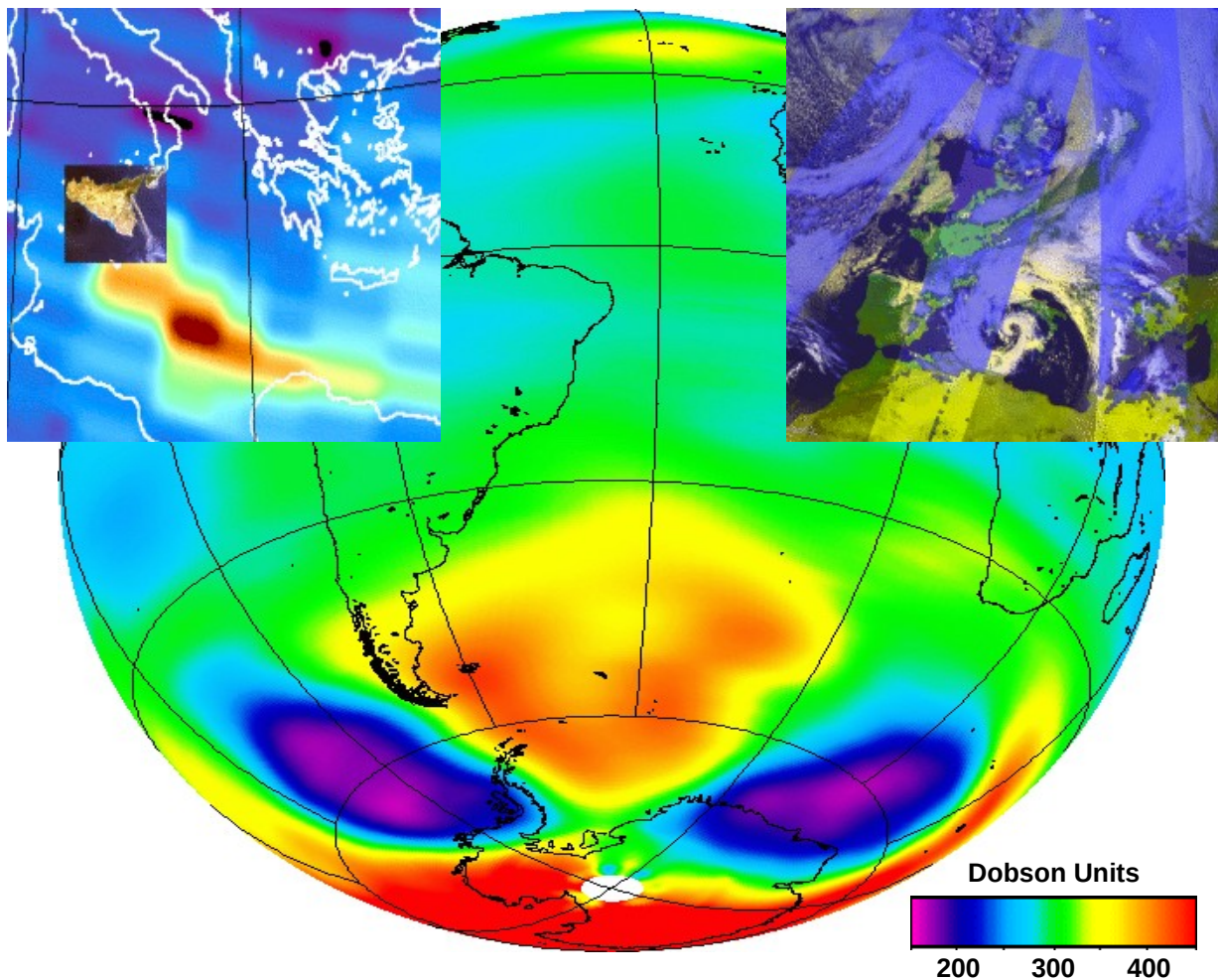




Product User Manual for GOME Total Columns of Ozone, NO_2 , tropospheric NO_2 , BrO, SO_2 , H_2O , HCHO, OCIO, and Cloud Properties

(O3M-SAF OTO and NTO)



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| GOME/ERS-2 Team | ESA, BIRA, RTS, AUTH, various |
| O3M-SAF Team | EUMETSAT, FMI, AUTH, BIRA, KNMI, various |



Document Change Log

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| 1 | A | 31 July 2004 to 20 July 2006 | all | HDF5 and BUFR output product format documents merged in this product user manual |
| 1 | B | 5 October 2006 | 4, 5 | Content of chapters added |
| 1 | C | 10 November 2006 | all | First official version of this document |
| 1 | D | 6 March 2007 | 5.7 6.2, 6.5 | Fix file name convention Added VCDQualityIndicator, QualityFlags, CloudMode, CloudType, AMFTTotal, AMFTTotal_Error, OrbitActualDuration, new receiving stations |
| 1 | E | 30 April 2008 | all 6 7 | Revised following ORR-A Added in HDF5 section: - IterativeVCDNumberOfIterations - a-priori O ₃ _Profile - T_Profile BUFR product update to BUFR version 4 |
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| | | 18 December 2009 | 6 | PixelFlag under Geolocation section is renamed to SurfaceConditionFlag. SurfaceConditionFlag definition added. H ₂ OFlag definition changed. |



| | | | | |
|---|---|-----------------|--------------|---|
| 2 | C | 23 April 2010 | 1.1 | Add reference to reprocessed GOME-2 |
| | | | 5.9.2 | Add new O3M-SAF logo and web page |
| | | | 6.4 | Finalized NO ₂ HDF5 entries |
| | | | 6.2 | Added PMD dataset descriptions |
| | | | 7.2 | Add WMO/GTS bulletin identifier |
| | | | 8 | New section |
| | | | 6.8.5 | New flag value added to SO ₂ _Flag |
| | | | 6.8.7 | New flag value added to HCHO_Flag |
| 2 | D | 25 March 2011 | 6.8.2 | Renamed SurfaceCondition_Flag to SurfaceConditionFlags |
| | | | 6.2 | Removed obsolete FittingFlag, AMFFlag and VCDFlag |
| | | | 6.8.6 | New definitions for H ₂ O_Flags |
| | | | 6.3 | Converted ViewMode to integer and added DescendingFlag |
| 2 | E | 8 August 2012 | 4.1 | Added new chapter GDP-5.0 used for GOME/ERS-2 O ₃ products |
| | | | 6.7 | |
| | | | 6.6.2 | Added NO ₂ entries: <ul style="list-style-type: none"> - 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 | 28 June 2013 | 6.6.4 | H ₂ O: <ul style="list-style-type: none"> - Add EastWestPostCorrectionFactorH2O - Removed RingCorrectionFactor |
| | | | 6.8.1 all | Added ViewMode description table Updates for GOME-2/MetOp-B Updated entry descriptions Various clarifications |



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1 Introduction

1.1 Purpose and Scope

DLR has been producing on an operational basis a range of total column trace gases and cloud products for GOME/ERS-2 in the framework of ESA's D-PAF project. In the same way, DLR produces total column trace gases and cloud products for GOME-2/MetOp in the framework of EUMETSAT's O3M-SAF.

DLR has a long experience in operational processing of GOME 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/ERS-2 and GOME-2/MetOp total column trace gases and cloud products available at DLR.

In this document, the terms GOME/ERS-2 and GOME-2/MetOp are used to reference the specific instruments. The general term GOME applies to both sensors.

The trace gases total column products are:

- Ozone (O₃) column
- Nitrogen dioxide (NO₂) column
- Bromide monoxide (BrO) column
- Sulphur dioxide (SO₂) column
- Water vapour (H₂O) column
- Formaldehyde (HCHO) column

Additionally DLR provides the following cloud properties derived from GOME 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 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 two weeks (up to four weeks in case of GOME/ERS-2) after sensing.

Additionally, DLR provides reprocessed products for climate applications. The complete

GOME/ERS-2 data record starting in 1995 has been reprocessed and validated on a regular basis using improved algorithms. In the same way, the complete GOME-2/MetOp data record starting in 2007 was already reprocessed and validated.

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 products. The “Hierarchical Data Format” (HDF) and the “Binary Universal Form for the Representation of meteorological data” (BUFR) have been selected for the GOME 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/ERS-2 and GOME-2/MetOp instruments 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] Product Requirements Document, SAF/O3M/FMI/RQ/PRD/001, Rev. 06, May 2008

1.2.1 Reference Documents

- [R1] P. Valks, D. Loyola, N. Hao, P. Hedelt, S. Slijkhuis, M. Grossi, Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, Tropospheric Ozone, NO₂, tropospheric NO₂, BrO, SO₂, H₂O, HCHO, OClO, and Cloud Properties (GDP 4.5 for O3M-SAF OTO and NTO), DLR/GOME-2/ATBD/01, Iss./Rev. 2/H, 2013.
- [R2] R. Spurr, M. van Roozendaal, D. Loyola, C. Lerot, J. van Geffen, J. van Gent, C. Fayt, J.-C. Lambert, W. Zimmer, A. Doicu, S. Otto, D. Balis, M. Koukouli, C. Zehner, GDP 5.0 Upgrade of the GOME Data Processor for Improved Total Ozone Columns — Algorithm Theoretical Basis Document, DLR/GOME/ATBD/GDP5, Iss./Rev. 1B, August 2012.
- [R3] “Algorithm Theoretical Basis Document for GOME Total Column Densities of Ozone and Nitrogen Dioxide, UPAS/GDOAS: GDP 4.0”, ERSE-DTEX-EOPG-TN-04-0007, Iss./Rev. 1/A, December 2004.
- [R4] J-C. Lambert, M. Koukouli, D. Balis, J. Granville, C. Lerot, and M. Van Roozendaal, GDP 5.0 Upgrade of the GOME Data Processor for Improved Total Ozone Columns — Validation Report, TN-IASB-GOME-GDP5-VR, Iss./Rev. 1B, August 2012.
- [R5] D. Balis, M. Koukouli, D. Loyola, P. Valks, N. Hao, GOME-2 O₃ total column validation report, SAF/O3M/AUTH/VR/O3/3, November 2009.



- [R6] J.-C. Lambert, G. Pinardi, J. Granville, K. Clemer, A. Delcloo, P. Valks, N. Hao, GOME-2 NO₂ total column validation report, SAF/O3M/IASB/VR/NO2/095, February 2011.
- [R7] J. van Geffen, M. Van Roozendael, M. Rix, P. Valks, GOME-2 SO₂ total column initial validation, TN-IASB-GOME2-O3MSAF-SO2-01.1, November 2008.
- [R8] M. Van Roozendael, N. Theys, N. Hao, P. Valks, GOME-2 BrO total column validation report, SAF/O3M/BIRA/VR/BRO/091, January 2009.
- [R9] N. Kalakoski, T. Wagner, K. Mies, S. Beirle, S. Slijkhuis, D. Loyola, GOME-2 H₂O total column validation report, SAF/O3M/FMI/VR/H2O/111, April 2011.
- [R10] "Delta Validation Report for ERS-2 GOME Data Processor upgrade to version 4.0", ERSE-CLVL-EOPG-TN-04-0001, Iss./Rev. 1.0, December 2004
- [R11] "Product Specification Document of the GOME Data Processor", ER-PS-DLR-GO-0016, Iss./Rev. 4/B, December 2004
- [R12] "GOME-2 Level 1 Product Format Specification", EPS/MIS/SPE/97232, 2008
- [R13] "GOME-2 Products Guide", EUM/OPS-EPS/MAN/05/0005, Issue 1.0, February 2005
- [R14] HDF5 File Format Specification <http://www.hdfgroup.org/HDF5/>
- [R15] BUFR Format Specification
<http://www.wmo.int/pages/prog/www/WDM/Guides/Guide-binary-1A.html>
- [R16] Eumetcast Dissemination Facility
<http://www.eumetsat.int/website/home/Data/DataDelivery/EUMETCast/index.html>
- [R17] Eoweb DLR Online User Service
<http://eoweb.dlr.de>

1.3 Abbreviations and Acronyms

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

| | |
|-----------|--|
| AAIA | Absorbing Aerosol Indicator Algorithm |
| 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 |
| O3M-SAF | SAF on Ozone and Atmospheric Chemistry Monitoring |
| 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) is a scanning spectrometer 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 0.4 nm.

The measured spectra are mainly used to derive ozone total column and vertical profile, nitrogen dioxide, bromine oxide, water vapour, oxygen, sulphur oxide 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.

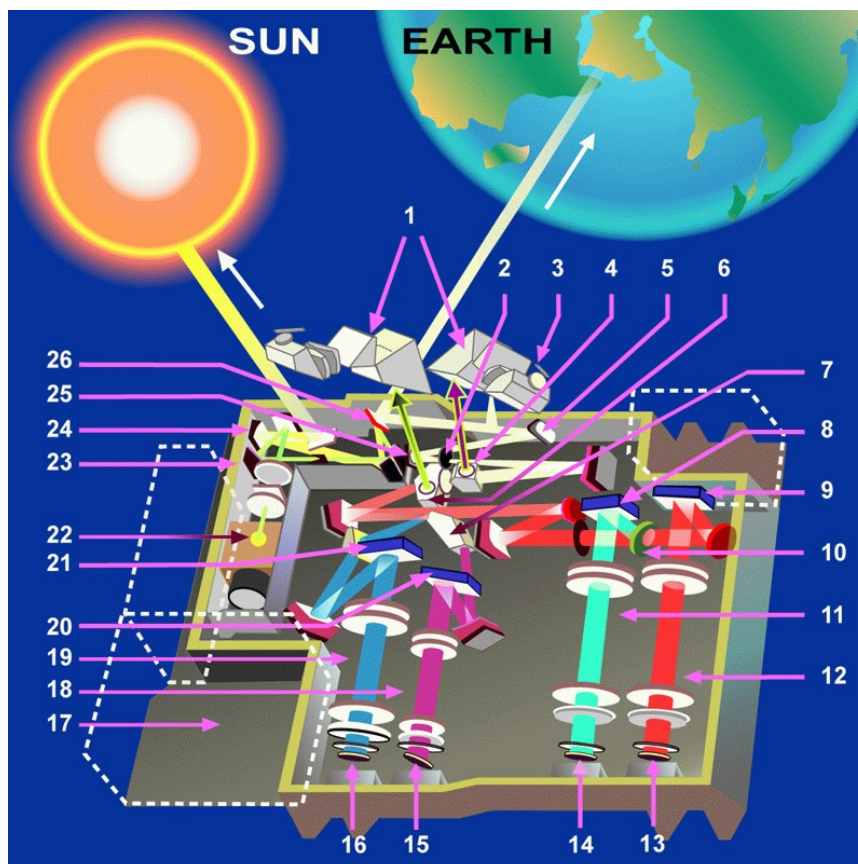


Figure 1: GOME optical layout (courtesy of ESA/ESTEC)



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 [R13].

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 (O3M-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>

<http://www.eumetsat.int/EPSCalValExtranet/Main/GOMECalVal/index.htm>

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 this calibrations are performed on the night side.

The effective optical throughput and the potential data rate for GOME-2/MetOp are much higher than those for GOME/ERS-2¹. The default integration times for GOME-2/MetOp is 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/ERS-2 and GOME-2/MetOp. The GDP 4.7 uses an optimised DOAS (Differential Optical Absorption Spectroscopy) algorithm to determine the trace gas slant column. 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. The latest development GDP 5 uses the GODFIT algorithm for the retrieval of total ozone from GOME/ERS-2. A detailed description of the GDP algorithms are given in [R1], [R2] and [R3].

3.2 Trace Gas and Cloud Products

The GOME/ERS-2 and GOME-2/MetOp trace gas column densities and cloud properties (level-2 product) are retrieved from GOME (ir)radiance and PMD data (level-1 product). The following table lists the trace gas column and cloud products provided by DLR, and the corresponding wavelength regions used for the retrieval.

| <i>Product</i> | <i>Wavelength region (nm)</i> |
|--|-------------------------------|
| O ₃ column | 325.0-335.0 |
| NO ₂ column | 425.0-450.0 |
| BrO column | 332.0-359.0 |
| SO ₂ column | 315.0-326.0 |
| H ₂ O column | 614.0-683.2 |
| HCHO column | 328.5-346.0 |
| Cloud fraction | 300-800 (PMD-p) |
| Cloud-top height (pressure) and albedo (cloud optical thickness) | 758.0-771.0 |

4 Processing

The Universal Processor for UV/VIS Atmospheric Spectrometers (UPAS) is the core GOME 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. O₃, NO₂, BrO, H₂O, SO₂, HCHO) 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 O₃, NO₂, and cloud retrieval 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/ERS-2

DLR has a processing chain for GOME/ERS-2 NRT and OL total column products that is being used operationally since 1995. It includes data ingestion, from level 1 to level 4 product generation, quality control, product archiving, data dissemination, and ordering.

The operational products from GOME are total ozone and NO₂ using GDP-5.0. In GDP-5.0 the new GODFIT algorithm for total ozone developed by BIRA/RTS/DLR and the DOAS algorithm for NO₂ are used. See [R2] and [R3].

GOME/ERS-2 images and value added products produced at DLR are available at <http://atmos.eoc.dlr.de/gome>.

4.2 GOME-2/MetOp

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 [R13] and received at DLR via EUMETCast ([R16]). 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 O3M-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.

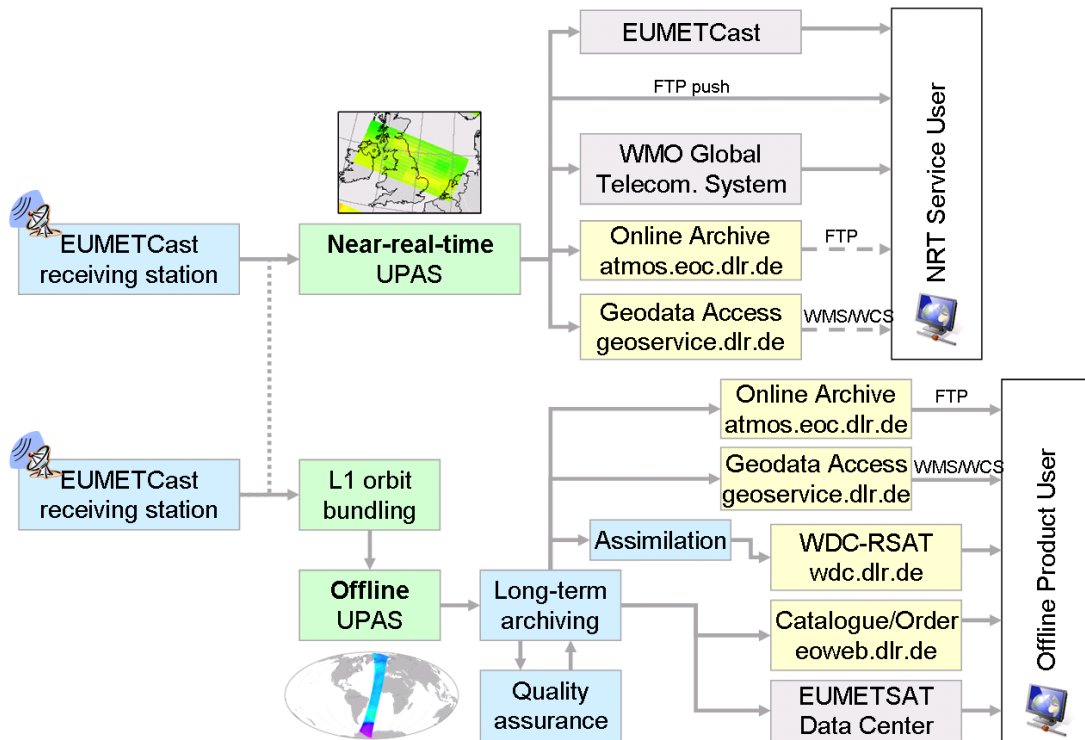


Figure 2: GOME-2/MetOp processing chain

4.3 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 O3M-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 [R17]).

4.4 Quality Control and Monitoring

The quality of the OL 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.

4.5 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, other satellite data, as well as data assimilation techniques. The validation results are publicly available on the Internet, see section 5.9.

4.6 User Services

Information about data and services are accessible through the websites given in section 5.9 and at the end of this section.

The interactive catalogue and ordering interface EOWEB® from DLR allows individual product searches and ordering.

Catalogue information from the O3M-SAF products generated at DLR are 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.

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>, left side of 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.

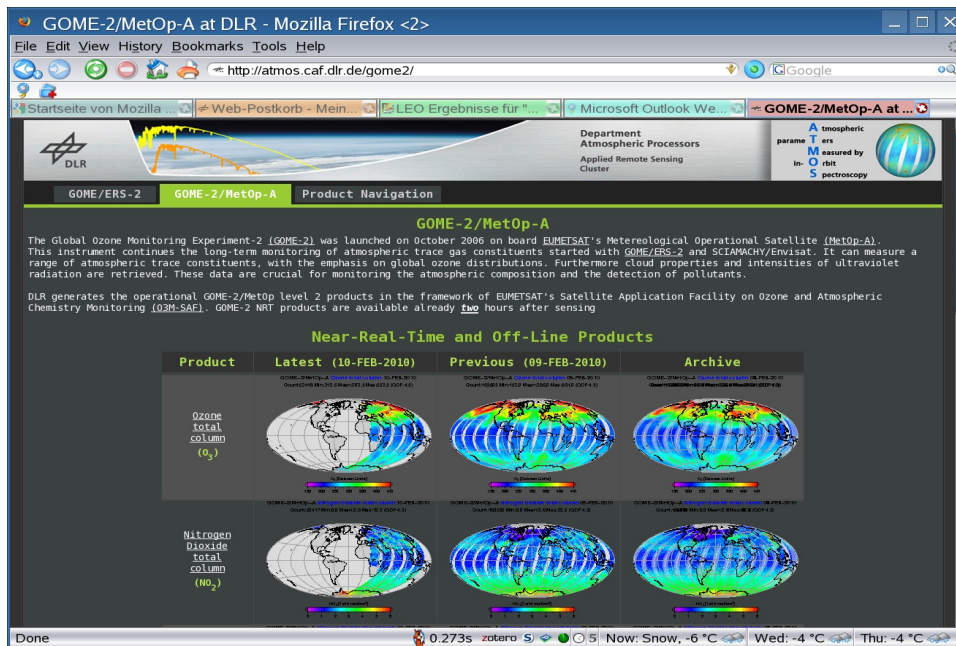


Figure 3: GOME-2/MetOp web page at DLR

5 Total Column Trace Gases and Cloud Products

The 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 ₂ O 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 [%] |

5.2 Geographical Coverage and Granularity

GOME/ERS-2 has a nominal global coverage at the equator after three days. 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, operational OL and reprocessed products have by default a global coverage. The coverage of trace gases available only under special conditions may be reduced, e.g. SO₂ measured during volcanic eruption.

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

5.3 Spatial Resolution

GOME/ERS-2 has three forward-scan pixels with a nominal resolution of 40 km x 320 km, and one back-scan pixel with a nominal resolution of 40 km x 960 km.

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.

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 level 0 or level 1 product.

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

The GOME-2/MetOp OL products are available two weeks after sensing. The GOME/ERS-2 OL products are available up to four weeks after sensing due to constraints on the current level 0 data dissemination.

Reprocessed GOME/ERS-2 and 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

The following table lists the GOME total column trace gases and cloud products provided by DLR together with estimated uncertainties.

| <i>Product</i> | <i>Acronym</i> | <i>Expected Accuracy</i> | <i>Expected Precision</i> |
|--|-----------------------|--|---|
| Total ozone column, | O ₃ | 3.6-4.3% (SZA < 80°) 6.4-7.2% (80° < SZA < 90°), see [R4] and [R5] | 2.4-3.3% (SZA < 80°) 4.9-5.9% (80° < SZA < 90°) |
| Total NO ₂ column | NO ₂ | 5-15% (unpolluted conditions), see [R6] | 3-15% (unpolluted conditions) |
| Tropospheric NO ₂ column | NO ₂ Tropo | 40-80% (polluted conditions) > 100% (unpolluted), see [R6] | 40-80% (polluted conditions) > 100% (unpolluted) |
| Total BrO column | BrO | 20-50%, see [R8] | 10-50% |
| Total SO ₂ column | SO ₂ | 50-100% (SZA < 70°) >100% (SZA > 70°), see [R7] | 20-50% (SZA < 70°) >50% (SZA > 70°) |
| Total H ₂ O column | H ₂ O | 10-25%, see [R9] | 5-20% |
| Total HCHO column, | HCHO | 50-100% (polluted conditions) > 100% (unpolluted) | 20-50% (polluted conditions) > 100% (unpolluted) |
| Cloud fraction | CF | < 10% | < 10% |
| Cloud-top height (cloud-top pressure) | CTH (CTP) | < 10% | < 10% |
| Cloud albedo (cloud optical thickness) | CTA (COT) | < 10% | < 10% |

NRT and OL products have the same accuracy and precision.



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 section 6 on page 25, and for the BUFR product in section 7 on page 42.

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-BrO” 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

For example, the following identifier denotes a GOME/ERS-2 off-line product:

GOME_O3-NO2_L2_20060723165752_023_ERS2_58855_DLR_05.HDF5

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

GOME_O3-NO2-BrO_L2_20070302111155_047_METOPA_01900_DLR_01.HDF5

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

S-O3M_GOME_O3-NO2-NO2Tropo-SO2_L2_20121205144758_003_METOPA_31808_DLR_03.HDF

S-O3M_GOME_O3-NO2-SO2_L2_20121205144758_003_METOPA_31808_DLR_03.BUFR

5.8 Product Dissemination

5.8.1 GOME/ERS-2

GOME/ERS-2 products are available at the D-PAF FTP-server:

eo-a-dp.eo.esa.int

The products are organized in directories as follows:

products/level_2_HDF5/YYYY/MM/DD

where *YYYY* is the year, *MM* the month, *DD* the day.

For requesting a FTP user account see 5.9.1.

5.8.2 GOME-2/MetOp

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 O3M-SAF Products is:

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

Additionally the GOME-2/MetOp NRT and OL (including reprocessed) products in HDF5 format are available at the DLR atmos FTP-server:

ftp://atmos.eoc.dlr.de/gome2nrt
ftp://atmos.eoc.dlr.de/gome2nt
ftp://atmos.eoc.dlr.de/gome2ol

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

For requesting a FTP user account see 5.9.2. Additionally, the NRT and OL products can be directly pushed to dedicated FTP servers located at the user's premises.

Following the O3M-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

5.9.1 GOME/ERS-2

GOME/ERS-2 total column products are generated at DLR's D-PAF on behalf of ESA.



For ordering/registration please contact:

ESA ESRIN - EO Help Desk
eohelp@esa.int

Current and historical quicklook images as well as value added products generated by DLR are available at:

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

5.9.2 GOME-2/MetOp

The GOME-2/MetOp total column products are generated at DLR in the framework of EUMETSAT's O3M-SAF.



For information and access to all O3M-SAF products, please refer to the O3M-SAF web page and help desk:

O3M-SAF Web page
<http://o3msaf.fmi.fi>

O3M-SAF Helpdesk
o3msaf@fmi.fi

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

<http://navigator.eumetsat.int>

Current and historical quicklook 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. O₃, NO₂, SO₂, 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 ([R11], [R12]) 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* group.

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, currently 2/F. 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.

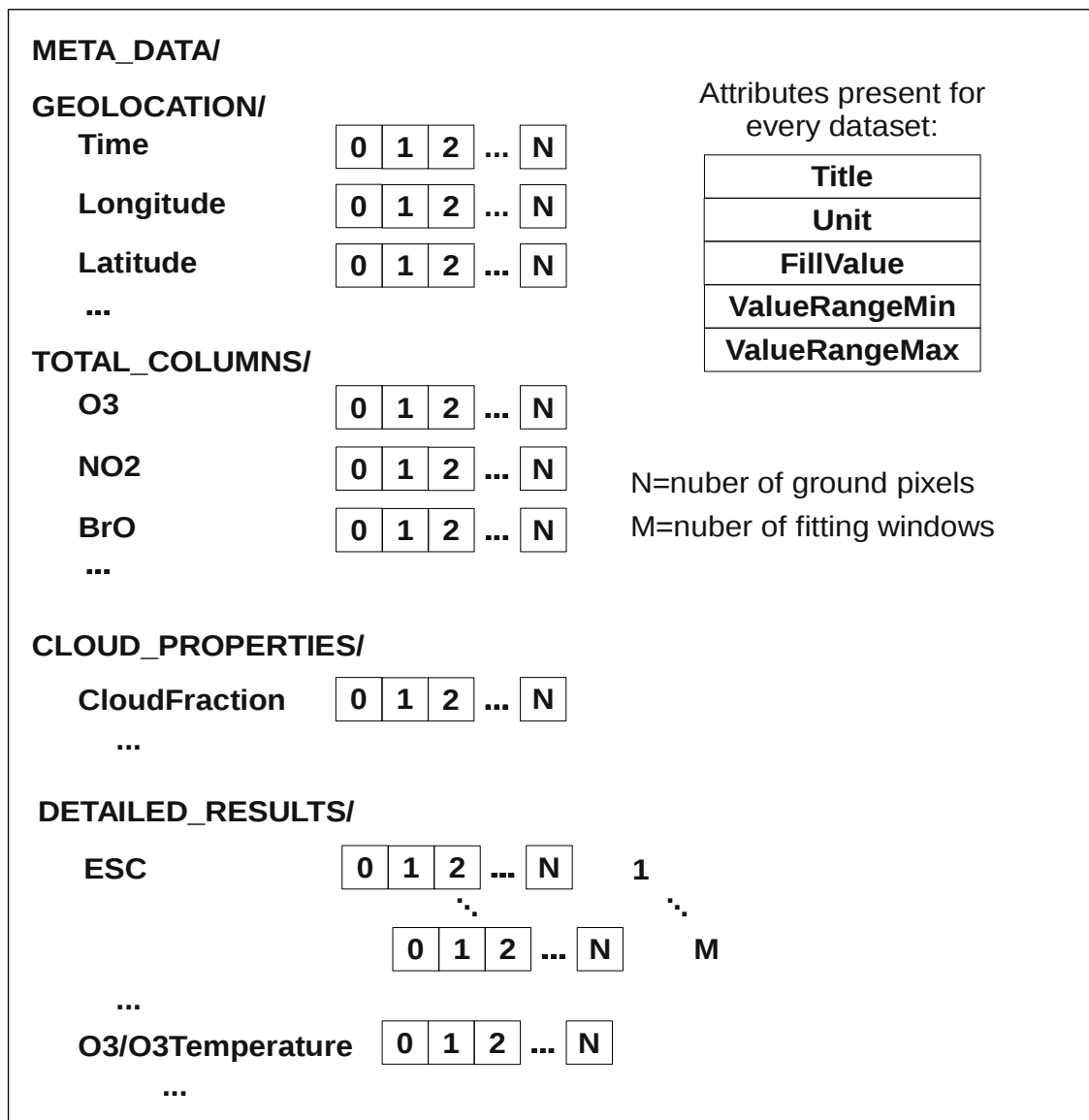


Figure 4: Organization of the GOME total column products in the HDF5 structure

Most datasets 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 (O₃/TemperatureProfile, containing one profile for every ground pixel) to three dimensional (for O₃/AveragingKernels), or there are even be subgroups (e.g. for the different plume heights of SO₂).

6.1.1 Description of Common Items

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

| <i>Attribute Name</i> | <i>Data Type</i> | <i>Description</i> |
|-----------------------|------------------|--|
| 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)

| <i>Attribute Name</i> | <i>Data Type</i> | <i>Description</i> | <i>Allowed Values GOME/ERS-2</i> | <i>Allowed Values GOME-2/Metop</i> |
|-----------------------|----------------------|--|---|---|
| ArchiveFacility | string | Centre where the data is archived. | D-PAF DLR OP | O3DLR |
| SatelliteID | string | Platform identifier (mission and spacecraft). | ERS-2 | Mnn |
| StartOrbitNumber | integer | Orbit number at the start of sensing, i.e. at the beginning of a dump. | <i>integer</i> | <i>integer</i> |
| InstrumentID | string | Instrument which acquired the product | GOME | GOME |
| InstrumentMode | VIEW_MODES structure | Specifies how many ground pixels were observed in the corresp. view modes. | <i>VIEW_MODES structure</i> | <i>VIEW_MODES structure</i> |
| SensingStartTime | CCSDS_ASCII | UTC date and time at sensing start. | <i>Date in CCSDS format (ASCII)</i> | <i>Date in CCSDS format (ASCII)</i> |
| SensingEndTime | CCSDS_ASCII | UTC date and time at sensing end. | <i>Date in CCSDS format (ASCII)</i> | <i>Date in CCSDS format (ASCII)</i> |
| ReceivingCentre | string | Centre that received the data. | KS, GS, DP, ES, MS | ECF (for EECF), FBK, FUC, GCA, PGS, RUS, SOC, SVL, UBI, WAL, WEC, WIV |
| ProcessingCentre | string | Centre that generated the data. | D-PAF DLR OP | O3DLR |
| ProcessingMode | string | Processing mode applied for generation of the product. | N (nominal), B (backlogged), R (reprocessed), V (validation) T (near-real-time) | 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. | <i>string</i> | <i>string</i> |
| ProductType | string | Description of the product type | ERSNTO, ERSOTO | O3MNTO, O3MOTO |



| <i>Attribute Name</i> | <i>Data Type</i> | <i>Description</i> | <i>Allowed Values</i> |
|--|------------------|--|---------------------------------|
| 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 |
| OrbitEccentricity | 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 |
| OrbitAscendingNodeCrossing DateTime | 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.

| <i>Attribute Name</i> | <i>Data Type</i> | <i>Description</i> | <i>Allowed Values</i> |
|------------------------|------------------|--|-----------------------|
| NumberOfFittingWindows | integer | Number of fitting windows used in processing | 1- M |

This table describes data sets containing information about the fitting windows:

| <i>Dataset Name</i> | <i>Data Type</i> | <i>Description</i> | <i>Allowed Values</i> |
|---------------------|------------------|--|-----------------------|
| 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 6.8.3) for this window | 0-100% |

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.

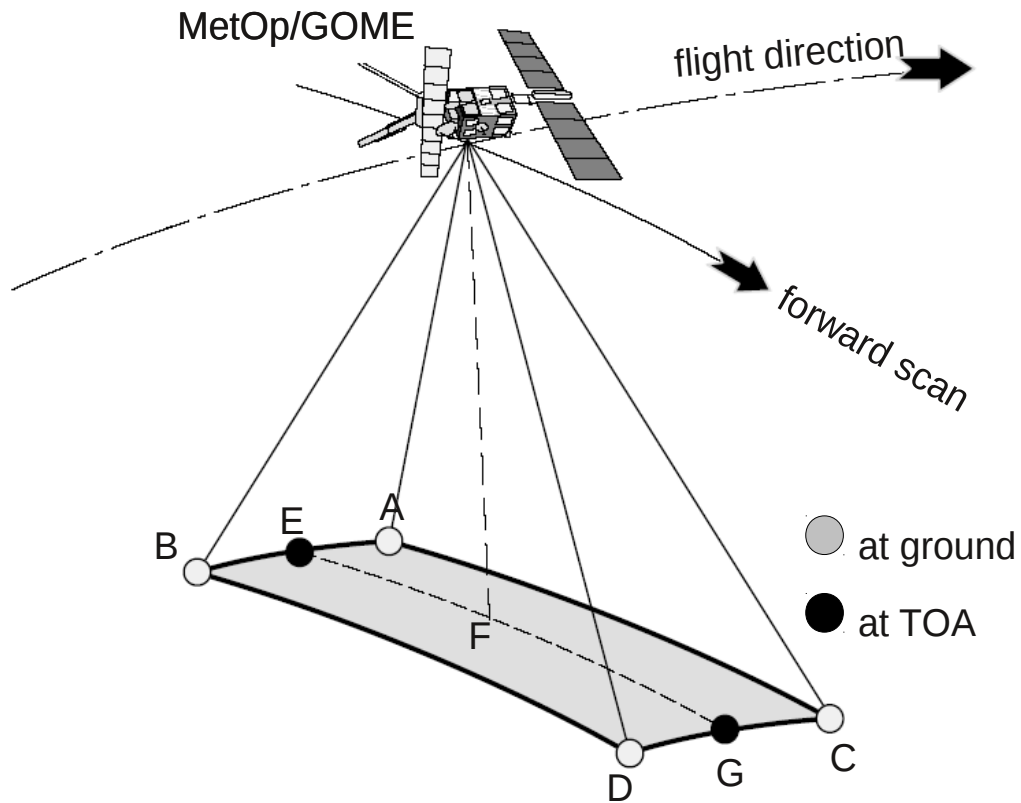


Figure 5: Ground Pixel Geometry

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:

| <i>Dataset Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
|---------------------------------|------------------|-------------|--|
| 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 |



| <i>Dataset Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
|---------------------|------------------|-------------|---|
| 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, (0-3 for GOME/ERS-2; 0 to 3, 7 or 31 for GOME-2/MetOp) |
| ViewMode | integer[pixels] | - | Scanning mode of the instrument at the time of acquisition (bits 0-7), geolocation flags (bit 8-31) See section 6.8.1 |

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 key trace gas total column information. 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.

| <i>Dataset Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
|---------------------|------------------|---------------------------|--|
| O3 | float[pixels] | Dobson Units | Total vertical column density of O3 |
| O3_Error | float[pixels] | % | Error on total vertical column density of O3 |
| NO2 | float[pixels] | molecules/cm ² | Initial total vertical column density of NO2 |
| NO2_Error | float[pixels] | % | Error on initial total vertical column density of NO2 |
| NO2Tropo | float[pixels] | molecules/cm ² | Tropospheric vertical column density of NO2 (cloud screened) |
| NO2Tropo_Error | float[pixels] | % | Error on tropospheric vertical column density of NO2 |
| BrO | float[pixels] | molecules/cm ² | Vertical column density of BrO |
| BrO_Error | float[pixels] | % | Error on vertical column density of BrO |
| SO2 | float[pixels] | Dobson Units | Vertical column density of SO2 for a plume height of 6 km |
| SO2_Error | float[pixels] | % | Error on vertical column density of SO2 |
| H2O | float[pixels] | kg/m ² | Vertical column density of H2O (cloud screened) |
| H2O_Error | float[pixels] | % | Error on vertical column density of H2O |
| HCHO | float[pixels] | molecules/cm ² | Vertical column density of HCHO (cloud screened) |
| HCHO_Error | float[pixels] | % | Error on vertical column density of HCHO |



6.5 CLOUD_PROPERTIES Group

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

| <i>Dataset Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
|-----------------------------|------------------|-------------|--|
| 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 |
| SurfaceAlbedo | float[pixels] | - | Surface albedo used for cloud retrieval |
| 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 on page 26) 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).

| <i>Dataset Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
|--------------------------------|--------------------------|---------------------|---|
| AAI | float[pixels] | - | Absorbing aerosol indicator |
| SurfaceHeight | float[pixels] | km | Surface altitude |
| 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 6.8.2) |
| SurfaceAlbedo | float[pixels][windows] | - | Surface albedo for the associated retrieval window |
| QualityFlags | integer[pixels][windows] | - | Quality flags for each pixel/gas (see 6.8.3) |
| VCD | float[pixels][windows] | mol/cm ² | Uncorrected vertical column density of main gas |
| VCD_Error | float[pixels][windows] | % | Error on vertical column density |
| IntensityWeightedCloudFraction | float[pixels][windows] | - | Cloud radiance fraction (weighting factor for clear-sky and cloudy AMFs) |
| ESC | float[pixels][windows] | mol/cm ² | Slant column density of main gas |
| ESC_Error | float[pixels][windows] | % | 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 |
| GhostColumn | float[pixels][windows] | mol/cm ² | Ghost column below cloud (only used for O3) |
| 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 |

The following subsections contain sub groups of the *DETAILED_RESULTS* group which contain trace gas specific data.



6.6.1 DETAILED_RESULTS/O3 Subgroup

In the following table, the number of atmospheric layers is denoted as “layers” in profile datasets.

| <i>Dataset Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
|--------------------------------|-----------------------|---------------------|---|
| ESCRingCorrected | float[pixels] | mol/cm ² | Ozone slant column density corrected for Ring-effect |
| O3Temperature | float[pixels] | K | Fitted ozone temperature |
| EastWestPostCorrectionFactor | 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 O ₃ profile used in the retrieval of O ₃ (layers=13, optional parameter) |
| TemperatureProfile | float[pixels][layers] | K | A priori temperature profile used in the retrieval of O ₃ (layers=13, optional parameter) |
| IterativeVCDNumberOfIterations | integer[pixels] | - | Number of iterations for the iterative VCD algorithm |

6.6.2 DETAILED_RESULTS/NO2 Subgroup

| <i>Dataset Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
|------------------------------|---------------------------|---------------------|--|
| 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 |
| VCDStrato | float[pixels] | mol/cm ² | Stratospheric vertical column density |
| VCDStrato_Error | float[pixels] | % | Error on stratospheric vertical column density |
| VCDTropo | float[pixels] | mol/cm ² | Tropospheric vertical column density (cloud screened) |
| VCDTropo_Error | float[pixels] | % | Error on tropospheric vertical column density |
| VCDCorrected | float[pixels] | mol/cm ² | Total vertical column density corrected for tropospheric contribution (cloud screened) |
| VCDCorrected_Error | float[pixels] | % | Error on corrected total vertical column density |
| NO2Tropo_Flag | integer[pixels] | - | Flag indexing tropospheric NO ₂ calculations (see 6.8.4 on page 40) |
| AveragingKernel | float[pixels] [layers] | - | Average Kernel for tropospheric NO ₂ (layers=24) |
| AveragingKernelPressureLevel | float[pixels] [layers] | - | Pressure levels of Average Kernel (layers=24) |

Please note that this section is empty for GOME/ERS-2 products.

For more information on the NO₂ parameters see section 8.

6.6.3 DETAILED_RESULTS/SO₂ Subgroup

The GOME SO₂ algorithm provides SO₂ vertical columns for several assumed plume heights. The number of plume heights is available in the field “NumberOfPlumeHeights”, which also describes the cardinality of the subsequent datasets (denoted as “heights”). The different height values are available in the dataset “PlumeHeights”.

| <i>Attribute Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
|-------------------------|------------------------|---------------------|---|
| NumberOfPlumeHeights | integer | - | Number of assumed plume heights (3) |
| <i>Dataset Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
| PlumeHeights | float[heights] | km | Assumed plume heights for retrieval (15, 6, 2.5 km) |
| ESCCorrected | float[pixels][heights] | mol/cm ² | SO ₂ slant column density (background 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] | mol/cm ² | Total vertical column density (background corrected) |
| VCDCorrected_Error | float[pixels][heights] | % | Error on total vertical column density |
| SO ₂ _Flag | integer[pixels] | - | Flag indexing SO ₂ calculations (see 6.8.5 on page 40) |

(*) for future use, not yet implemented

6.6.4 DETAILED_RESULTS/H₂O Subgroup

| <i>Dataset Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
|---------------------------------|------------------|---------------------|--|
| ESC_O2 | float[pixels] | mol/cm ² | O ₂ slant column density |
| ESC_O4 | float[pixels] | mol/cm ² | O ₄ slant column density |
| EastWestPostCorrectionFactorH2O | float[pixels] | - | Correction factor for scan angle dependency in retrieved H ₂ O column |
| H ₂ O_Flag | integer[pixels] | - | Flag indexing H ₂ O calculations (see 6.8.6 on page 41) |

6.6.5 DETAILED_RESULTS/HCHO Subgroup

| <i>Dataset Name</i> | <i>Data Type</i> | <i>Unit</i> | <i>Description</i> |
|---------------------|------------------|---------------------|--|
| ESCCorrected | float[pixels] | mol/cm ² | Slant column density (background corrected) |
| ESCRefSector | float[pixels] | mol/cm ² | Slant column density for Reference Sector (Pacific Region between 160-240°E) |
| ESCRefSectorEquator | float[pixels] | mol/cm ² | Slant column density for the Equatorial Reference Sector (Pacific Equator Region) |
| VCD0 | float[pixels] | mol/cm ² | A priori vertical column density for the Reference Sector (Pacific Region (160-240°E)) from IMAGES model |
| VCDCorrected | float[pixels] | mol/cm ² | Total vertical column density (background corrected) |
| HCHO_Flag | integer[pixels] | - | Flag indexing HCHO calculations (see 6.8.7 on page 41) |



6.7 DETAILED_RESULTS_GODFIT Group

As the GDP-5 algorithm is different to GDP-4, an additional output section was introduced for each trace gas processed with GDP-5. For O₃ (DETAILED_RESULTS_GODFIT/O3), it contains the following datasets (layers=13):

| Dataset Name | Data Type | Unit | Description |
|--------------------------|-----------------------|------|---|
| O3Profile | float[pixels][layers] | DU | A priori O ₃ profile used in the retrieval of O ₃ |
| TemperatureProfile | float[pixels][layers] | K | A priori temperature profile used in the retrieval of O ₃ |
| FitPar1_O3 | float[pixels] | DU | O3 column |
| FitPar2_TemperatureShift | float[pixels] | K | Temperature shift |
| FitPar3_Albedo1 | float[pixels] | - | Internal closure parameter 1 |
| FitPar4_Albedo2 | float[pixels] | - | Internal closure parameter 2 |
| FitPar5_Albedo3 | float[pixels] | - | Internal closure parameter 3 |
| FitPar6_Ring | float[pixels] | - | Fitted ring spectrum |
| FitPar7_Undersampling | float[pixels] | - | Fitted undersampling |
| FitPar8_WavelengthShift | float[pixels] | nm | Fitted earthshine spectrum shift |
| NumberOfIterations | float[pixels] | - | Number of fitting iterations |
| FittingRMS | float[pixels] | - | Final RMS of the fit |
| O3Temperature | float[pixels] | K | Fitted ozone temperature, including T-Shift |
| GhostColumn | float[pixels] | DU | Associated ghost column |
| CovarianceMatrix | float[pixels][8][8] | - | Covariance and Correlation results matrix (see below) |
| AveragingKernels | float[pixels][layers] | - | Averaging kernels for each atmosphere layer |

For the fitting parameters, the general name scheme is “FitParN_<name>”, where “N” is the number of the fitting parameter, and “<name>” the corresponding name. With this approach, the desired dataset can be retrieved from the product even if the position in the fitting vector should change in the future.

The Covariance dataset contains a square matrix with the dimensions of the fitting vector. In the lower/left triangle, the covariance is available, the diagonal contains the variance, and the upper/right triangle contains the correlation:

$$\text{cor}_{ij} = \text{cov}_{ij} / \sqrt{(\text{cov}_{ii} * \text{cov}_{jj})} \text{ for } j > i \text{ (upper/right triangle)}$$

6.8 Detailed Flag Description

6.8.1 ViewMode

| 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 |

6.8.2 SurfaceConditionFlags

| Flag | Value | Description |
|------|-------|---|
| 0 | 1 | Land/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 |

These flags give additional information about the surface state during the retrieval.

6.8.3 QualityFlags

| Flag | Value | Description | Specified Valid Conditions | | | | | | | |
|------|-------|---|------------------------------------|--|--|--------------------|-------------------------|--|---|--------------------|
| | | | O ₃ | NO ₂ | BrO | SO ₂ | H ₂ O | HCHO | OClO | |
| 0 | 1 | Validity of total column (VCD) If the retrieved total column is invalid, it is replaced with the fill value and this flag is set, together with flags 1 and 2 | retrieval possible and result >= 0 | retrieval possible | retrieval possible | retrieval possible | retrieval possible | retrieval possible | retrieval possible | retrieval possible |
| 1 | 2 | Total column (VCD) out of range Set if the total column retrieved for this ground pixel is outside the specified range | 75-700 DU | 0-5*10 ¹⁶ mol/cm ² | 0-1.5*10 ¹⁴ mol/cm ² | -10-1000 DU | 0-100 kg/m ² | < 1.0*10 ¹⁷ mol/cm ² | -0.3 - 100*10 ¹⁵ mol/cm ² | |
| 2 | 4 | Large error in slant column (ESC) Set if the <i>ESC_Error</i> value of this ground pixel exceeds the specified threshold | <=2% | <=50% | <=100% | Not applicable | <= 50% | Not applicable | Not applicable | Not applicable |



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 and 2) 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.

See *VCDQualityIndicator* in 6.2 on page 28 for the percentage of pixels which have been flagged as an overall quality indicator for the whole orbit.

6.8.4 NO₂Tropo_Flags

| Flag | Value | Description |
|------|-------|--|
| 0 | 1 | Polluted condition: <i>VCDTropo</i> and <i>VCDCorrected</i> values are available. <ul style="list-style-type: none"> • <i>DETAILED_RESULTS/VCD</i> contains the total column density based on an unpolluted AMF (initial total VCD) • <i>DETAILED_RESULTS/NO2/VCDCorrected</i> contains the pollution corrected total column density. • <i>DETAILED_RESULTS/NO2/VCDTropo</i> contains the tropospheric column density. Note: <i>IntensityWeightedCloudFraction</i> < 50% |
| 1 | 2 | Unpolluted condition: <i>VCDTropo</i> and <i>VCDCorrected</i> not available (fill-values). <ul style="list-style-type: none"> • <i>DETAILED_RESULTS/VCD</i> contains the total column density based on an unpolluted AMF (initial total VCD) Note: <i>IntensityWeightedCloudFraction</i> < 50%. |
| 2 | 4 | Cloudy condition: <i>VCDTropo</i> and <i>VCDCorrected</i> not available (fill-values). <ul style="list-style-type: none"> • <i>DETAILED_RESULTS/VCD</i> contains the total column density based on an unpolluted AMF (initial total VCD) Note: <i>IntensityWeightedCloudFraction</i> > 50% |
| 3 | 8 | Measurement in polar regions (Lat > 70 deg): <i>VCDTropo</i> and <i>VCDCorrected</i> not available (fill-values). <ul style="list-style-type: none"> • <i>DETAILED_RESULTS/VCD</i> contains the total column density based on an unpolluted AMF (initial total VCD) |
| 4 | 16 | NO₂ column data not available: <ul style="list-style-type: none"> • <i>VCD</i>, <i>VCDTropo</i> and <i>VCDCorrected</i> contain fill-values • <i>TOTAL_COLUMNS/NO2</i> contain fill-values |

For more information on the NO₂ parameters see Section 8.

6.8.5 SO₂_Flags

| Flag | Value | Description |
|------|-------|---|
| 0 | 1 | Measurement in polar regions (SZA > 75 deg): <ul style="list-style-type: none"> • reduced quality of SO₂ total column |
| 1 | 2 | SO₂ column data not available: <ul style="list-style-type: none"> • <i>DETAILED_RESULTS/VCD</i> and <i>DETAILED_RESULTS/SO2/VCDCorrected</i> contain fill-values • <i>TOTAL_COLUMNS/SO2</i> contain fill-values |
| 2 | 4 | SO₂ column data not available due to unfulfilled external data dependency. <ul style="list-style-type: none"> • <i>VCD</i> and <i>VCDCorrected</i> contain fill-values • <i>TOTAL_COLUMNS/SO2</i> contain fill-values |

6.8.6 H₂O_Flags

| <i>Flag</i> | <i>Value</i> | <i>Description</i> |
|-------------|--------------|---|
| 0 | 1 | Measurement in cloudy conditions <ul style="list-style-type: none"> reduced quality of H₂O total column <i>TOTAL_COLUMNS/H₂O</i> contain fill-values |
| 1 | 2 | Measurement in cloudy and/or elevation conditions (small O ₂ column): <ul style="list-style-type: none"> reduced quality of H₂O total column <i>TOTAL_COLUMNS/H₂O</i> contain fill-values |

6.8.7 HCHO_Flags

| <i>Flag</i> | <i>Value</i> | <i>Description</i> |
|-------------|--------------|---|
| 0 | 1 | Measurement with high solar zenith angle (SZA > 70 deg): <ul style="list-style-type: none"> reduced quality of HCHO total column <i>TOTAL_COLUMNS/HCHO</i> contain fill-values |
| 1 | 2 | Cloudy conditions: <ul style="list-style-type: none"> reduced quality of HCHO total column <i>TOTAL_COLUMNS/HCHO</i> contain fill-values Note: CloudFraction > 40% |
| 2 | 4 | HCHO column data not available: <ul style="list-style-type: none"> <i>DETAILED_RESULTS/VCD</i> contains fill-values <i>TOTAL_COLUMNS/HCHO</i> contain fill-values |
| 3 | 8 | HCHO column data not available due to unfulfilled external data dependency. <ul style="list-style-type: none"> <i>DETAILED_RESULTS/VCD</i> contain fill-values <i>TOTAL_COLUMNS/HCHO</i> contain fill-values |

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 ([R11], [R12]) 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 O3M-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

| <i>Octet</i> | <i>Description</i> | <i>Allowed Values</i> |
|--------------|--|-----------------------|
| 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

| <i>Octet</i> | <i>Description</i> | <i>Allowed/Used Values</i> |
|--------------|--|----------------------------|
| 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

| <i>Octet</i> | <i>Description</i> | <i>Allowed/Used Values</i> |
|--------------|---|----------------------------|
| 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

| <i>Descriptor</i> | <i>Description</i> | <i>Value</i> |
|-------------------|--|-------------------------|
| 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.

| <i>Octet</i> | <i>Description</i> | <i>Allowed Values</i> |
|--------------|---|-----------------------|
| 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

| <i>Octet</i> | <i>Description</i> | <i>Allowed Values</i> |
|--------------|--|-----------------------|
| 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:

| <i>Trace gas</i> | <i>Trace gas name</i> | <i>Atmospheric Chemical No. (08 043 descriptor)</i> | <i>CAS Registry Number (08 044 descriptor)</i> |
|------------------|-----------------------|---|--|
| 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 ₂ O | 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 section contains practical information on using the GOME 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.

The H₂O entry in the *TOTAL_COLUMNS* group of the HDF5 products is set to fill-value for measurements under cloudy conditions. The retrieval values are nevertheless available in the *DETAILED_RESULTS* group under the VCD entry. The BUFR products contain all H₂O retrievals, but it is recommended not to use measurements under cloudy conditions (*cloud_fraction* * *cloud_top_albedo* < 0.6).

The NO₂ entry in the *TOTAL_COLUMNS* group contains the same value as the VCD entry (for the NO₂ window) in *DETAILED_RESULTS*. These two entries contain the total NO₂ column density based on an unpolluted AMF. The VCDcorrected entry in *DETAILED_RESULTS/NO2* contains the pollution corrected total NO₂ column density (available only for measurements with an intensity weighted cloud fraction < 50% and for latitudes < 70 deg). Note that VCDcorrected >= VCD. 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 NO₂ column density (available only for measurements with an intensity weighted cloud fraction < 50% and for latitudes < 70 deg). The VCDStrato entry in *DETAILED_RESULTS/NO2* contains the stratospheric NO₂ column density (as derived with a spatial filtering approach and available only for latitudes < 70 deg).

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 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>

A Appendixes

A.1 HDF5 Data Types

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

| <i>Data type</i> | <i>HDF5 predefined data type</i> |
|------------------|---|
| 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-DDThh: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.

| <i>EECF Short Name</i> | <i>Attribute Name</i> | <i>Notes</i> |
|-------------------------|--------------------------------------|---|
| 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 O3M-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 <i>ProductAlgorithmVersion</i> , <i>InitializationFileVersion</i> , <i>InternalProcessorRevision</i> , and <i>Revision</i> |
| 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.