EUMETSAT AC SAF ATMOSPHERIC COMPOSITION MONITORING

PRODUCT USER MANUAL

GOME-2 Total Columns of Ozone, NO_2, BrO, HCHO, SO_2, H_2O, OClO and Cloud Properties

(GDP 4.8 for AC SAF OTO and NTO)

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Distribution List

Function	*Organization*
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Document Change Log

Issue	*Rev*	*Date*	*Section*	*Description of Change*
1/A	1	31 July 2004 to 20 July 2006	all	HDF5 and BUFR output product format documents merged in this product user manual
1/B	1	5 October 2006	4, 5	Content of chapters added
1/C	1	10 November 2006	all	First official version of this document
1/D	1	6 March 2007	5.7 6.2, 6.5	Fix file name convention Added VCDQualityIndicator, QualityFlags, CloudMode, CloudType, AMFTotal, AMFTotal_Error, OrbitActualDuration, new receiving stations
1/E	1	30 April 2008	all 6 7	Revised following ORR-A Added in HDF5 section: – IterativeVCDNumberOfIterations – a-priori O3_Profile – T_Profile BUFR product update to BUFR version 4
2/A	1	9 December 2008 28 January 2009	all 6	Revised following ORR-B Finalized HDF5 product format: – Moved trace gas specific datasets into groups inside DETAILED_RESULTS – Moved cloud properties into own group
2/B	1	16 November 2009	6	Update H2O and HCHO format, new sections 6.6.4, 6.6.5, 6.7.4, 6.7.5 Minor corrections: – SurfaceAlbedoRW → SurfaceAlbedo – Total Columns and BrO cleanup
		18 December 2009	6	PixelFlag under Geolocation section is renamed to SurfaceConditionFlag. SurfaceConditionFlag definition added. H2OFlag definition changed.

2/C	1	23 April 2010	1.1	Add reference to reprocessed GOME-2
				Add new O3M-SAF logo and web page
			6	Finalized NO2 HDF5 entries
			6	Added PMD dataset descriptions
			7.2	Add WMO/GTS bulletin identifier
			8	New section
			6.7.7	New flag value added to SO2_Flag
			0	New flag value added to HCHO_Flag
2/D	1	25 March 2011	6	Renamed SurfaceCondition_Flag to SurfaceConditionFlags
			6	Removed obsolete FittingFlag, AMFFlag and VCDFlag
			6.7.8	New definitions for H2O_Flags
			6.3	Converted ViewMode to integer and added DescendingFlag
2/E	1	8 August 2012	6	Added CHOCHO entries for future use (globally)
			6	Added NO_2 entries: – AMF Tropo Error field – AMF Tropo To Ground Error field – AMF Tropo To Cloud Error field – VCD Corrected Error field – VCD Strato Error field – Averaging Kernel field – Averaging Kernel Pressure field
		5 December 2012	5.7	Updated file name examples
2/F	1	28 June 2013	6.6.4	H_2O: – Add EastWestPostCorrectionFactorH2O – Removed RingCorrectionFactor
			6	Added ViewMode description table
			all	Updates for GOME-2/MetOp-B Updated entry descriptions Various clarifications
3/A	1	6 March 2017	all	Update for GDP 4.8
3/A	2	27 June 2017	all	Include OClO product Change SAF naming to AC SAF

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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 is to process, archive, validate and disseminate atmospheric composition products (O_3, NO_2, SO_2, BrO, HCHO, H_2O and OClO), 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 and Metop-B 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 OClO
- Offline ozone profiles
  - coarse and high-resolution
- Offline absorbing aerosol indexes
  - from main science channels and polarization measurement detectors
- Offline surface UV

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 and -B in the framework of EUMETSAT's AC SAF.

DLR has a long experience in operational processing of GOME and GOME-2 data and has developed a generic software for this purpose: the Universal Processor for UV/VIS Atmospheric Spectrometers (UPAS) [A1] system. This document is the user manual for the GOME-2/MetOp total column trace gases and cloud products available at DLR.

The GOME-2 trace gases total column products are:

- Ozone (O_3) column
- Nitrogen dioxide (NO_2) column (total and tropospheric)
- Bromide monoxide (BrO) column
- Sulphur dioxide (SO_2) column
- Water vapour (H_2O) column
- Formaldehyde (HCHO) column
- Chlorine dioxide (OClO) column

Additionally DLR provides the following cloud properties derived from GOME-2 measurements:

- Cloud fraction (CF)
- Cloud-top albedo (CTA) and cloud optical thickness (COT)
- Cloud-top height (CTH) and cloud-top pressure (CTP)

DLR provides near-real-time (NRT), off-line (OL), and reprocessed products. 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 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.

GOME/ERS-2, GOME-2/MetOp-A and GOME-2/MetOp-B provide a unique data record of atmospheric measurements covering a time frame of around 25 years. DLR together with the partner organizations ESA and EUMETSAT will assure the continuity between GOME/ERS-2 and GOME-2/MetOp total column products. In this framework it is important to provide to the users a unified data format for accessing the GOME-2

products. The “Hierarchical Data Format” (HDF) and the “Binary Universal Form for the Representation of meteorological data” (BUFR) have been selected for the GOME-2 total column products. HDF and BUFR are self-describing, machine-independent file formats commonly used for storage and transfer of scientific and meteorological data.

The present document is divided into the following sections:

- Overview of the GOME-2 instruments on MetOp-A and -B including instrument modes
- Summary of the algorithms used for the retrieval of trace gases total columns and cloud properties
- Summary of the processing steps
- Product description including the used HDF5 and BUFR format
- Appendixes

1.2 References

1.2.1 Applicable Documents

[A1] Design Document for the GOME-2 Universal Processor for Atmospheric Spectrometers, SAF/O3M/DLR/DD/001, Issue 2.0, October 2003

[A2] EECF to PAF Interface Specifications, ER IS EPO GE 0102, Issue 3.0, January 1990

[A3] UMARF to SAFs Interface Control Document, EUM/UMA/ICD/004, Issue 3.12, April 2006

[A4] AC SAF Product Requirements Document, Issue 1.0, SAF/AC/FMI/RQ/PRD/001, Hovila et al., 2017.

1.2.2 Reference Documents

[R1] 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 for AC SAF OTO and NTO), SAF/AC/DLR/ATBD/01, Iss. 3/A, Rev. 2, Valks, P., et al., 2017.

[R2] GOME-2 GDP 4.8 total ozone validation report, SAF/O3M/AUTH/VRR/O3, Koukouli et al., December 2015.

[R3] GOME-2 GDP 4.8 NO_2 total and tropospheric column validation report, SAF/O3M/IASB/VR/NO2, Pinardi et al., October 2015.

[R4] GOME-2 GDP 4.8 SO_2 column validation report, SAF/O3M/IASB/VR/SO2, Theys et al., December 2015.

[R5] GOME-2 GDP 4.8 BrO total column validation report, SAF/O3M/BIRA/VR/BRO, Theys et al., October 2015.

[R6] GOME-2 GDP 4.8 HCHO column validation report, SAF/O3M/BIRA/VR/HCHO, De Smedt et al., October 2015.

[R7] GOME-2 GDP 4.8 H2O total column validation report, SAF/O3M/DLR/ORR/H2O, Gross et al., October 2015.

[R8] GOME-2 GDP 4.8 OClO slant column validation report, SAF/AC/IASB/VR/OClO, Pinardi et al., June 2017.

[R9] "GOME-2 Level 1 Product Format Specification", EPS/MIS/SPE/97232, v9D, March 2012.

[R10] "GOME-2 Products Guide", EUM/OPS-EPS/MAN/07/0445, Issue 3.0, March 2011

[R11] HDF5 File Format Specification
http://www.hdfgroup.org/HDF5/

[R12] BUFR Format Specification
http://www.wmo.int/pages/prog/www/WDM/Guides/Guide-binary-1A.html

[R13] Eumetcast Dissemination Facility
http://www.eumetsat.int/website/home/Data/DataDelivery/EUMETCast/index.html

[R14] Eoweb DLR Online User Service
http://eoweb.dlr.de

[R15] Mateer, C. L., and J. J. DeLuisi, A new Umkehr inversion algorithm, J. Atmos. Terr. Phys., 54, 537-556, 1992.

1.3 Abbreviations and Acronyms

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

AAIA	Absorbing Aerosol Indicator Algorithm
AC SAF	SAF on Atmospheric Chemistry Monitoring
AMF	Air Mass Factor
BIRA-IASB	Belgian Institute for Space Aeronomy
BUFR	Binary Universal Form for the Representation of meteorological data
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
EPS	EUMETSAT Polar System
ERS-2	European Remote Sensing Satellite-2
ESA	European Space Agency
ESC	Effective Slant Column
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GDOAS	GODFIT-DOAS
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
HDF	Hierarchical Data Format
IMF	Remote Sensing Technology Institute
MetOp	Operational Meteorological Satellite
NRT	Near-Real-Time
NT	Nominal-Time
NTO	Identifier used for near-real-time total column and cloud products
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
SZA	Solar Zenith Angle
TBD	To be Defined
TOA	Top of Atmosphere
UMARF	Unified Meteorological Archiving and Retrieval Facility
UV	Ultra Violet
UPAS	Universal Processor for UV/VIS Atmospheric Spectrometers
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 captures 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 vapor, sulphur dioxide and other trace gases, as well as cloud properties and aerosols.
The next figure shows a schematic representation of GOME optical layout. A scan mirror (26) directs the light emitted from the Earth's atmosphere or the Sun diffuser (24) into the instrument. The spectrometer splits incoming light into four channels (11, 12, 18, 19) using a complex array of telescopes (5, 25), prisms (4, 6) and gratings (8, 9, 20, 21). Detectors at the end of each optical path (13 to 16) collect information about the signal in each channel.

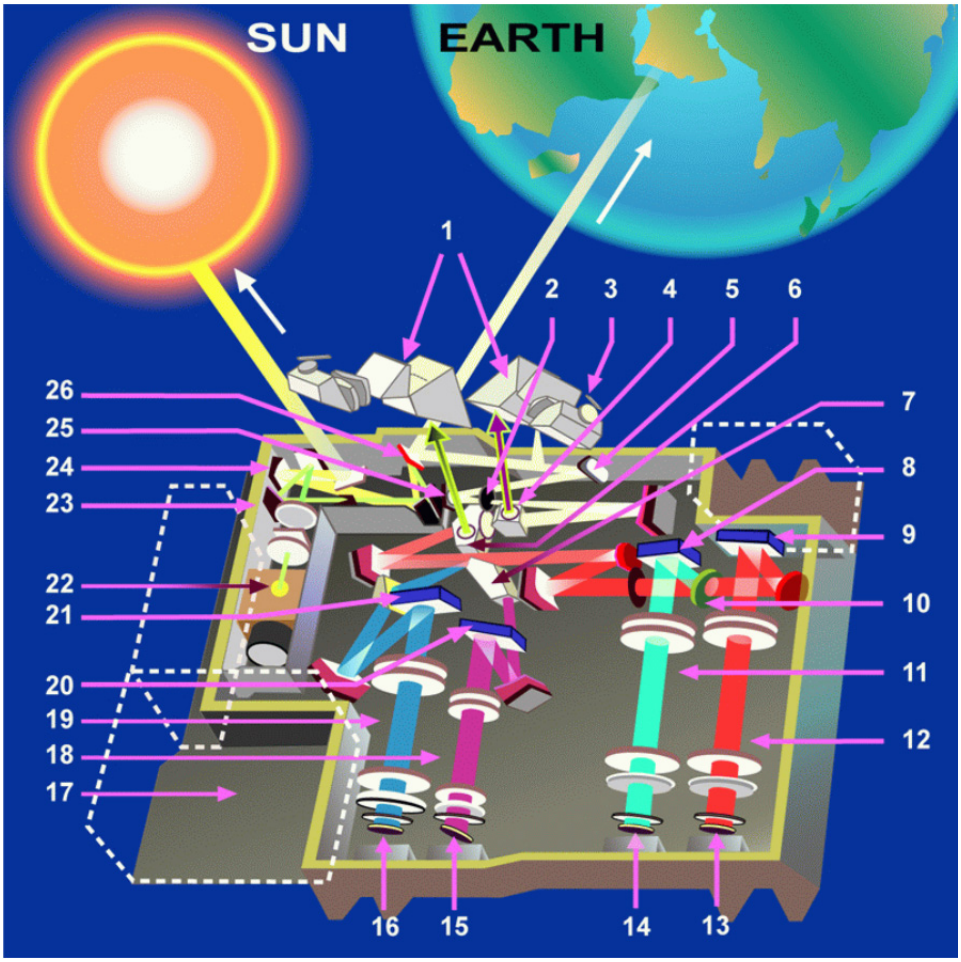

Figure 1: GOME optical layout (courtesy of ESA/ESTEC)

2.2 GOME/ERS-2

In June 1990, the ESA Council approved the satellite project to follow the first European Remote Sensing Satellite (ERS-1). The ERS-2 satellite was intended to provide data continuity between ERS-1 and the European polar platforms. ERS-2 was launched on 21 April 1995.
In addition to the ERS-1 mission objectives, ERS-2 was scheduled to make a significant contribution to atmospheric chemistry. To meet this need, ERS-2 carried GOME, an instrument designed to measure a range of atmospheric trace constituents in the troposphere and stratosphere.
GOME/ERS-2 is a nadir viewing spectrometer, which in its normal mode scans across track in three steps. The field of view of each step may be varied in size from 40 km x 40 km to 320 km x 40 km, with five options allowed. The mode with the largest footprint (three steps with a total coverage of 960 km x 40 km) provides global coverage at the equator within 3 days.
DLR developed the GOME Data Processor (GDP) system, the operational ground segment for GOME/ERS-2. GDP incorporates a Level 0-to-1 processing chain, the complete GOME/ERS-2 data archive, a DOAS-based total column retrieval process (Level 1-to-2), and processing chain for the generation of value added products.

2.3 GOME-2/MetOp

On 30 January 1998, the ESA Earth Observation Programme Board gave its final go-ahead for the MetOp Programme. 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 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 [R9].
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 which may be retrieved from GOME-2/MetOp level 1b products.

2.4 Measurement Scenarios, Timelines and Instrument Modes

GOME/ERS-2 and GOME-2/MetOp follow in general the same operational scenarios, 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.

The effective optical throughput and the potential data rate for GOME-2/MetOp are higher than those for GOME/ERS-2[1]. The default integration times for GOME-2/MetOp are 4 to 8 times smaller than those for GOME/ERS-2.

1 The effective optical throughput is enhanced by approximately a factor of 2, and co-adding (as used for GOME/ERS-2) is not required because of the higher data rate (10 times faster).

3 Algorithm Description

3.1 Summary

The GOME Data Processor (GDP) operational algorithm is the baseline algorithm for the trace gas column retrievals from GOME-2/MetOp. The GDP 4.8 uses an optimized DOAS (Differential Optical Absorption Spectroscopy) algorithm to determine the trace gas slant columns. The DOAS slant column fitting is followed by Air Mass Factor (AMF) conversions to generate vertical columns. Cloud information used in the trace gas retrieval is obtained with the OCRA and ROCINN algorithms. A detailed description of the GDP 4.8 algorithm is given in [R1].

3.2 Trace Gas and Cloud Products

The GOME-2/MetOp trace gas column densities and cloud properties (level-2 product) are retrieved from GOME-2 (ir)radiance and PMD data (level-1 product).
Tables 1 and 2 list the near real time (NRT) and off-line (OL) trace gas column and cloud products provided by DLR in the framework of the AC SAF, and the corresponding wavelength regions used for the retrieval. In addition, the AC SAF provides reprocessed data records of all the GOME-2 trace gas column products. Table 3 lists the time period of the data records and the corresponding DOI. Note that GOME-2 OClO slant column data is currently only available as a reprocessed data record.

Table 1 Near real time (NRT) GOME-2 trace gas column and cloud products from MetOp-A and –B provided by the AC SAF

Near real time product	*AC SAF identifier*	*Wavelength region (nm)*
O_3 column	O3M-01,-41	325.0-335.0
NO_2 column (total and tropospheric)	O3M-02,-50,-36,-52	425.0-450.0
SO_2 column	O3M-54,-55	315.0-326.0
HCHO column	O3M-176,-177	328.5-346.0
Cloud fraction	N.A.	300.0-800.0 (PMD-p)
Cloud-top height and albedo	N.A.	758.0-771.0

Table 2 Offline (OL) GOME-2 trace gas column and cloud products from MetOp-A and –B provided by the AC SAF

Off-line products	*AC SAF identifier*	*Wavelength region (nm)*
O_3 column	O3M-06,-42	325.0-335.0
NO_2 column (total and tropospheric)	O3M-07,-51,-37,-53	425.0-450.0
BrO column	O3M-08,-82	332.0-359.0
SO_2 column	O3M-09,-56	315.0-326.0
H_2O column	O3M-12,-86	614.0-683.2
HCHO column	O3M-10,-58	328.5-346.0
Cloud fraction	N.A.	300.0-800.0 (PMD-p)
Cloud-top height and albedo	N.A.	758.0-771.0

Table 3 Reprocessed (RP) GOME-2 trace gas column data records from MetOp-A and –B provided by the AC SAF

Reprocessed data record	*Period*	*AC SAF identifier*	*DOI*
O_3 column	23.01.2007 – 16.11.2016	O3M-110	10.15770/EUM_SAF_O3M_0009
Total NO_2 column	23.01.2007 – 16.11.2016	O3M-114	10.15770/EUM_SAF_O3M_0010
Tropospheric NO_2 column	23.01.2007 – 16.11.2016	O3M-123	10.15770/EUM_SAF_O3M_0018
BrO column	23.01.2007 – 16.11.2016	O3M-115	10.15770/EUM_SAF_O3M_0011
SO_2 column	23.01.2007 – 16.11.2016	O3M-117	10.15770/EUM_SAF_O3M_0013
H_2O column	23.01.2007 – 16.11.2016	O3M-121	10.15770/EUM_SAF_O3M_0017
HCHO column	23.01.2007 – 16.11.2016	O3M-118	10.15770/EUM_SAF_O3M_0014
OClO column	23.01.2007 – 16.11.2016	O3M-119	10.15770/EUM_SAF_O3M_0015

4 Processing

The Universal Processor for UV/VIS Atmospheric Spectrometers (UPAS) is the core GOME-2 retrieval system at DLR [A1]. UPAS is a new-generation Level 2 system for the processing of operational near-real-time and off-line trace gas and cloud properties products. UPAS takes as input the calibrated and geolocated Level 1 radiances from different sensors (e.g. GOME/ERS-2 and GOME-2/MetOp) and produces total columns of trace gases (e.g. O_3, NO_2, BrO, H_2O, SO_2, HCHO and OClO) and cloud properties (cloud fraction, cloud-top albedo and height).
The UPAS system is based on a scalable client/server architecture, which makes it possible to run the system with an unlimited number of processing nodes. The average UPAS processing time for the trace gas column and cloud retrievals includes ~15% on pre-processing tasks, ~15% on DOAS, ~60% on explicit calls to the radiative transfer model LIDORT for AMF calculations, and the rest on Level 1 loading and other tasks.

4.1 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 [R9] and received at DLR via EUMETCast ([R13]). DLR generates GOME-2/MetOp level 2 total column and cloud products using UPAS.
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 primary 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.

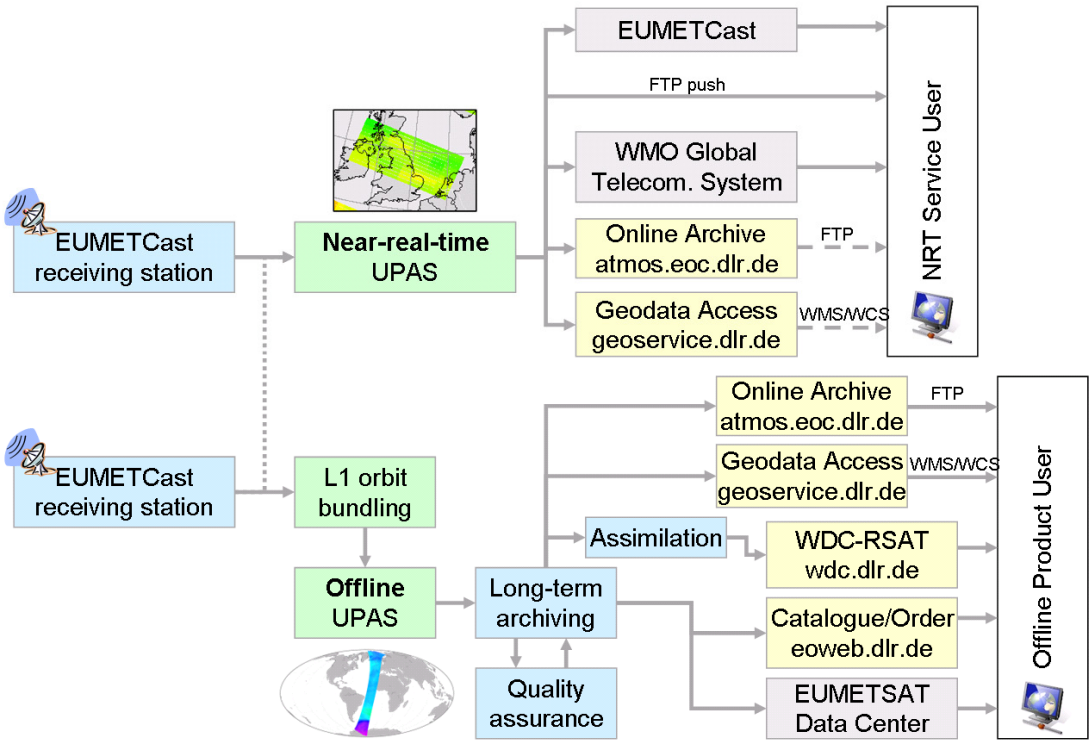

Figure 2: GOME-2/MetOp processing chain

4.2 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 and by individual ordering and delivery through DLR's on-line user services EOWEB® (Figure 2 and [R14]).

4.3 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.

4.4 Geophysical Validation

The geophysical validation of the official GOME products is performed by independent partner organizations: AUTH, BIRA, and FMI. The validation is accomplished using ground-based measurements available through the World Ozone and Ultraviolet radiation Data Centre, ground-based measurements from the NDACC network and MAX-DOAS networks, other satellite data, as well as data assimilation techniques. The validation results [R2-R8] are publicly available on the Internet, see Sect. 5.9.

4.5 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 the GOME-2 L2 trace gas column data is the AC SAF web-portal at FMI: http://acsaf.org.
Catalogue information from the AC-SAF products generated at DLR is regularly made available to the central EUMETSAT facility UMARF. The users can query the catalogue of the UMARF and submit their request, the UMARF facility will then send to each SAFs orders requested by the end users about SAF products catalogued in UMARF. DLR's data management system will then deliver the requested products to the user.
The interactive catalogue and ordering interface EOWEB® from DLR allows individual product searches and ordering. DLR operates additionally on-line user services on remote sensing data in the framework of the World Data Center for Remote Sensing of the Atmosphere (WDC-RSAT http://wdc.dlr.de, see Figure 2).
GOME-2/MetOp images and value added products produced at DLR and partner organizations are available at http://atmos.eoc.dlr.de/gome2 , see Figure 3.

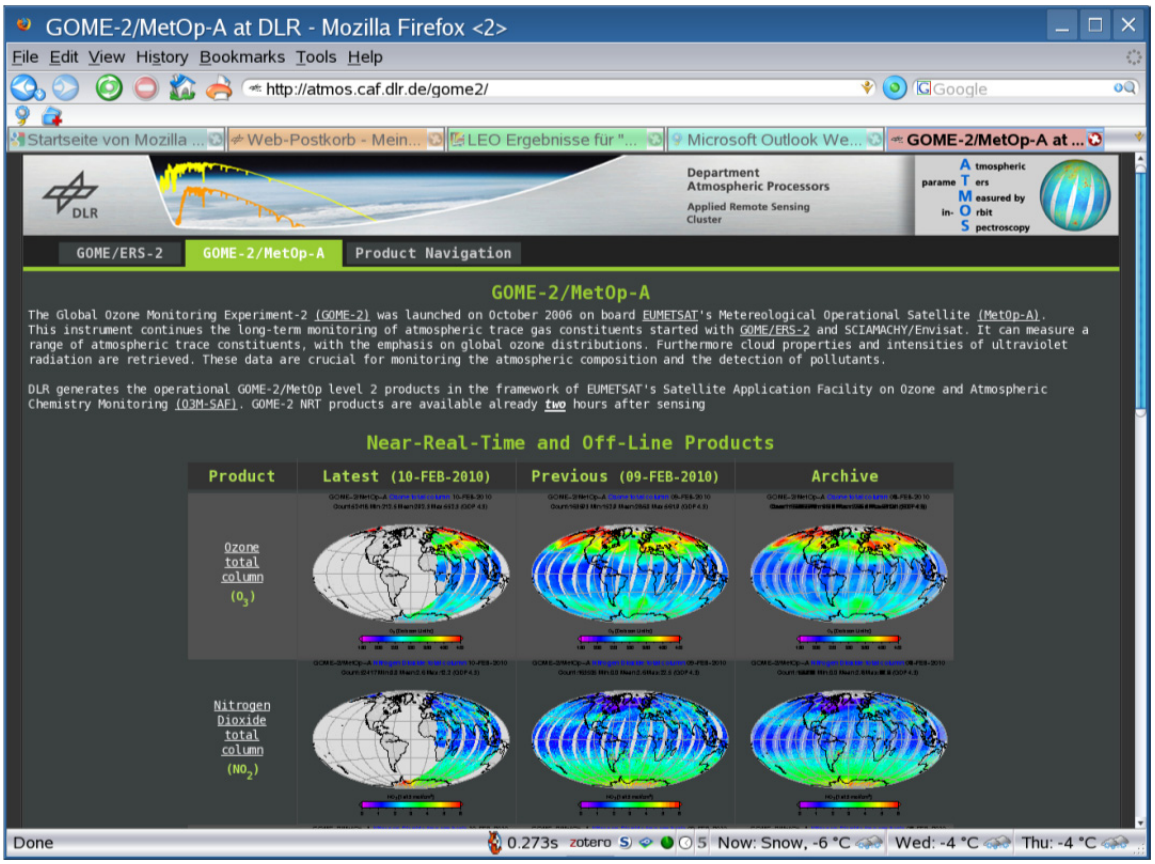

Figure 3: GOME-2/MetOp web page at DLR

5 Total Column Trace Gases and Cloud Products

The GOME-2 level 2 total column products generated with the UPAS system 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.

5.1 Units

Dataset	Units
Total ozone and SO_2 column amount	[DU] and [molecules/cm^2]
Total H_2O column amount	[kg/m^2] and [molecules/cm^2]
Other trace gas column amounts	[molecules/cm^2]
Cloud fraction and cloud-top albedo (optical thickness)	(unitless) [-]
Height	[km]
Pressure	[hPa]
Angles are given at satellite and at Top-of-Atmosphere (TOA) (70 km)	[0 to 360 degrees]
Geographical Coordinates	longitude [0 to 360 degrees] latitude [–90 to +90 degrees]
Errors	relative values [%] and absolute values [molecules/cm^2] or [DU]

5.2 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 products have by default a global coverage. The coverage of trace gases available only under special conditions may be reduced, e.g. SO_2 measured during volcanic eruption.
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.

5.3 Spatial Resolution

GOME-2/MetOp has 24 forward-scan pixels with a nominal resolution of 40 km x 80 km, and 8 back-scan pixels with a nominal resolution of 40 km x 240 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 operates 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. Both forward- and back-scan pixels are generally processed and written to the products.

5.4 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 using the latest level 1 data and improved retrieval algorithms are available on a regular basis.

5.5 Expected Accuracy

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

5.6 Product Formats

The format of the product file is either HDF5 or BUFR. A detailed description of the HDF5 product format is given in Chap. 6, and for the BUFR product in Chap. 7.

5.7 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. The acronyms from the above table are used, e.g. "O3-NO2-SO2" is a products containing these three trace gases
- *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: ERS2, METOPA, METOPB, METOPC
- ##### 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: HDF5 or BUFR

The following example is a typical name for a GOME-2/MetOp-A off-line product:

GOME_O3-NO2-NO2Tropo-BrO-SO2-H2O-HCHO_L2_20070302111155_047_METOPA_ 01900_DLR_04.HDF5

The following example is a typical name for a GOME-2/MetOp-A reprocessed data product (including OClO slant columns):

GOME_O3-NO2-NO2Tropo-BrO-SO2-H2O-HCHO-OClO_L2_20070302111155_047_ METOPA_ 01900_DLR_04.HDF5

Note: The GOME-2/MetOp NRT products disseminated via EUMETCast have a fixed prefix file name: S-O3M_, see the following examples for MetOp-A:

S-O3M_GOME_O3-NO2-NO2Tropo-SO2_HCHO_L2_20121205144758_003_METOPA_ 31808_DLR_04.HDF

S-O3M_GOME_O3-NO2-SO2_L2_20121205144758_003_METOPA_ 31808_DLR_04.BUFR

5.8 Product Dissemination

The primary dissemination mean of GOME-2/MetOp NRT products is EumetCast using the BUFR and HDF5 format.

The NRT products in BUFR format are additionally disseminated via WMO/GTS. The corresponding bulletin identifier for the AC-SAF Products is:

Region	RTH	Country	TTAAii	CCCC	CodeForm
6	OFFENBACH	GERMANY	IUCX01	EDLR	FM 94-XIII

Additionally the GOME-2/MetOp NRT, OL and reprocessed products in HDF5 format are available at the DLR ATMOS FTP–server (after registration):

ftp://atmos.eoc.dlr.de/

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

A FTP user account can be obtained at the AC SAF web-portal: http://acsaf.org (see next section). In addition, the NRT and OL products can be directly pushed to dedicated

FTP servers located at the user's premises.

Following the AC SAF strategy, reprocessed products replace off-line products in the local archive and FTP server. The reasoning behind is that the reprocessed products are the best possible products and their quality is at least as good as the off-line products.

5.9 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://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 as well as value added products generated by DLR are available at:

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

6 HDF5 Product Format Description

The product content comprises the following groups:

- *META_DATA*
  - Product Metadata
- *GEOLOCATION*
  - Date & Time (all retrievals)
  - 4 Corner Coordinates & Centre of Ground Pixel
  - Solar, Line-of-Sight Zenith, and relative Azimuth angles at TOA
  - Orbit information
- *TOTAL_COLUMNS*
  - Total and tropospheric column amounts of the various trace gases with corresponding (relative) errors
- *CLOUD_PROPERTIES*
  - Retrieved cloud properties
- *DETAILED_RESULTS*
  - Geophysical parameters (surface, cloud and aerosol values)
  - Vertical column, slant column, and AMF values with corresponding errors
  - Fitting diagnostics (chi-square, RMS, etc.)
  - Various subgroups for trace gas specific data (e.g. O_3, NO_2, SO_2, etc.)

6.1 Structure

The data in the HDF5 file is organized in five groups: *META_DATA, GEOLOCATION, TOTAL_COLUMNS, DETAILED_RESULTS, CLOUD_PROPERTIES* (Figure 4). The values in all groups are either copied from the level 1 [R9] or other input data, or calculated by the UPAS level 1-to-2 processor. The *META_DATA* group contains parameters required by EECF [A2] or UMARF [A3], and general information about the product. The data related to each ground pixel is divided into three groups: *GEOLOCATION, TOTAL_COLUMNS* and *DETAILED_RESULTS*. The *GEOLOCATION* group contains all information related to geolocation of the pixel. Pixel processing information is stored in the *TOTAL_COLUMNS* and *DETAILED_RESULTS* groups. Cloud properties derived are stored in the CLOUD_PROPERTIES and *DETAILED_RESULTS* groups.
The last three groups mentioned above contain all pixel information, stored in arrays with length equal to the number of ground pixels in one granule (orbit or PDU). Data values may occur more than once for a given ground pixel, and these will be separated by fitting windows. The information for each entry is stored as a matrix. Elements in these matrices are not always atomic: they can contain variable length data structures.

When entries for a pixel or pixel-window combination cannot be calculated using the normal processing procedure, “fill-in” values are written to the arrays. Also, not all datasets defined here have to exist in every product.
Please note that this description is only valid for the actual version of the product format. The version of a GOME HDF5 level 2 product can reliably be read from the field *META_DATA/ProductFormatVersion*, therefore a reader can implement several versions in parallel.
Each dataset has five associated attributes: *Title*, *Unit*, *FillValue*, *ValueRangeMin* and *ValueRangeMax* (Figure 4). These are used to describe the contents of the array.
Values in the *META_DATA* group are stored as attributes of the group.

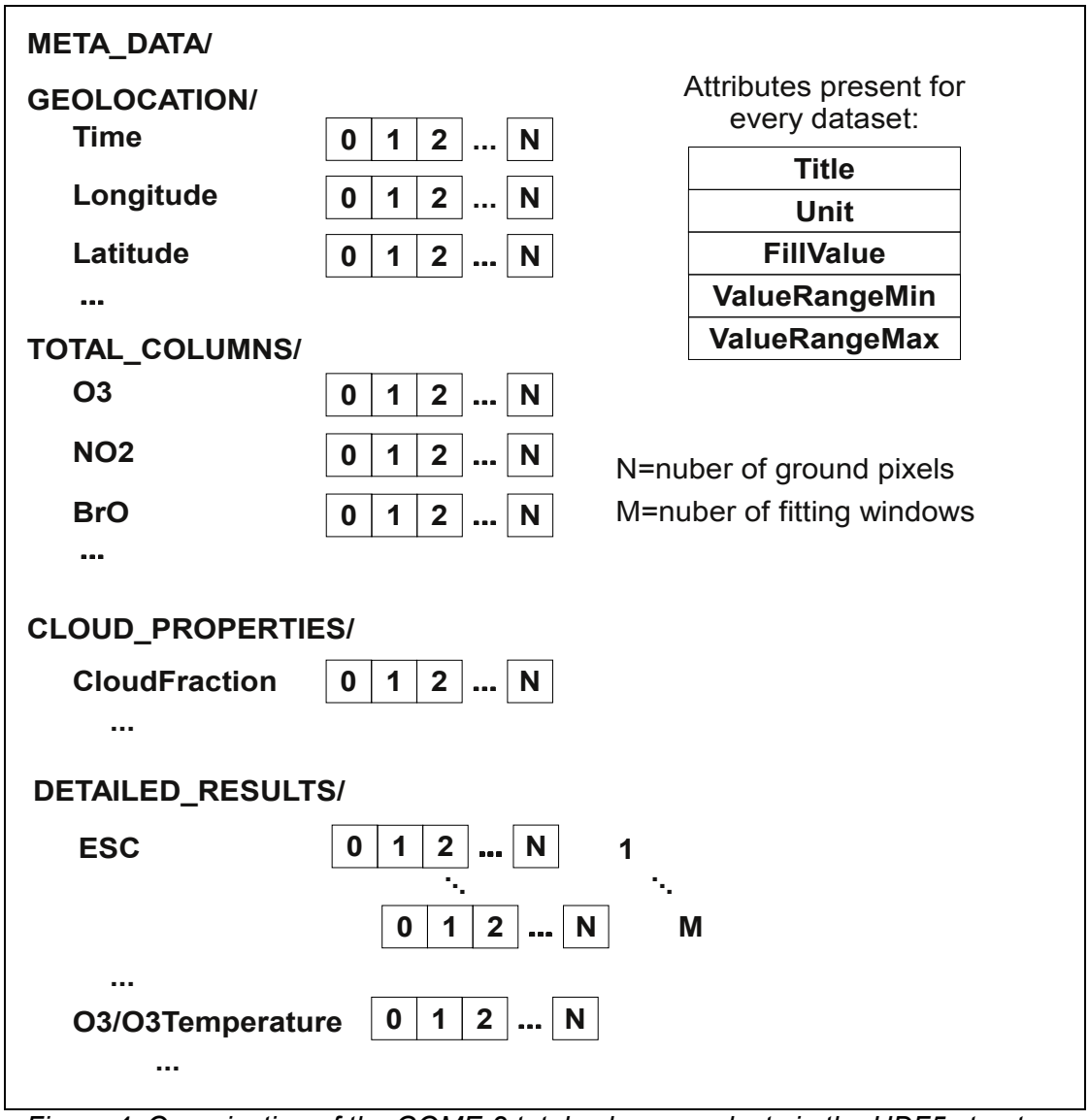

Figure 4: Organization of the GOME-2 total column products in the HDF5 structure

Most dataset are one dimensional, containing one value for every ground pixel. In the

DETAILED_RESULTS group however, every dataset contains an additional dimension for the fitting window. In the subgroups of detailed results, the dimensions of the datasets vary considerably, being one-dimensional (ground pixel number only), over two dimensional (e.g. for O3/O3Profile, containing one profile for every ground pixel), or there are subgroups (e.g. for the different plume heights of SO_2).

6.1.1 Description of Common Items

In the *GEOLOCATION, TOTAL_COLUMN* and DETAILED_RESULTS groups, all datasets have a set of attached attributes. These are shown in the table below.

Attribute Name	*Data Type*	*Description*
Title	string	Description of the dataset, e.g. “Ozone total column”
Unit	string	Unit of the values in the array, e.g. “DU”
FillValue	same as dataset	Value in the array, if actual data value is missing
ValueRangeMin	same as dataset	Minimum value in this dataset (present only when applicable)
ValueRangeMax	same as dataset	Maximum value in this dataset (present only when applicable)

6.2 *META_DATA* Group

The content of the *META_DATA* group is shown in the following tables. Allowed values for parameters required by EECF and UMARF are consistent with requirements given in [A2] and [A3]. Allowed values specified in italics indicate any value of the given type (e.g. *string* means that the attribute can contain any string within the UMARF size limit).

Attribute Name	*Data Type*	*Description*	*Allowed Values*
ArchiveFacility	string	Centre where the data is archived.	O3DLR
SatelliteID	string	Platform identifier (mission and spacecraft).	M*nn*
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
InstrumentMode	VIEW_MODES structure	Specifies how many ground pixels were observed in the corresp. 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	O3MNTO, O3MOTO

Attribute Name	Data Type	Description	Allowed Values
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
BaseProducts	string	Name of the base products.	string
ProductAlgorithmVersion	string	Version of the algorithm that produced the product.	string
InitializationFileVersion	string	Version of the configuration file used for processing.	string
InternalProcessorRevision	string	Version of the processor used to generate this product.	string
ProductFormatType	string	Data format of the product.	“HDF5”
ProductFormatVersion	string	Version number of the product format.	string
ProductContents	string	Trace gases included in the product (comma-separated list).	string
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	Long. 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	Long. 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
OrbitUTCDaysSince1950	integer	UTC days since 1.1.1950	int
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 (UMARF notation)
OrbitActualDuration	integer	Orbit duration in minutes, only counting valid pixels	0...~60
SolarSpectraDate	CCSDS_ASCII	Date and time of the solar spectra	CCSDS Date
NumberOfGroundPixels	integer	Number of ground pixels in the product	int
DegradedRecordCount	integer	Number of records which could not be processed	int
DegradedRecordPercentage	integer	Percentage of records, which could not be processed	0-100%
MissingDataCount	integer	Number of missing data records.	int
MissingDataPercentage	integer	Percentage of missing data records.	0-100%

The next table contains metadata specific to the total column products:

Attribute Name	Data Type	Description	Allowed Values
NumberOfFittingWindows	integer	Number of fitting windows used in processing	1- M

The following table describes data sets containing information about the fitting windows:

Dataset Name	*Data Type*	*Description*	*Allowed Values*
FWName	string[windows]	Names of fitting windows	string
FWLowerBound	float[windows]	Lower wavelength bound of a fitting window in nm	240-780
FWUpperBound	float[windows]	Upper wavelength bound of a fitting window in nm	240-780
MainSpecies	string[windows]	Name of the main reference species retrieved in this fitting window	string
VCDQualityIndicator	float[windows]	Percentage of flagged pixels (see QualityFlags 0-2 in Sect. 6.7.3) for this window	0-100%
DOI	string	Digital Object Identifiers (DOIs) for the trace gas column products included in the product (comma-separated list). For reprocessed data records only.	string

6.3 *GEOLOCATION* Group

The *GEOLOCATION* group contains information for seven different points for the ground pixel, denoted by letters A to G in Figure 5.

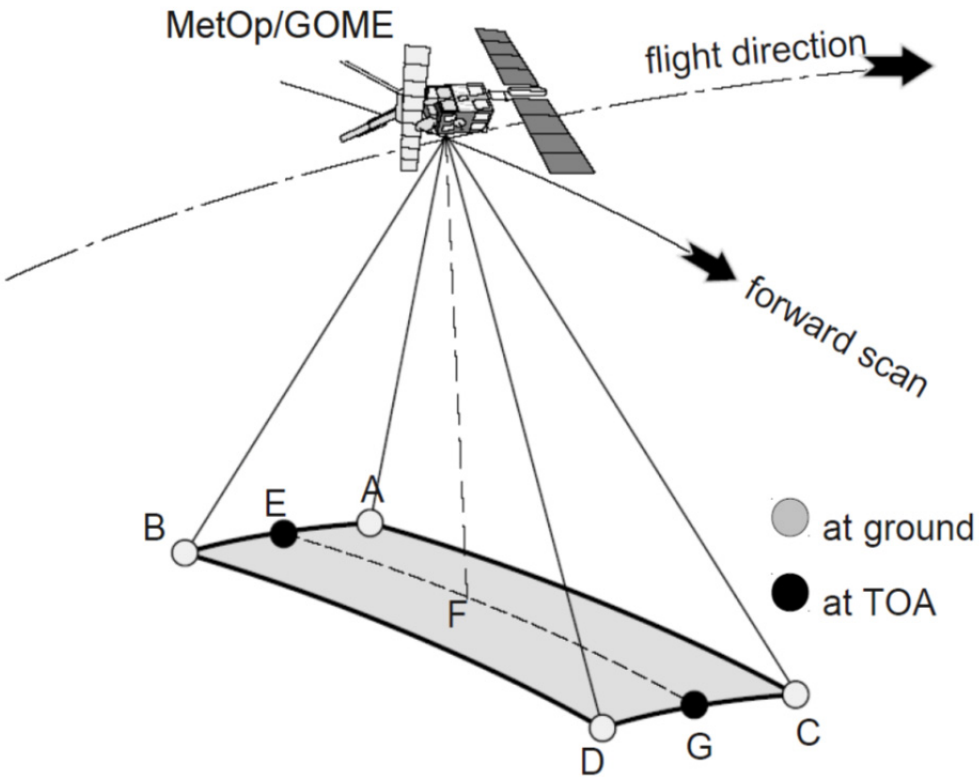

Figure 5: Ground Pixel Geometry

The term ”pixels” denote the number of ground pixels, whereas the term “PMDpixels” denote the total number of PMD subpixels.

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

Dataset Name	Data Type	Unit	Description
InternalPixelId	integer[pixels]	-	Internal ground pixel number
Time	UTC[pixels]	ms	Time of the observation in UTC format
LongitudeCentre	float[pixels]	degrees	Longitude of the centre of the ground pixel (Point F)
LatitudeCentre	float[pixels]	degrees	Latitude of the centre of the ground pixel (Point F)
LongitudeA	float[pixels]	degrees	Longitude (Point A)
LatitudeA	float[pixels]	degrees	Latitude (Point A)
LongitudeB	float[pixels]	degrees	Longitude (Point B)
LatitudeB	float[pixels]	degrees	Latitude (Point B)
LongitudeC	float[pixels]	degrees	Longitude (Point C)
LatitudeC	float[pixels]	degrees	Latitude (Point C)
LongitudeD	float[pixels]	degrees	Longitude (Point D)
LatitudeD	float[pixels]	degrees	Latitude (Point D)
PMDCenterLon	float[PMDpixels]	degrees	Longitude (Point F) of forward scan PMD subpixel center
PMDCenterLat	float[PMDpixels]	degrees	Latitude (Point F) of forward scan PMD subpixel center
PMDPixelMap	integer[pixels]	-	Mapping from ground pixel to PMD pixel (-1 for backscan)
SolarZenithAngleE	float[pixels]	degrees	Solar zenith angle at TOA (Point E)
SolarZenithAngleCentre	float[pixels]	degrees	Solar zenith angle at TOA (Point F)
SolarZenithAngleG	float[pixels]	degrees	Solar zenith angle at TOA (Point G)
LineOfSightZenithAngleE	float[pixels]	degrees	Line-of-sight zenith angle at TOA (Point E)
LineOfSightZenithAngleCentre	float[pixels]	degrees	Line-of-sight zenith angle at TOA (Point F)
LineOfSightZenithAngleG	float[pixels]	degrees	Line-of-sight zenith angle at TOA (Point G)
RelativeAzimuthE	float[pixels]	degrees	Relative azimuth at TOA (Point E)
RelativeAzimuthCentre	float[pixels]	degrees	Relative azimuth at TOA (Point F)
RelativeAzimuthG	float[pixels]	degrees	Relative azimuth at TOA (Point G)
SolarZenithAngleSatE	float[pixels]	degrees	Solar zenith angle at satellite (Point E)
SolarZenithAngleSatCentre	float[pixels]	degrees	Solar zenith angle at satellite (Point F)
SolarZenithAngleSatG	float[pixels]	degrees	Solar zenith angle at satellite (Point G)
LineOfSightZenithAngleSatE	float[pixels]	degrees	Line-of-sight zenith angle at satellite (Point E)
LineOfSightZenithAngleSatCentre	float[pixels]	degrees	Line-of-sight zenith angle at satellite (Point F)
LineOfSightZenithAngleSatG	float[pixels]	degrees	Line-of-sight zenith angle at satellite (Point G)
RelativeAzimuthSatE	float[pixels]	degrees	Relative azimuth at satellite (Point E)
RelativeAzimuthSatCentre	float[pixels]	degrees	Relative azimuth at satellite (Point F)
RelativeAzimuthSatG	float[pixels]	degrees	Relative azimuth at satellite (Point G)
SubSatellitePointLongitude	float[pixels]	degrees	Geodetic longitude of subsatellite point
SubSatellitePointLatitude	float[pixels]	degrees	Geodetic latitude of subsatellite point
SatelliteAltitude	float[pixels]	km	Geodetic altitude of satellite
EarthRadius	float[pixels]	km	Radius of the Earth

Dataset Name	Data Type	Unit	Description
IndexInScan	integer[pixels]	-	Index of the pixel within the scan (0-2 forward scan, 0-east part of scan, 1-centre part of scan, 2-west part of scan; 3 backward scan)
SubPixelInScan	integer[pixels]	-	Subpixel within the scan (0 to 3, 7 or 31)
ViewMode	integer[pixels]	-	Scanning mode of the instrument at the time of acquisition (bits 0-7), geolocation flags (bit 8-31) Allowed values: - Nominal (0), Narrow (1), Static (2), SouthPolar (3), NorthPolar (4) - DescendingFlag (bit 8): set if the pixel is located in the descending part of the orbit see also Sect. 6.7.1
SwathMode(*)	integer[pixels]	-	Scanning mode of the instrument at the time of Acquisition. Allowed values: - Nominal (0), Narrow (1), Static (2), SouthPolar (3), NorthPolar (4)
OrbitalMode(*)	integer[pixels]	-	Orbital mode of measurement (0: Measurement on ascending node, 1: Measurement on descending node)
SAAFlag	integer[pixels]	-	Set to 1 if measurement taken in SAA region, otherwise 0
SolarEclipseFlag	Integer[pixels]	-	If set to 1 high probability that data quality is reduced due to solar eclipse, otherwise 0

(*) SwathMode and OrbitalMode are the datasets which together form the ViewMode dataset. They are provided as of version GDP 4.8 in order to facilitate the usage of the dataset (see Sect. 6.7.1).

6.4 *TOTAL_COLUMNS* Group

The data sets in the *TOTAL_COLUMNS* group are given in the following tables. Attributes attached to all data sets in this group are the same as those for the *GEOLOCATION* group.
This group contains the main key trace gas total column information and represents the final results (i.e. including all corrections). Data sets are arrays of size N, where N is the number of ground pixels in the product granule.
All entries starting with the name of the trace gas are only included if the trace gas total column has been retrieved, in which case it is included in the /META_DATA/MainSpecies attribute.

Dataset Name	Data Type	Unit	Description
O3	float[pixels]	Dobson Units	Total vertical column density of O_3
O3_Error	float[pixels]	%	Relative error on total vertical column density of O_3
NO2	float[pixels]	molecules/cm^2	Initial total vertical column density of NO_2
NO2_Error	float[pixels]	molecules/cm^2	Error on initial total vertical column density of NO_2
NO2Tropo	float[pixels]	molecules/cm^2	Tropospheric vertical column density of NO_2 (cloud screened)
NO2Tropo_Error	float[pixels]	molecules/cm^2	Error on tropospheric vertical column density of NO_2
BrO	float[pixels]	molecules/cm^2	Vertical column density of BrO
BrO_Error	float[pixels]	molecules/cm^2	Error on vertical column density of BrO
SO2(*)	float[pixels]	Dobson Units	Vertical column density of SO_2 for a volcanic plume height of 6 km
SO2_Error(*)	float[pixels]	Dobson Units	Error on vertical column density of SO_2
H2O	float[pixels]	kg/m^2	Vertical column density of H_2O (cloud screened)
H2O_Error	float[pixels]	%	Relative error on vertical column density of H_2O
HCHO	float[pixels]	molecules/cm^2	Vertical column density of HCHO (cloud screened)
HCHO_Error	float[pixels]	molecules/cm^2	Error on vertical column density of HCHO
OClO	float[pixels]	molecules/cm^2	Slant column density of OClO
OClO_Error	float[pixels]	molecules/cm^2	Error on slant column density of OClO

(*) Note that for SO_2 only the vertical column density for a volcanic plume at 6 km is stored in this group. The dataset for other SO_2 scenarios can be found in the DETAILED_RESULTS/SO2 group

6.5 *CLOUD_PROPERTIES* Group

In this group, the main cloud properties of each pixel are stored.

Dataset Name	Data Type	Unit	Description
CloudFraction	float[pixels]	-	Cloud fraction
CloudFraction_Error	float[pixels]	%	Error on cloud fraction
CloudTopAlbedo	float[pixels]	-	Cloud-top albedo (-1 if clear sky)
CloudTopAlbedo_Error	float[pixels]	%	Error on cloud-top albedo (-1 if clear sky)
CloudTopHeight	float[pixels]	km	Cloud-top height (-1 if clear sky)
CloudTopHeight_Error	float[pixels]	%	Error on cloud-top height (-1 if clear sky)
CloudOpticalThickness	float[pixels]	-	Cloud optical thickness (-1 if clear sky)
CloudOpticalThickness_Error	float[pixels]	%	Error on cloud optical thickness (-1 if clear sky)
CloudTopPressure	float[pixels]	hPa	Cloud-top pressure (-1 if clear sky)
CloudTopPressure_Error	float[pixels]	%	Error on cloud-top pressure (-1 if clear sky)
CloudType	integer[pixels]	-	ISCCP cloud type classification (-1 if clear sky): 1 = cirrus, 2 = cirrostratus, 3 = deep convection, 4 = altocumulus, 5 = altostratus, 6 = nimbostratus, 7 = cumulus, 8 = stratocumulus, 9 = stratus
CloudMode	integer[pixels]	-	Mode in which cloud parameters have been calculated 0=normal mode, 1=snow/ice mode
PMDCloudFraction	float[PMDpixels]	-	Cloud fraction for forward-scan PMD subpixels

6.6 *DETAILED_RESULTS* Group

The following table lists ancillary surface/aerosol data and detailed processing results, as stored in the *DETAILED_RESULTS* group. Data sets (see Figure 4) are represented either as arrays of size N, where N is the number of ground pixels in the product, or as matrices of dimensions NxM, for N the number of ground pixels (denoted as "pixels" in the following tables) and M the number of fitting windows (denoted as "windows" in the following tables).
Note that this group provides the results after the DOAS fit of the main species, i.e. no additional corrections are applied. The final retrieval results can be found in the TOTAL_COLUMNS group as well as in the subgroup of each gas, as described below.

Dataset Name	*Data Type*	*Unit*	*Description*
AAI	float[pixels]	-	Absorbing aerosol indicator
SurfaceHeight	float[pixels]	km	Ground Surface Height
SurfacePressure	float[pixels]	hPa	Pressure at the surface level
SurfaceConditionFlags	integer[pixels]	-	Flag for different pixel retrieval conditions, e.g. land/sea, sun glint or snow/ice (see section 6.7.2)
SurfaceAlbedo	float[pixels][windows]	-	Surface albedo for the associated retrieval window
QualityFlags	integer[pixels][windows]	-	Quality flags for each pixel/gas (see section 6.7.3)
VCD(***)	float[pixels][windows]	molec/cm^2	Uncorrected vertical column density of main gas calculated from fitted ESC and AMF total
VCD_Error(*)	float[pixels][windows]	%	Relative error on vertical column density
IntensityWeightedCloudFraction	float[pixels][windows]	-	Cloud radiance fraction (weighting factor for clear-sky and cloudy AMFs)
ESC	float[pixels][windows]	molec/cm^2	Fitted slant column density of main gas
ESC_Error(*)	float[pixels][windows]	%	Relative error on slant column density
FittingRMS	float[pixels][windows]	-	RMS of the DOAS fit
FittingChiSquare	float[pixels][windows]	-	ChiSquare of the DOAS fit
FittingGoodness	float[pixels][windows]	-	Goodness of the DOAS fit
FittingNumberOfIterations	integer[pixels][windows]	-	Number of iterations in the DOAS fit
AMFToGround(***)	float[pixels][windows]	-	AMF to ground for main gas
AMFToGround_Error(**)	float[pixels][windows]	%	Error on AMF to ground
AMFToCloudTop(***)	float[pixels][windows]	-	AMF to cloud-top for main gas (-1 if clear sky)
AMFToCloudTop_Error(**)	float[pixels][windows]	%	Error on AMF to cloud-top (-1 if clear sky)
AMFTotal(***)	float[pixels][windows]	-	Total AMF for main gas
AMFTotal_Error(**)	float[pixels][windows]	%	Total AMF error

(*) Note that for SO_2, HCHO and OClO, the relative error can be unphysically high, since VCDs around zero are commonly retrieved for these gases. The absolute errors for these trace gases can however be found in the TOTAL_COLUMNS group as well as in the DETAILED_RESULTS subgroups.
(**) AMF errors are only available for O_3, NO_2 and H_2O
(***) For SO_2 only the (uncorrected) vertical column density and AMF values for a plume at 6km are stored in this group. The datasets for other plume scenarios can be found in the DETAILED_RESULTS/SO2 subgroup (see section 6.6.3). For OClO, only slant column densities are available.

The following subsections contain sub groups of the *DETAILED_RESULTS* group which contain trace gas specific data. In these groups also the final retrieval results are provided.

6.6.1 *DETAILED_RESULTS/O3* Subgroup

Dataset Name	Data Type	Unit	Description
ESCRingCorrected	float[pixels]	molec/cm^2	Ozone slant column density corrected for Ring-effect
O3Temperature	float[pixels]	K	Fitted ozone temperature
EastWestPostCorrectionFactor O3	float[pixels]	-	Correction factor for scan angle dependency in retrieved ozone column
RingCorrection	float[pixels]	-	Ring correction factor
O3Profile(*)	float[pixels][layers]	DU	A priori ozone profile (partial columns) used in the total ozone retrieval (layers=13)
O3ProfilePressure(*)	float[pixels][layers]	hPa	Pressure of the ozone profile layer interfaces
O3_Volcano_Flag	float[pixels]	-	Flag indexing volcanic SO_2 affecting total ozone retrieval (see Sect.6.7.4)
IterativeVCDNumberOf Iterations	integer[pixels]	-	Number of iterations for the iterative VCD algorithm
VCDCorrected	float[pixels]	molec/cm^2	Corrected total vertical column density of ozone
VCDCorrected_Error	float[pixels]	%	Relative error of total vertical column density of ozone
GhostColumn	float[pixels]	molec/cm^2	Ghost column below cloud

(*) The a priori ozone profile is described as a function of Umkehr Layer. The first value in O3Profile represents Umkehr Layer #12-15 (Top-of-Atmosphere), the second value is for Umkehr Layer #11, etc. and the last value represents Umkehr Layer #0 (surface layer). The Umkehr Layer definition can be found in [R14].

6.6.2 *DETAILED_RESULTS/NO2* Subgroup

Dataset Name	Data Type	Unit	Description
AMFTropoToGround	float[pixels]	-	Tropospheric AMF to ground (clear-sky)
AMFTropoToGround_Error	float[pixels]	%	Error on Tropospheric AMF to ground (clear-sky)
AMFTropoToCloudTop	float[pixels]	-	Tropospheric AMF to cloud-top (-1 if clear sky)
AMFTropoToCloudTop_Error	float[pixels]	%	Error on tropospheric AMF to cloud-top (-1 if clear sky)
AMFTropo	float[pixels]	-	Total tropospheric AMF
AMFTropo_Error	float[pixels]	%	Error on total tropospheric AMF
AMFStrato			Stratospheric AMF
AMFStrato_Error	float[pixels]	%	Error on total stratospheric AMF
AMFStratoToGround	float[pixels]	-	Stratospheric AMF to ground (clear-sky)
AMFStratoToGround_Error	float[pixels]	%	Error on Stratospheric AMF to ground (clear-sky)
AMFStratoToCloudTop	float[pixels]	-	Stratospheric AMF to cloud-top (-1 if clear sky)
AMFStratoToCloudTop_Error	float[pixels]	%	Error on Stratospheric AMF to cloud-top (-1 if clear sky)
VCDInit	float[pixels]	molec/cm^2	Total initial vertical column density
VCDInit_Error	float[pixels]	molec/cm^2	Error on total initial vertical column density
VCDStrato	float[pixels]	molec/cm^2	Stratospheric vertical column density
VCDStrato_Error	float[pixels]	molec/cm^2	Error on stratospheric vertical column density
VCDTropo	float[pixels]	molec/cm^2	Tropospheric vertical column density
VCDTropo_Error	float[pixels]	molec/cm^2	Error on tropospheric vertical column density
VCDCorrected	float[pixels]	molec/cm^2	Total vertical column density corrected for tropospheric contribution
VCDCorrected_Error	float[pixels]	molec/cm^2	Error on corrected total vertical column density
NO2Tropo_Flag	integer[pixels]	-	Flag indexing tropospheric NO_2 calculations (see Sect. 6.7.5)
AveragingKernel	float[pixels][layers]	-	Averaging Kernel (layers=24)
AveragingKernelPressureLevel	float[pixels][layers]	-	Pressure levels of Averaging Kernel (layer center)
AprioriNO2Profile	float[pixels][layers]	vmr	A priori NO_2 profile (volume mixing ratio)

For more information on the Averaging Kernel parameters see Chap. 8.

6.6.3 *DETAILED_RESULTS/SO2* Subgroup

The GOME SO_2 algorithm provides SO_2 vertical columns for four scenarios - three assumed volcanic SO_2 scenarios and one scenario of anthropogenic pollution in the PBL. The number of scenarios is available in the group attribute "NumberOfScenarios", which also describes the cardinality of the subsequent datasets (denoted as "heights"). The different height values are available in the dataset "Scenarios". Note that for the anthropogenic pollution scenario a 'height' of 1km is indicated. The user is advised to only use data with cloud fractions <20% when using this data.

For low cloud fractions (<30%) clear sky conditions are considered (i.e. a cloud fraction of 0% is assumed and only AMFtoGround is used) in order to avoid errors from the unstable cloud-top pressure

Dataset Name	*Data Type*	*Unit*	*Description*
PlumeHeights	float[heights]	km	Assumed SO_2 height for each scenario in the retrieval. For volcanic scenarios the height is the SO_2 plume height, for the polluted scenario a 1km height is indicated
ESCCorrected	float[pixels][heights]	molec/cm^2	SO_2 slant column density (background and temperature corrected)
AMFToGround	float[pixels][heights]	-	AMF to ground
AMFToGround_Error (*)	float[pixels][heights]	%	Error on AMF to ground
AMFToCloudTop	float[pixels][heights]	-	AMF to cloud-top (-1 if clear sky)
AMFToCloudTop_Error (*)	float[pixels][heights]	%	Error on AMF to cloud-top (-1 if clear sky)
AMFTotal	float[pixels][heights]	-	Total AMF
AMFTotal_Error (*)	float[pixels][heights]	%	Total AMF error
VCDCorrected	float[pixels][heights]	molec/cm^2	Total vertical column density (background corrected)
VCDCorrected_Error	float[pixels][heights]	molec/cm^2	Error on total vertical column density
SO2_Flag	integer[pixels]	-	Flag indexing quality of SO_2 calculations (see Sect 6.7.6)
SO2_Volcano_Flag	integer[pixels]	-	Flag indexing increased SO_2 values with potential volcanic origin (see Sect. 6.7.7).

(*) for future use, not yet implemented

6.6.4 *DETAILED_RESULTS/H2O* Subgroup

Dataset Name	***Data Type***	***Unit***	***Description***
ESC_O2	float[pixels]	molec/cm^2	O_2 slant column density
ESC_O2Corrected	float[pixels]	molec/cm^2	O_2 slant column density (saturation corrected)
ESC_O4	float[pixels]	molec/cm^2	O_4 slant column density
ESCCorrected	float[pixels]	molec/cm^2	H_2O slant column density (saturation corrected)
EastWestPostCorrectionFactorH2O	float[pixels]	-	Correction factor for scan angle dependency in retrieved H_2O column
H2O_Flag	integer[pixels]	-	Flag indexing H_2O calculations (see Sect. 6.7.8)
VCDCorrected	float[pixels]	molec/cm^2	Corrected H_2O vertical column
VCDCorrected_Error	float[pixels]	%	Relative error on corrected H_2O vertical column

6.6.5 *DETAILED_RESULTS/HCHO* Subgroup

Dataset Name	*Data Type*	*Unit*	*Description*
ESCCorrected	float[pixels]	molec/cm^2	Slant column density (background corrected)
ESCRefSector	float[pixels]	molec/cm^2	Slant column density for Reference Sector (Pacific Region between 160-240°E)
ESCRefSectorEquator	float[pixels]	molec/cm^2	Slant column density for the Equatorial Reference Sector (Pacific Equator Region)
VCD0	float[pixels]	molec/cm^2	A priori vertical column density for the Reference Sector (Pacific Region (160-240°E)) from IMAGESv2 model
VCDCorrected	float[pixels]	molec/cm^2	Total vertical column density (background corrected)
VCDCorrected_Error	float[pixels]	molec/cm^2	Error of total vertical column density (background corrected)
HCHO_Flag	integer[pixels]	-	Flag indexing HCHO calculations (see Sect. 6.7.9)
AveragingKernel	float[pixels][layers]	-	Averaging Kernel (layers=40)
AveragingKernelPressureLevel	float[pixels][layers]	-	Pressure levels of Averaging Kernel (layer center)
AprioiHCHOProfile	float[pixels][layers]	vmr	A priori HCHO profile (volume mixing ratio)

For more information on the Averaging Kernel parameters see Chap. 8.

6.6.6 *DETAILED_RESULTS/BrO* Subgroup

Dataset Name	*Data Type*	*Unit*	*Description*
ESCCorrected	float[pixels]	molec/cm^2	Slant column density (background corrected)
VCDCorrected_Error	float[pixels]	molec/cm^2	Error on corrected vertical column density
VCDCorrected	float[pixels]	molec/cm^2	Vertical column density (background corrected)

6.6.7 *DETAILED_RESULTS/OClO* Subgroup

Dataset Name	*Data Type*	*Unit*	*Description*
ESCCorrected	float[pixels]	molec/cm^2	Slant column density (background corrected)
ESCCorrected_Error	float[pixels]	molec/cm^2	Error on corrected slant column density
OClO_Flag	integer[pixels]	-	Flag indexing OClO calculations (see Sect. 6.7.10)

6.6.8 *DETAILED_RESULTS/Clouds* Subgroup

Dataset Name	*Data Type*	*Unit*	*Description*
Alpha	float[pixels]	-	Regularization parameter
CloudFractionAPriori	float[pixels]	-	A priori cloud fraction from OCRA
ConditionNumber	float[pixels]	-	Condition number
DegreesOfFreedom	float[pixels]	-	Fitting degrees of freedom
Flag	integer[pixels]	-	Flag for retrieval diagnostics (e.g. convergence)
Iterations	integer[pixels]	-	Number of iterations during fit
NoiseVariance	float[pixels]	-	Noise variance of O2A sun-normalized radiances
Residual	float[pixels]	-	Fitting residual
ShannonInformationContent	float[pixels]	-	Shannon Information Content
SurfaceAlbedo	float[pixels]	-	Surface Albedo used for cloud retrieval
SurfaceAlbedoAPriori	float[pixels]	-	A priori surface albedo
SurfaceAlbedoError	float[pixels]	-	Surface albedo error
WavelengthShift	float[pixels]	nm	Wavelength shift
WavelengthShiftError	float[pixels]	-	Wavelength shift error

6.7 Detailed Flag Description

This section gives an overview of all flag datasets. In Sect. 6.7.11 a detailed description on how the flag data can be interpreted can be found.

6.7.1 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. 6.2 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

6.7.2 SurfaceConditionFlags

These flags give additional information about the surface state during the retrieval. See Sect. 6.7.11 for an example how to use this flag.

Bit	*Value*	*Description*
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
2	4	Snow/Ice

6.7.3 QualityFlag

The QualityFlag dataset provides flags if the measured data is valid. These flags give additional information about the quality of the total column retrieval. If for example the fitting of the slant column does not succeed (or in case of ozone the fitting results

produce negative values), flag 0 (and also flag 1, 2 and 3) is set to indicate this condition, and the total column field will contain the fill value.

If the total column has been retrieved, but is out of the specified range, flag 1 is set. If the associated slant column error exceeds a specific threshold, flag 2 is set. If for SO_2, BrO or HCHO the correction of the VCD failed, flag 3 is set.

See *VCDQualityIndicator* in Sect. 6.2 for the percentage of pixels which have been flagged as an overall quality indicator for the whole orbit.

Bit	*Value*	*Description*
0	1	**Invalid total column (VCD)** If the retrieved total column is invalid, it is replaced with the fill value and this bit is set, together with bits 1, 2 and 3
1	2	**Total column (VCD) out of range** Set if the total column retrieved for this ground pixel is outside the specified range
2	4	**Large error in slant column (ESC)** Set if the *ESC_Error* value of this ground pixel exceeds the specified threshold
3	8	**VCD correction failed** Set if the correction of the VCD failed. Corrected VCD values in all subgroups contain fill values. This flag is only set for SO_2, BrO, HCHO and OClO.

Note that SO_2, HCHO and OClO are gases for which VCDs around zero are common (background conditions). Corresponding relative errors (as stored in the ESC_Error dataset) can thus become unphysically high. Absolute errors for these trace gases can however be found in the TOTAL_COLUMNS group as well as in the DETAILED_RESULTS subgroups.

The following table lists the valid conditions for each gas

	O_3	*NO_2*	*BrO*	*SO_2*	*H_2O*	*HCHO*	*OClO*
Total column (Flag 1)	75-700 DU	0–5*10^{16} molec/cm^2	0–1.5*10^{14} molec/cm^2	-10 – +1000 DU	0–100 kg/m^2	< 1.0*10^{17} molec/cm^2	N.A.
Slant column error (Flag 2)	<2%	<50%	<100%	N.A.	<50%	N.A.	N.A.

6.7.4 O3_Volcano_Flag

The O_3_Volcano_Flag indicates whether a GOME-2 pixel is affected by large SO_2 abundances (SO_2 emissions during a volcanic eruption). When the O3_Volcano_Flag is set to 1, total ozone column densities are overestimated (by a few percent), due to the strong SO_2 absorption.

Bit	*Value*	*Description*
0	1	***Measurement in strong SO_2 absorption (SO_2 column > 75 DU)*** • Reduced quality of total ozone column

6.7.5 NO2Tropo_Flag

The NO_2 entry in the *TOTAL_COLUMNS* group contains the same value as the VCD

entry (for the NO_2 window) in *DETAILED_RESULTS.* These two entries contain the initial total NO_2 column density based on a stratospheric (unpolluted) AMF.

The NO2Tropo entry in the *TOTAL_COLUMNS* group contains the same value as the VCDTropo entry in *DETAILED_RESULTS/NO2.* These two entries contain the tropospheric NO_2 column density. The tropospheric NO_2 column is only available for measurements with latitude < 70º and SZA < 80º. The error in the retrieved tropospheric NO_2 columns can become (very) large for measurements with cloud fractions > 20% (cloud radiance fraction > 50%), and these tropospheric NO_2 measurements should normally not be used. Therefore, the NO2Tropo entry in the *TOTAL_COLUMNS* group is not available for these cloudy conditions (the tropospheric NO_2 columns for cloudy conditions remain available via the VCDTropo entry in *DETAILED_RESULTS/NO2* to facilitate detailed data analyses).

The VCDcorrected entry in *DETAILED_RESULTS/NO2* contains the pollution corrected total NO_2 column density (available only for measurements with latitudes < 70º and SZA < 80º). The error in the pollution corrected NO_2 columns can become (very) large for measurements with cloud fractions > 20%, and these measurements should normally not be used.

The VCDStrato entry in *DETAILED_RESULTS/NO2* contains the stratospheric NO_2 column density as derived with a spatial filtering approach (available only for measurements with latitudes < 70º and SZA < 80º).

Bit	Value	Description
0	1	***Polluted condition***: ● *DETAILED_RESULTS/VCD* and TOTAL_COLUMNS/NO2 contain the initial total column density based on the stratospheric (unpolluted) AMF. ● *DETAILED_RESULTS/NO2/VCDTropo* and TOTAL_COLUMNS/NO2Tropo contain the tropospheric column density. ● *DETAILED_RESULTS/NO2/VCDCorrected* contains the pollution corrected total column density. Note: *IntensityWeightedCloudFraction* < 50%
1	2	***Unpolluted condition***: ● *DETAILED_RESULTS/VCD* and TOTAL_COLUMNS/NO2 contain the initial total column density based on the stratospheric (unpolluted) AMF. ● The tropospheric column densities in *DETAILED_RESULTS/NO2/VCDTropo* and TOTAL_COLUMNS/NO2Tropo are zero or negative. Note: *IntensityWeightedCloudFraction* < 50%.
2	4	***Cloudy condition*** (*Cloud radiance fraction* > 50%): ● *DETAILED_RESULTS/VCD* and TOTAL_COLUMNS/NO2 contain the initial total column density based on the stratospheric (unpolluted) AMF. ● *Large error in DETAILED_RESULTS/NO2/VCDTropo and DETAILED_RESULTS/NO2/VCDCorrected* ● TOTAL_COLUMNS/NO2Tropo contains fill-values. Note: *IntensityWeightedCloudFraction* > 50%
3	8	***Measurement in polar regions*** (Lat > 70º or SZA > 80º): ● *DETAILED_RESULTS/VCD* and TOTAL_COLUMNS/NO2 contain the initial total column density based on the stratospheric (unpolluted) AMF. ● *DETAILED_RESULTS/NO2/VCDTropo* and TOTAL_COLUMNS/NO2Tropo not available (fill-values) ● *DETAILED_RESULTS/NO2/VCDCorrected* not available (fill-values). ● *DETAILED_RESULTS/NO2/VCDStrato* not available (fill-values)
4	16	***Tropopsheric NO_2 column retrieval failed***: ● *DETAILED_RESULTS/NO2/VCDTropo* and TOTAL_COLUMNS/NO2Tropo not available (fill-values) ● *DETAILED_RESULTS/NO2/VCDCorrected* not available (fill-values). ● *DETAILED_RESULTS/NO2/VCDStrato* not available (fill-values)

Normally the tropospheric NO_2 column and pollution corrected total NO_2 column should only be used for measurements with *NO2Tropo_Flag* set to *1* or *2*.

6.7.6 SO2_Flag

Bit	Value	Description
0	1	***Measurement in polar regions*** (SZA > 75°): • reduced quality of SO_2 total column
1	2	**Measurement in the SAA region** • reduced quality of SO_2 total column
2	4	***SO_2 column data not available***: • *VCD* and *VCDCorrected* contain fill-values due to retrieval problems
3	8	***SO_2 column data not available due to unfulfilled external data dependency.*** • *VCD* and *VCDCorrected* contain fill-values due to e.g. missing O_3 data (needed for AMF calculation)

6.7.7 SO2_Volcano_Flag

The SO2_Volcano_Flag indicates whether a pixel shows increased SO_2 values due to a volcanic eruption. A pixel is flagged when the total vertical column exceeds a certain threshold SO_2 value and this also true for a certain amount of neighboring pixels. Different threshold values in the vicinity of volcanoes, close to anthropogenic pollution hot spots or in areas with high noise are used to avoid false-positive detections. Since sometimes a false-positive detection can still occur especially in the Norilsk area, in the SAA region or at high SZA, these pixels are flagged separately.
Note that during a solar-eclipse false-positive detections can occur. The user is advised to use the *SolarEclipseFlag* in the *GEOLOCATION* group (see Section 6.3) in combination with the SO2_Volcano_Flag.

Value	Description
0	***No detection***
1	***Volcanic SO_2 detection*** • Pixel as well as >50% of the neighboring pixels exceed a threshold SO_2 value of 1.2 DU. In the vicinity of known volcanoes the threshold is set to 0.7 DU
2	***Volcanic SO_2 detection in polluted region*** • Pixel as well as >50% of the neighboring pixels exceed a threshold SO_2 value of 2 DU in the polluted areas of Bohai (China, 20-45°N, 100-130°E) or Norilsk (Russia, 60-80°N, 60-120° E)
3	***Volcanic SO_2 detection in SAA region or at high SZA (>70deg)*** • Pixel as well as >66% of the neighboring pixels exceed a threshold SO_2 value of 3 DU in the South Atlantic Anomaly region (SAA, 60-100°S, 100-0°) or for SZA angles >70°

6.7.8 H2O_Flags

Bit	Value	Description
0	1	***Measurement in cloudy conditions*** • Reduced quality of H_2O total column
1	2	***Measurement in cloudy and/or elevation conditions*** (small O_2 column): • Reduced quality of H_2O total column

The H_2O entry in the *TOTAL_COLUMNS* group is set to fill-value for measurements under cloudy conditions (Bit 0 is set). The retrieval values are nevertheless available in the *DETAILED_RESULTS/H2O* Subgroup. Note that the BUFR products (see Chap. 7) contain all H_2O retrievals, but it is recommended not to use measurements under cloudy conditions (cloud_fraction * cloud_top_albedo < 0.6).

6.7.9 HCHO_Flags

Bit	Value	Description
0	1	***Measurement with large solar zenith angle*** (SZA > 70°): ● reduced quality of HCHO total column
1	2	***Cloudy conditions (cloud fraction > 40%)***: ● reduced quality of HCHO total column
2	4	***HCHO column data not available***: ● *HCHO* contains fill-values
3	8	***HCHO column data not available due to unfulfilled external data dependency.*** ● *HCHO* contain fill-values

6.7.10 OClO_Flag

This flag indicates if OClO can be observed. As OClO photolyses rapidly, it can only be observed at large solar zenith angles, usually during twilight. Therefore, valid (enhanced) OClO column values can only be expected for measurements with *OClO_Flag* set to *1* or *2*. Note that for OClO only slant column densities are provided (no conversion to vertical columns).

Bit	Value	Description
0	1	***Measurement (daylight) with large solar zenith angle*** (85 ° < SZA < 89°) • Note: OClO can only be observed at large solar zenith angles
1	2	***Measurement during twilight*** (89 ° < SZA < 92°) • Note: OClO can only be observed at large solar zenith angles
2	4	***OClO column data (background corrected) not available*** • ESCCorrected contains fill-values

6.7.11 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. 6.7.2) in order to explain how to read and interpret these datasets.

In the SurfaceConditionFlag several scenarios can appear: Land/Sea, Sun glint as well as Snow/Ice. In principle for a single pixel several scenarios can occur e.g. a pixel over the sea which is subject to sun glint. When represented in binary form then it would look like:

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

0 1 1 Value 2 1 0 Bit Integer value: 3 (2^1+2^0, first and second bit set)	Pixel over sea, sun glint (both flags set), no snow/ice
1 0 0 Value 2 1 0 Bit Integer value: 4 (2^2)	Pixel over land, no sun glint, snow/ice flag set
1 0 1 Value 2 1 0 Bit Integer value: 5 (2^2+2^0)	Pixel over sea, no sun glint, snow/ice flag set
1 1 0 Value 2 1 0 Bit Integer value: 6 (2^2+2^1)	Pixel over land, sun glint flag set, snow/ice flag set
1 1 1 Value 2 1 0 Bit Integer value: 7 ($2^2+2^1+2^0$)	All flags 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 snow/ice flag bit is set the user has to do the operation 2^{bit} AND SurfaceConditionFlag(Pixel). The snow/ice flag is stored in the 2^{nd} bit, hence the operation would be 2^2 AND SurfaceConditionFlag(Pixel). If for example for this pixel the SurfaceConditionFlag would have the integer value 7 (all flags set) then the resulting check would be 2^2 AND 7 or 4 AND 7. In this case the result would be 4 since the binary AND compares the following:

2	1	0	Bit
1	0	0	Check value 2^2 (2^{nd} bit set)
1	1	1	SurfaceConditionFlag(pixel)
1	**0**	**0**	**AND result: $2^{bit}=2^2=4$**

In case the snow/iceflag would not be set, the result of this operation would be zero:

2	1	0	Bit
1	0	0	Check value 2^2 (2^{nd} bit set)
0	1	1	SurfaceConditionFlag(pixel)
0	**0**	**0**	**AND result = 0**

Hence in order to select all pixels with the Snow/Ice flag set, the user has to search for all pixels which fulfill the condition 4 AND 7 > 0.

As a second example we describe how to use the ViewMode dataset (Sect.6.7.1). 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 9^{th} 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 2^8 AND ViewMode > 0 must be fulfilled. For the pixels on the ascending node the condition 2^8 AND ViewMode = 0 applies

Here we give some examples:
Nominal swath, ascending orbit: (255 AND ViewMode) = 0 & (256 AND ViewMode) =0
Nominal swath, descending orbit: (255 AND ViewMode) = 0 & (256 AND ViewMode) >0
Narrow swath, ascending orbit: (255 AND ViewMode) = 1 & (256 AND ViewMode) =0
Narrow swath, descending orbit: (255 AND ViewMode) = 1 & (256 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)

7 BUFR Product Format Description

7.1 Structure

The data in the BUFR file is organized in six sections: *INDICATOR SECTION, IDENTIFICATION, OPTIONAL SECTION, DATA DESCRIPTION, DATA SECTION* and *END SECTION*. The values in all sections are either copied from the level 1 ([R12], [R13]) or other input data, or calculated by the level 1-to-2 processor. Each of the sections of a BUFR message is made up of a series of octets. The term octet, meaning 8 bits, was coined to avoid having to continually qualify byte as an 8-bit byte.
The *DATA DESCRIPTION* section contains a list of descriptors defining the structure and the format of data following in *DATA SECTION*. This is called “self-descriptive” nature of BUFR. The strength of this self-descriptive feature is in accommodating change. For example, if new observations or observational platforms are developed, there is no need to invent a new code form to represent and transmit the new data; all that is necessary is the publication of additional data description tables. Similarly for the deletion of possibly outdated observations: instead of having to send “missing” indicators for a long period while awaiting a change to a fixed format code, the “missing” data are simply not sent in the message and the data description section is adjusted accordingly. The data description tables are not changed, however, so that archives of old data may be retrieved.
The data encoded in BUFR format is purely binary or bit oriented, thus making it both machine dependent and, at the same time, machine independent. The dependency comes in the construction or interpretation of BUFR messages: there is not much for a human to look at as all the numbers in a message, whether data descriptors or the data themselves, are binary integers. And that, of course, leads to the machine independence: with BUFR consisting entirely of binary integers any brand of machine can handle BUFR as well as any other.
Theoretically there is no upper limit to the size of a BUFR message but, by convention, BUFR messages are restricted to 15000 octets or 120000 bits. This limit is to allow an entire BUFR message to be contained within memory of most computers for decoding. It is also a limit set by the capabilities of the Global Telecommunications System (GTS) of the WMO. In UPAS the length of a single BUFR message is limited to 200 ground pixels, that gives approximately 10Kbytes for storing one message. The file contains the information corresponding to a single orbit and can contain an unlimited number of consecutive BUFR messages.

7.2 WMO/GTS Bulletin Identifier

The BUFR products from the AC-SAF can be accessed using the following identifier:

Region	RTH	Country	TTAAii	CCCC	CodeForm
6	OFFENBACH	GERMANY	IUCX01	EDLR	FM 94-XIII

7.3 Section 0 - Indicator Section

Octet	Description	Allowed Values
1-4	"BUFR" (coded according to the CCITT International Alphabet No. 5)	"BUFR"
5-7	Total length of BUFR message, in octets (including Section 0)	0-15000
8	BUFR edition number (currently 4)	1-4

7.4 Section 1 - Identification Section

Octet	Description	Allowed/Used Values
1-3	Length of section, in octets	int value
4	BUFR master table (zero if standard WMO FM 94 BUFR tables are used - provides for BUFR to be used to represent data from other disciplines, and with their own versions of master tables and local tables)	0
5-6	Originating centre: code table 0 01 031	210
7-8	Originating sub-centre	0
9	Update sequence number (zero for original BUFR messages; incremented for updates)	1
10	Bit 1 = 0 No optional section = 1 Optional section included Bits 2 - 8 set to zero (reserved)	0
11	Data Category type (BUFR Table A)	3
12	Data Category sub-type (defined by local ADP centres)	255
13	Local data sub-category	206
14	Version number of master tables used (currently 2 for WMO FM 94 BUFR tables)	11
15	Version number of local tables used to augment the master table in use	0
16-17	Year	2xxx
18	Month	1-12
19	Day	1-31
20	Hour	0-23
21	Minute	0-59
22	Second	0-59

7.5 Section 3 - Indicator Section

Octet	Description	Allowed/Used Values
1-3	Length of section, in octets	
4	Set to zero (reserved)	
5-6	Number of data subsets	200
7	Bit 1 = 1 observed data = 0 other data Bit 2 = 1 compressed data = 0 non-compressed data Bit 3 - 8 set to zero (reserved)	192
8-	A collection of descriptors which define the form and content of individual data elements comprising one data subset in the data section.	

7.6 Section 3 - UPAS Level-2 Specific List of Descriptors

Descriptor	Description	Value
0 01 007	Satellite Identifier	5 = Metop-2
0 02 019	Satellite Instruments	220 = GOME-2
3 01 011	Date in format YYYY-MM-DD (0 04 001, 0 04 002, 0 04 003)	
3 01 013	Time in format HH-MM-SS (0 04 004, 0 04 005, 0 04 006)	
3 01 021	Latitude / Longitude Centre (0 05 001, 0 06 001)	
1 02 004	Repeat next 2 fields 4 times (for four corners of a pixel)	
0 27 001	Latitude (High Accuracy)	
0 28 001	Longitude (High Accuracy)	
0 10 001	Height of land surface	
0 14 019	Surface Albedo	0.0-1.0
0 07 025	Solar zenith angle	
0 10 080	Viewing Zenith Angle	
0 05 023	Sun to satellite azimuth difference	
0 20 010	Cloud Cover (Total)	[%]
0 08 003	Vertical significance	2 = Cloud top
0 07 004	Pressure	[pa]
0 14 026	Albedo at the top of clouds	0.0-1.0
0 20 014	Height of top of clouds	[km]
0 13 093	Cloud optical thickness	
0 31 001	Delayed descriptor replication factor	2
0 07 004	Pressure	Top
0 07 004	Pressure	Bottom
0 08 043	Atmospheric chemical or physical constituent type	see table below
0 08 044	CAS registry number	see table below
0 15 021	Integrated mass density	[kg/m^2]
2 24 000	First order statistics follow	
2 36 000	Backward reference bitmap	
0 31 001	Delayed descriptor replication factor	2
0 31 031	Data present indicator	0/1
0 01 031	Identification of originating/generating centre	254 (Eumetsat)
0 01 032	Generating Application Defined by local Generating Centre	1
0 08 023	First order statistics	7 = Mean absolute error
0 31 001	Delayed descriptor replication factor	2
0 15 021	Scaled Integrated mass density	[kg/m^2]

7.7 Section 4 - Indicator section.

Octet	Description	Allowed Values
1-3	Length of section, in octets	
4	Set to zero (reserved)	
5-	Binary data as defined by descriptors which begin at octet 8, Section 3	

7.8 Section 5 - End Section

Octet	Description	Allowed Values
1-4	"7777" (coded according to the CCITT International Alphabet No. 5)	„7777“

7.9 Trace Gas Table

The following field values are used for the different trace gases:

Trace gas	Trace gas name	Atmospheric Chemical No. (08 043 descriptor)	CAS Registry Number (08 044 descriptor)
O_3	Ozone	0	10028-15-6
NO_2	Nitrogen dioxide	5	10102-44-0
BrO	Bromine oxide	9	15656-19-6
SO_2	Sulfur dioxide	8	7446-09-5
H_2O	Water Vapour	1	7732-18-5
HCHO	Formaldehyde	7	50-00-0
OClO	Chlorine dioxide	10	10049-04-4
CHOCHO	Glyoxal	TBD	107-22-2

8 Using the Products

This chapter contains practical information on using the GOME-2 trace gas column products.

As a general advise, it is strongly recommended to use only the forward-scan pixels and discard the back-scan pixels. Back-scan pixels are not only redundant, but they are less accurate than the forward-scan pixels due to their larger footprint size. The IndexInScan attribute from the *GEOLOCATION* group in the HDF5 products has values of 0,1,2 for East/Nadir/West forward-scan pixels; back-scan pixels can be easily filtered-out checking that IndexInScan<3. Back-scan pixels are not included in the BUFR products.

8.1 Confidence Flags and Ancillary Fields

The users should check the quality flags associated with each trace gas and cloud product. Detailed information is given in the corresponding tables.

8.2 Averaging Kernels

For the tropospheric NO_2 and HCHO columns, averaging kernels are provided together with the error budget for each individual GOME-2 pixel. The column averaging kernels A_l are calculated for optically thin absorbers (such as NO_2 and HCHO) 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.

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 NO_2 and HCHO profiles as used in the retrieval (pressure level at layer center). The a priori NO_2 and HCHO profiles (in volume mixing ratios) are also provided in the GOME-2 product.

8.3 Software and Tools for reading the products

The HDF5 products can be read using the standard HDF software and tools available at:

http://www.hdfgroup.org/products/hdf5_tools

the above Web page contains HDF5 libraries for a number of programming languages. The BEAT and VISAN tools for ingesting, processing, and analyzing atmospheric

remote sensing data fully support the GOME HDF5 products:

http://www.stcorp.nl/beat

ECMWF provides software for decoding BUFR products, see:

http://www.ecmwf.int/products/data/software/bufr.html

9 Appendixes

A.1 HDF5 Data Types

The following table shows the correspondence between Product data types and HDF5 data types

Data type	*HDF5 predefined data type*
Char	H5T_STD_I8LE
Integer	H5T_STD_I32LE
Float	H5T_IEEE_F32LE
Double	H5T_IEEE_F64LE
String	H5T_C_S1
UTC	H5T_COMPOUND { H5T_STD_I32LE Day, H5T_STD_I32LE MillisecondOfDay }, where Day denotes number of days since 1st of January, 1950

VIEW_MODES	H5T_COMPOUND {
	H5T_STD_I32LE NominalPixels,
	H5T_STD_I32LE StaticPixels,
	H5T_STD_I32LE NarrowPixels,
	H5T_STD_I32LE PolarSouthPixels,
	H5T_STD_I32LE PolarNorthPixels
	}

CCSDS_ASCII	The format for ASCII Time Code is *YYYY-MM-DD*T*hh:mm:ss.ddd*, where: *YYYY* = Year in four-character subfield with values 0001-9999 *MM* = Month in two-character subfield with values 01-12 *DD* = Day of month in two-character subfield with values 01-28,-29, -30, or -31 "T" = Calendar-Time separator *hh* = Hour in two-character subfield with values 00-23 *mm* = Minute in two-character subfield with values 00-59 *ss* = Second in two-character subfield with values 00-59 *ddd* = Decimal fraction of second where each d has values 0-9

POS_VEC	H5T_COMPOUND {
	H5T_IEEE_F64LE X,
	H5T_IEEE_F64LE Y,
	H5T_IEEE_F64LE Z
	}

A.2 Traceability Matrix of HDF5 Metadata to EECF Parameters

The EECF metadata parameters [A2] which are applicable to the D-PAF products are stored in the HDF5 file as attributes in the *META_DATA* group. The tracing of EECF parameters to the attributes in the product file is indicated in the following table. Attributes can only take values which are allowed by EECF.

EECF Short Name	*Attribute Name*	*Notes*
SATELLITE_ID	SatelliteID	possible values: ERS; M01, M02... for METOP
SENSOR_ID	InstrumentID	GOME
ORBIT_NO	StartOrbitNumber	
ACQUISITION_FACILITY_ID	ReceivingCentre	ECF, FBK, FUC, GCA, PGS, RUS, SOC, SVL, UBI, WAL, WEC, WIV
PROCESSING_FACILITY_ID	ProcessingCentre +ArchiveFacility	D-PAF DLR OP (ERS), O3DLR (METOP)
PROCESSING_DATE_TIME	ProcessingTime	

TEMPORAL_COVERAGE_START	SensingStartTime	
TEMPORAL_COVERAGE_STOP	SensingEndTime	
SOFTWARE_VERSION	ProductAlgorithmVersion	
AUX_DATA	InitializationFileVersion	
PRODUCT_TYPE	ProcessingLevel	“02” or “03”
REVISION	Revision	
SOURCE_ITEM	BaseProducts	

A.3 Traceability Matrix of HDF5 Metadata to UMARF Parameters

The UMARF metadata parameters [A3] applicable to the AC-SAF products are stored in the HDF5 file as attributes in the *META_DATA* group. The mapping of UMARF parameters to product file attributes is shown below; again, attributes can only take values allowed by UMARF.

UMARF Short Name	***Attribute Name***	***Notes***
AARF	ArchiveFacility	possible values: D-PAF DLR OP (ERS), O3DLR (METOP)
ABID	ProductContents	Spectral Band Ids
AIID	InstrumentID	GOME
APAS	Applicable (*)	Product Size
APNA	Applicable (*)	Product Name
APNM	ProductType	e.g. O3MOTO, O3MNTO
APPN	BaseProducts	Parent Product Name
ASTI	SatelliteID	possible values: ERS; M01, M02, M03 for METOP
AVBA	BaseProductAlgorithmVersion	
AVPA	ProductAlgorithmVersion	Concatenation of the HDF5 attributes *ProductAlgorithmVersion*, *InitializationFileVersion*, *InternalProcessorRevision*, and *Revision*
GDMD	Applicable (*)	Disposition Mode: T, O, or P
GGTP	Applicable (*)	GranuleType: “DP”
GNFV	ProductFormatVersion	
GORT	Applicable (*)	OrbitType: “LEO”
GPLV	ProcessingLevel	“02” or “03”
GPMD	ProcessingMode	N, B, R, V
LLAE	SubSatellitePointEndLat	-90.0000 to +89.9999
LLAS	SubSatellitePointStartLat	-90.0000 to +89.9999
LLOE	SubSatellitePointEndLon	-180.0000 to +179.9999
LLOS	SubSatellitePointStartLon	-180.0000 to +179.9999
LONS	StartOrbitNumber	
LSVL	OrbitAscendingNodeLongitude	-180.0000 to +179.9999
LSVT	OrbitAscendingNodeCrossingDateTime	CCSDS date
PPRC	ProcessingCentre	possible values: D-PAF DLR OP (ERS), O3DLR (METOP)
PPST	Processing End Date and Time	CCSDS date
QDLC	MissingDataCount	
QDLP	MissingDataPercentage	
QDRC	DegradedRecordCount	
QDRP	DegradedRecordPercentage	
QQAI	Applicable (*)	Associated Quality Information
QQOV	Applicable (*)	Overall quality flag: OK/NOK
RRCC	ReceivingCentre	ECF, FBK, FUC, GCA, PGS, RUS, SOC, SVL, UBI, WAL, WEC, WIV
SMOD	InstrumentMode	e.g. NARROW, NORMAL or STATIC
SNIT	Applicable (*)	CCSDS date
SSBT	SensingStartTime	CCSDS date
SSST	SensingEndTime	CCSDS date

(*) Parameter is not contained in the HDF5 product, but will be provided by DIMS.