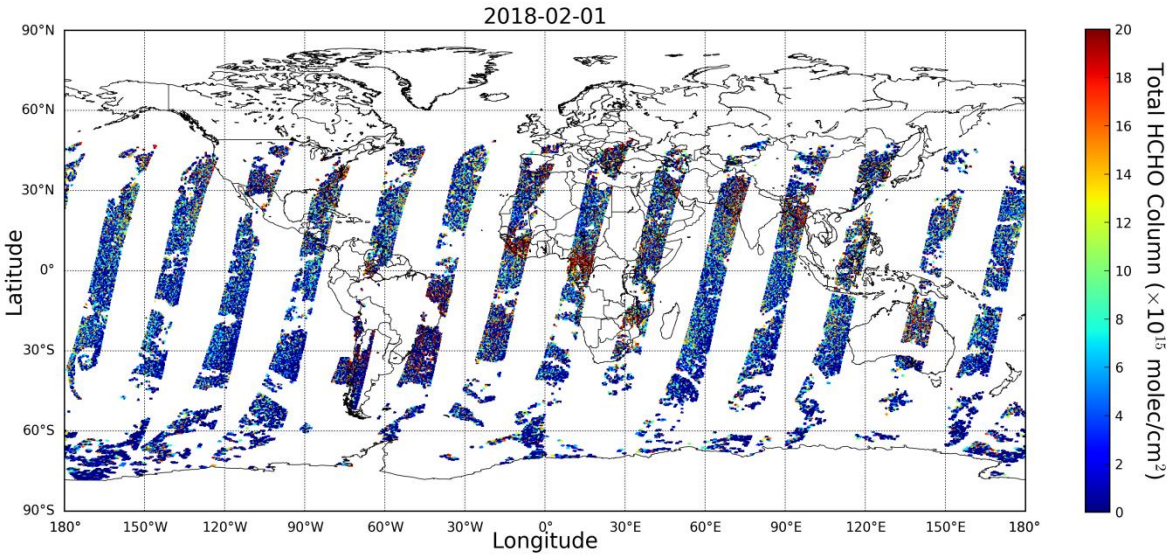

Figure 3.5: Geographical distribution of total HCHO columns derived from GOME-2/Metop-A measurements on 1 February 2018. Missing data is due to cloud filtering.

3.7 Level 3 mapped BrO parameters

The daily averaged GOME-2 total BrO column for each grid cell is given in the PRODUCT group. The temporal resolution of the product is daily. Grid maps coordinates range from -180.0° to +180.0° in longitude and from -90.0° to 90.0° in latitude. Both the mean errors associated to the L2 measurements and the standard deviations associated to the observed values are computed. An area weighted tessellation technique is used to compute the total BrO column and the associated standard deviation, as described in Sect. 3.1

Table 3.6: List of Level 3 mapped BrO products

Variable name	**Unit**	**Size**	**Description**
latitude	Degree north	720 / 0.25°	Centre of the gridded data Latitudinal resolution
longitude	Degree east	1440 / 0.25°	Centre of the gridded data Longitudinal resolution
group: PRODUCT			
bro	molec cm^{-2}	720 × 1440	averaged total BrO column
bro_err	molec cm^{-2}	720 × 1440	averaged error associated to the total BrO column
bro_stddev	molec cm^{-2}	720 × 1440	total BrO column standard deviation
bro_nobs	-	720 × 1440	number of individual observations in the grid cell
group: SUPPORT_DATA			
group: DETAILED_RESULTS			
CLOUD_PARAMETERS		Table 3.7	
SURFACE_PROPERTIES		Table 3.8	

Figure 3.6 shows an example of the daily gridded total BrO column (parameter *BrO* in PRODUCT group) derived from GOME-2/Metop-A measurements on 1 February 2018. As expected, elevated BrO columns are observed at higher latitudes in both Northern and Southern hemisphere, while lower BrO levels are observed over the tropics.

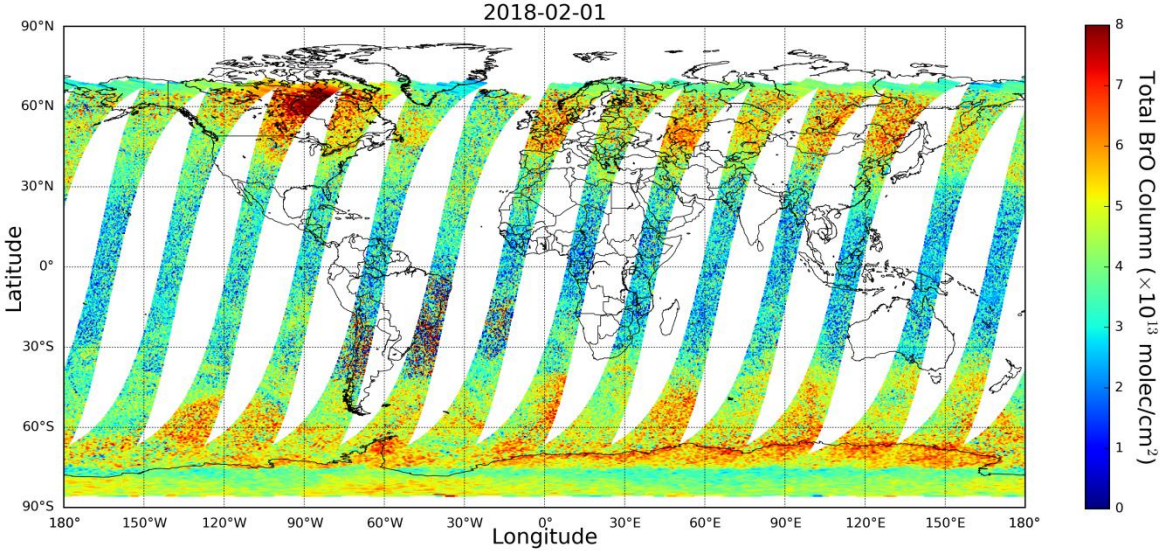

Figure 3.6: Geographical distribution of total BrO columns derived from GOME-2/Metop-A measurements on 1 February 2018.

3.8 Cloud properties

The L3 mapped products are computed from GOME-2 measurements of trace gas columns which are not flagged as cloud contaminated in the L2 data. Tropospheric species, such as water vapour, tropospheric NO_2, SO_2 and HCHO, only observations with cloud radiance fraction < 50% are used (see also Sect. 2.2).

The effects of a residual cloud contamination on observations of tropospheric trace gases can be investigated by looking at the averaged cloud parameters (cloud fraction, cloud height and cloud albedo) associated to the cloud screened observations in a given grid cell (see Table 3.7). The standard deviations for each of these parameters are also given to appreciate how much variation there is from the average. The number of individual observation in each grid cell (*nobs*) is provided in the PRODUCT group.

Table 3.7: Averaged Level 3 cloud parameters.

Variable name	Unit	Size	Description
cloud_fraction	-	720 x 1440	average cloud fraction
cloud_fraction_std	-	720 x 1440	cloud fraction standard deviation
cloud_height	km	720 x 1440	average cloud height
cloud_height_std	km	720 x 1440	cloud height standard deviation
cloud_albedo	-	720 x 1440	average cloud top albedo
cloud_albedo_std	-	720 x 1440	cloud top albedo standard deviation

3.9 Surface properties

The surface height and albedo for each grid cell, and a surface condition flag is provided in the SURFACE_PROPERTIES group. The surface properties from the L2 data are averaged to the resolution on the L3 product. The number of individual observation in each grid cell (*nobs*) is provided in the PRODUCT group.

Table 3.8: Averaged Level 3 surface properties.

Variable name	Unit	Size	Description
surface_albedo	-	360 x 720 / 720 x 1440	average surface albedo
surface_height	km	360 x 720 / 720 x 1440	average surface height
surface_flag	-	360 x 720 / 720 x 1440	land sea flag (see Table 3.9)

3.9.1 Surface condition flag

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 different pixels of the GOME-2 Level-2 product. Also PMD subpixels affected by sunglints are considered to derive the surface flag. To distinguish smaller land masses (e.g. Hawaii or Indonesia) in the resolution of the L3 product (0.25º×0.25º / 0.5º×0.5º), a “coastal” value was introduced.

Table 3.9: Land / sea flag

Flag value	Description	Threshold
0	Land	if less than 20 % of all GOME-2 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

REFERENCES

Applicable documents

[ATBD] Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, NO_2, BrO, SO_2, H_2O, HCHO, OClO and Cloud Properties (GDP 4.8/4.9), SAF/AC/DLR/ATBD/01, Iss. 3/B, Valks, P., et al., 2019. Download: https://acsaf.org/pums.php

[PUM] Product User Manual for GOME-2 Total Columns of Ozone, NO_2 , BrO, HCHO, SO_2, H_2O and Cloud Properties, DLR/GOME-2/PUM/01, Rev. 3/B, Valks, P., et. al., 2019. Download: https://acsaf.org/atbds.php

[PRD] AC SAF Product Requirements Document, SAF/AC/FMI/RQ/PRD/001/Rev. 1.7, J. Hovila, et. al., 2020.

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