The EUMETSAT Network of Satellite Application Facilities

O3M SAF
Ozone and Atmospheric Chemistry Monitoring

PRODUCT USER MANUAL

NRT and Offline Vertical Ozone Profile and Tropospheric Ozone Column Products

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DOCUMENT STATUS SHEET

Issue	Date	Modified Items / Reason for Change
0.1	2007-05-14	First draft version
0.2	2007-06-06	Revised after ORR-A2 comments
0.3	2007-08-30	Revised after ORR-A2 review
0.4	2007-10-30	Revised after ORR-A2 CloseOut
0.5	2008-01-31	Revised product format: Data.QualityProcessingFlags has new flags, different ordering, and different meaning. The flags now positively indicate overall convergence, and convergence on state and cost separately.; MetaData.ProductSoftwareVersion added. New Product Format Version number: 3.3
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0.7	2008-09-30	Revisions for ORR-B. No retrieval is indicated by fill values (e.g.: -999) in QualityProcessingFlags. Fixed typo: AprioriErrorCovariance (P→p); Some references to GOME-1 hidden.; New Product Format Version Number: 3.5
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0.9	2009-10-21	Updated Threshold/Target/Breakthrough levels. PCloudAdjustedToPSurface flag added to the QualityInputFlags record. Added IntegratedVerticalProfile and -Error to Datagroup. Softwareversion 1.20 / OPF v3.6, 20091021.
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1.01	2010-05-25	Added info on O3MSAF.
1.10	2011-11-16	Updates: added to DataGroup: Tropospheric and Stratospheric ozone columns (with errors), tropopause (model-) level. Added to GeolocationGroup: ScanDirection. Suitable for use with SoftwareVersion 1.25 / OPF v3.9, 20110916. Updates to the versions table.
1.11	2012-03-19	Revisions from ORR/PCR review. Made text more generic, introduced separation between coarse and high res retrievals where applicable.
1.12	2012-05-11	Naming conventions of High Resolution product have changed on request of ORR-board (2012-03-20). Should be applicable from SoftwareVersion 1.26 onwards

1.13	2013-05-28	Valid for: Algorithm version 1.11, Software version 1.28, OPF version 3.10. Added in Geolocation: EndUTCTime; Added in Data: AltitudeProfile_Raw, PressureProfile_Raw, TemperatureProfile_Raw, TropopausePressure_Raw. Applicable to GOME-2 on Metop-A and Metop-B. Text changes for NHP/OHP where applicable. BUFR file name convention and BUFR/HDF file sizes.
1.14	2013-06-16	Changes based on ORR RIDs
1.15	2014-04-11	Added Cross track and Along track co-adding factors in Product_Specific_MetaData. Indicated in Red.
1.16	2014-09-02	Added conversion of ozone values to DU in section on BUFR product. Updated list of product version numbers.
1.17	2014-11-12	Added Acknowledgement instructions to the Further Information section
1.18	2015-02-09	Relates to Software version 1.32, Algorithm version 1.12, OPF version 3.20. Added in Data group: IntegratedVerticalProfileSurfaceTo500hPa and IntegratedVerticalProfileErrorSurfaceTo500hPa, TropopausePressure_Thermal_Raw, TropopausePressure_PV (if available)
1.20	2015-05-20	Addition of DOI and ProductID in MetaData group
1.30	2015-07-01	Changes based on RIDs of the TrO3 review.

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1. INTRODUCTION

1.1 Purpose

This document is the Product User Manual for the Near Real Time and Offline Ozone Profiles, as well as the Tropospheric Ozone Column retrieved within the context of the Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring (O3M SAF). This document first presents a little background and a description on how the retrieval algorithm works. After that, the document provides information and guidance to the user on how to use and interpret the ozone profile data product.

1.2 Scope

This PUM provides information on the near real time (NRT) and offline vertical ozone profile in coarse and high resolution and the tropospheric ozone column product of the O3MSAF. This document does not go into much detail with regard to the algorithm or design of the software; please refer to the Algorithm Theoretical Basis Document (ATBD).

1.3 Definitions, acronyms and abbreviations

1.3.1 Acronyms

AAI	Absorbing Aerosol Index
ATBD	Algorithm Theoretical Basis Document
BOA	Bottom Of Atmosphere
DFS	Degrees of Freedom for Signal
ECMWF	European Centre for Medium-range Weather Forecast
ERS	European Remote Sensing Satellite
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FRESCO	Fast Retrieval Scheme for Cloud Observables
FWHM	Full Width Half Maximum
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Instrument
HDF	Hierarchical Data Format
HNP	High resolution NRT Ozone Profile
HOP	High resolution Ozone profile (offline)
IPA	Independent Pixel Approximation
IPA-Lamb	IPA- Lambertian

IPA-Scat	IPA- scattering layer
KNMI	Royal Netherlands Meteorological Institute
LIDORT	LInearized Discrete Ordinate Radiative Transfer
LUT	Look Up Table
MetOP	Meteorological Operational satellite
MDR	Measurement Data Record
NHP	NRT High resolution ozone Profile
NOP	NRT Ozone Profile (in coarse resolution)
NTO	NRT Total Ozone
O3MSAF	Ozone Monitoring and Atmospheric Chemistry SAF
OE	Optimal Estimation
OHP	Offline High resolution ozone Profile
OMI	Ozone Monitoring Instrument
OOP	Offline Ozone Profile (in coarse resolution)
OPERA	Ozone Profile Retrieval Algorithm
PDU	Product Dissemination Unit
PGE	Product Generation Element
PMD	Polarization Measurement Device
PUM	Product User Manual
RMS	Root Mean Square
RTM	Radiative Transfer Model
SAA	Solar Azimuth Angle
SAF	Satellite Application Facility
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CartograpHY
StrOC	Stratospheric Ozone Column
SW	Software
SZA	Solar Zenith Angle
TBA	To Be Added
TBC	To Be Confirmed
TBD	To Be Defined
TOA	Top Of Atmosphere
TOC	Total Ozone Column
TOMS	Total Ozone Mapping Spectrometer
TrOC	Tropospheric Ozone Column
UMARF	Unified Meteorological Archiving and Retrieval Facility
UV	Ultra Violet
VAA	Viewing Azimuth Angle
VIS	Visible
VZA	Viewing Zenith Angle

1.3.2 Definition of Terms

Attribute	A small dataset that can be used to describe the nature and/or the intended usage of the object it is attached to.
Dataset	A multi-dimensional array of data elements, together with supporting metadata.
Group	A structure containing zero or more HDF5 objects, together with supporting metadata. The two primary HDF5 objects are datasets and groups.
HDF 5 File	A container for storing grouped collections of multi-dimensional arrays containing scientific data.
Pixel	The term pixel is used in this document for ground pixels, i.e. integration intervals in the scan line.
Product generation element	An independent SW that processes a product to another product type. For example, NTO processor reads level 1b product and outputs level 2 total ozone product.
Independent Pixel Approximation	Treatment of clouds in radiative transfer: separate radiances are computed for cloud-free and clouded part of pixel, results are weighted with cloudfraction.
IPA- Lambertian	Clouds are treated as a Lambertian reflector
IPA- scattering layer	Clouds are treated as a layer of scattering particles

1.4 Applicable and Reference Documents

1.4.1 Applicable Documents

[AD1] Ozone SAF Detailed Design Document for Ozone Profile and Aerosol Processors, SAF/O3M/KNMI/DD/001, Issue 2.1, 21-10-2002

[AD2] Ozone SAF Software Requirements Document, SAF/O3M/SSF/RQ/001, Issue 2.2, 21 Oct 2002

[AD3] UMARF to SAFs Interface Control Document, EUM/UMA/ICD/004, Issue 3.3, 7 Feb 2003

[AD4] EPS Mission Conventions Document, EPS/SYS/SPE/990002, Issue 1.0 Draft D, 20 Aug 1999

1.4.2 Reference Documents

[RD1] Gome-2 Level 1 Product Format Specification, EUM/MIS/SPE/97232, Issue 7.0, 19 March 2004, or a later version

[RD2] The HDF5 File Format Specification from the HDF group website: http://hdf.ncsa.uiuc.edu/HDF5/doc/H5.format.html

[RD3] Gome-2 Level 1 Product Generation Specification, EPS.SYS.SPE.990011, Issue 6.0, 19 March 2004, or a later version

[RD4] Rodgers, C.D., Inverse methods for atmospheric sounding, World Scientific Publishing Pte Ltd, New York, 2000

[RD5] Algorithm Theoretical Basis Document for Opera, version 1.12, dated 2012-03-19, or later version.

2. INTRODUCTION TO EUMETSAT SATELLITE APPLICATION FACILITY ON OZONE AND ATMOSPHERIC CHEMISTRY MONITORING (O3M SAF)

2.1 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.

2.2 Objectives

The main objectives of the O3M SAF is to process, archive, validate and disseminate atmospheric composition products (O3, NO2, SO2, OClO, HCHO, BrO, H2O), aerosols and surface ultraviolet radiation utilising the satellites of EUMETSAT. The majority of the O3M SAF products are based on data from the GOME-2 spectrometer onboard the MetOp satellite series.

Another important task of the O3M 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.

2.3 Product families

Near real-time Total Column (NTO)

O3, NO2, O3Tropo, NO2Tropo

Near real-time Ozone Profile (NOP, NHP)

Near real-time UV Index (NUV)

Offline Total Column (OTO)

O3, NO2, O3Tropo, NO2Tropo, SO2, BrO, H2O, HCHO, OClO

Offline Ozone Profile (OOP/OHP)

Offline Surface UV (OUV)

Aerosols in NRT and offline (NAR/ARS // NAP/ARP)

2.4 Product 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 (NOP, NHP, NTO), GTS (NOP, NHP, NTO) or Internet (NUV).

Offline products are available in two weeks from the measurement and they are archived at the O3M SAF archives in Finnish Meteorological Institute (OOP, OHP, OUV, ARS) and German Aerospace Center (OTO).

Only products with “pre-operational” or “operational” status are disseminated. Up-to-date status of the products and ordering info is available on the O3M-SAF website given below.

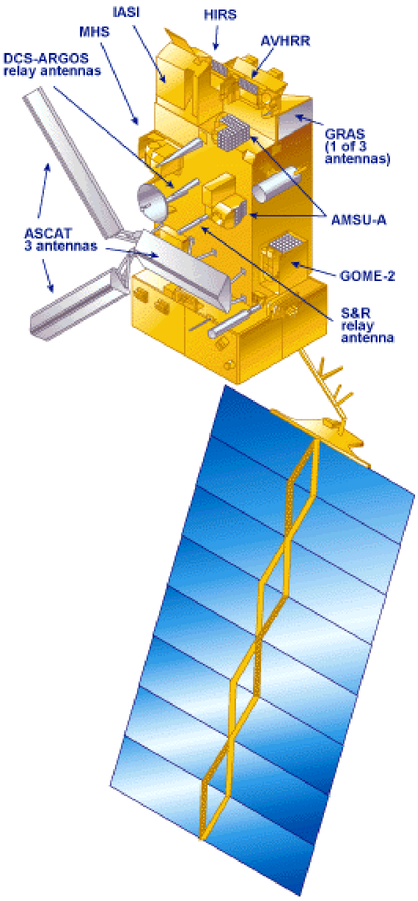
2.5 Information

Information about the O3M SAF project, about its various atmospheric and aerosol products and services can be found at the following web address: http://o3msaf.fmi.fi/

The O3M SAF Helpdesk can be contacted via e-mail at: o3msaf@fmi.fi

3. METOP AND GOME-2

3.1 MetOp



The MetOp satellite series is the core element of the EUMETSAT Polar System (EPS), developed in partnership with the European Space Agency. It carries a complement of new European instruments, as well as versions of operational instruments flown on the corresponding NOAA satellites of the USA.

The EUMETSAT programme includes provision for the development of the MetOp spacecraft in conjunction with the European Space Agency (ESA), the construction and launch of three new MetOp spacecraft, the development of the corresponding instruments and ground infrastructure, and provision for routine operations over a period of 15 years from the date of first launch. This polar system is complementary to EUMETSAT's existing Meteosat satellites in geostationary orbit.

The two EPS MetOp satellites (MetOp-A and MetOp-B) fly in a sun-synchronous polar orbit at an altitude of about 840 km, circling the planet 14 times each day and crossing the equator at 09:30 local (sun) time on each descending (south-bound) orbit. Successive orbits are displaced westward due to the Earth's own rotation, giving global coverage of most parameters at least twice each day, once in daylight and once at night.

The spacecraft carries a comprehensive set of instrumentation, designed primarily to support operational meteorology and climate monitoring, but also supporting many additional applications.

3.2 GOME-2

METOP carries a number of instruments including the Global Ozone Monitoring Experiment-2 (GOME-2). This instrument is designed to measure the total column and profiles of atmospheric ozone and the distribution of other key atmospheric constituents. GOME-2 is a nadir viewing across-track scanning spectrometer with a swath width of 1920 km. It measures the radiance back-scattered from the atmosphere and the surface of the Earth in the ultraviolet and visible range. The instrument uses four channels to cover the full spectral range from 200 to 790 nm with a spectral sampling of 0.11 nm at the lower end of the range, rising to 0.22 nm at the higher end. The instrument employs a mirror mechanism which scans across the satellite track with a maximum scan angle that can be varied from ground control, and three multi-spectral samples per scan. The ground pixel size of GOME-2 is 80 x 40 km² for the shortest integration times, but is usually 8 times larger for the detector measuring the shortest UV wavelengths.

Table 1; GOME-2 properties (values for Metop-A)

Spectrometer type	double spectrometer with pre-disperser prism and four holographic gratings
Spectral range	240 –790 nm
Field of view	0.286° (across track) x 2.75° (along track)
Entrance slit	0.2 mm (across track) x 9.6 mm (along track)
Channels (Bands) & sampling & resolution	1a: 203 – 306 nm & 0.14 - 0.11 nm & 0.24 – 0.29 nm 1b: 306 – 322 nm & +/- 0.11 nm & 0.24 – 0.29 nm 2a: 290 – 399 nm & +/- 0.13 nm & 0.26 – 0.28 nm 2b: 299 – 412 nm & +/- 0.13 nm & 0.26 – 0.28 nm 3: 391 – 607 nm & +/- 0.22 nm & 0.44 – 0.53 nm 4: 584 – 798 nm & +/- 0.22 nm & 0.44 – 0.53 nm
Polarisation monitoring unit	250 detector pixels 312 – 790 nm in 12 programmable bands spectral resolution: 2.8 nm at 312 nm to 40 nm at 790 nm
Swath widths	1920 km (nominal mode), 960 km, 320 km, 240 km, 120 km
Solar calibration	Once per day
Spectral calibration	fixed angle (once per day to once per month)
White Light Source Dark signal	fixed angle (night side of the orbit)
Default spatial resolution and integration time	Band 1a: 640 km x 40 km (1920 km swath and integration time of 1.5 s) Band 1b – 4: 80 km x 40 km (1920 km swath and int. time of 0.1875 s) PMD: 10 km x 40 km (for polarisation monitoring)

4. ALGORITHM DESCRIPTION

4.1 Ozone profile retrieval from nadir UV earthshine spectra

The development of ozone profile retrieval methods from space-borne measurements has started with the ozone profile retrieval from UV ground measurements with the Umkehr technique. *Singer & Wentworth* [1957] were the first to realize that, by using artificial satellites that measure the backscattered solar UV radiation emerging from the Earth atmosphere, information on the vertical distribution of ozone can be obtained. They proposed to use observations at different solar angles. *Twomey* [1961] made an important step towards a practical method by showing how to retrieve the ozone profile from a single earthshine spectrum. The method solves an inverse problem: the ozone profile determines the spectrum, but the spectrum is measured and the ozone profile is to be retrieved from it. Information on the vertical distribution of ozone is contained in the earth radiance measured from space in the wavelength range between about 260 to 340 nm. This is due to the strongly varying ozone absorption cross section in this range. It varies from a maximum of 0.3 DU^{-1} at 260 nm to 0.01 DU^{-1} at 300 nm to 0.001 DU^{-1} at 315 nm.

Considering that a typical total ozone column varies between 150 and 500 DU, the atmosphere varies from almost completely opaque to transparent regarding ozone absorption in this wavelength interval. At 260 nm only molecular (Rayleigh) scattering from the top layer of the atmosphere containing a few DU of ozone contributes to the back-scattered radiance since the solar light does not penetrate any deeper. Moving to longer wavelengths, deeper layers start to contribute to the back-scattered radiance. Between 300–310 nm a sizeable fraction of the solar light reaches the surface, depending on the solar zenith angle. The combination of earthshine radiances in the spectral range [260–310 nm] therefore yields information on the column-amount of scattering agents (mainly air molecules) as a function of ozone column, counted from the top. Since the column density of air molecules above a pressure level is proportional to the pressure, due to hydrostatic equilibrium, the ozone profile information in the spectrum is primarily the functional relation of pressure and ozone column density. Scattering by aerosol, extinction by molecular scattering and multiple scattering complicate this simple picture somewhat, but it captures the essence of the ozone profile retrieval.

4.2 Purpose and general description of the algorithm

The vertical ozone profile products are generated using Opera, which stands for Ozone ProfilE Retrieval Algorithm. Opera is capable of calculating (retrieving) an ozone profile from backscattered light in the UV-VIS spectral range measured by nadir viewing satellite instruments. The method Opera uses for its retrieval is a ‘physical algorithm’, which means that the laws of radiative transfer are used to calculate the radiance values from atmospheric parameters (like pressure, optical scattering and absorbing cross-sections and densities). A so called forward radiative transfer model and inversion are used iteratively to improve knowledge of the state of the atmosphere. In contrast to the physical method used by Opera, there are also ozone profile retrieval methods using a neural network approach.

The vertical ozone profile retrieved by Opera consists of a value for the ozone column density for each layer in a multi-layered atmosphere. In a configuration file the operator determines the position and the vertical extent of the layers by setting the atmospheric pressure levels, which form the boundaries of the layers. These levels are only adjusted at the bottom over elevated terrain and, in case the scene is (partially) clouded, at the top or middle of the cloud.

The absorption cross section of ozone decreases steeply with wavelength between 270 and 340 nm, especially in the region 290-310 nm. Scattered sunlight detected by the satellite at short wavelengths experiences strong absorption by ozone and therefore has only reached the top layers of the atmosphere: it thus carries only information on the ozone distribution in these layers. At larger wavelengths the photons reach deeper layers: at 340 nm most of the scattered radiation has reached the surface. So, the earthshine spectrum between 270-340 nm contains information on the vertical ozone profile. Opera retrieves the ozone profile from this spectrum.

In the case GOME-2 this spectral range is given in the data records of bands 1a, 1b, 2a and 2b. Band 1a usually has a longer integration time than the other Main Science Channel (MSC) bands (1.5s vs 0.1875s). For High Resolution retrievals we combine one large band 1a with one smaller band 1b pixel and project the final result on the band 1b footprint. For coarse resolution retrievals we need to average all radiance measurements onto an extended surface footprint with the integration time of the band 1a measurement. For GOME-2 this means that typically eight pixels of bands 1b-2b are averaged. In short:

- GOME-2: **1** band 1a pixel (1.5 s) is combined with **8** band 1b-2b pixels (0.1875 s)

Other co-adding modes are also possible which lead to different combinations of band 1a and band 1b pixels. Usually, if pixels are co-added, the spectral information is averaged per wavelength (where valid) and the result is projected on the footprint of the smallest pixel.

Opera uses an iterative method in the retrieval process to match a simulated radiance spectrum to the measured earthshine spectrum: non-linear optimal estimation. Initial values for a set of fit parameters (the state vector: ozone profile and possibly other parameters, such as surface albedo) are used for a first simulation by the radiative transfer model (RTM). The state vector is updated after each optimal estimation inversion step. Optimal estimation requires *a priori* information (value and error covariance) for the state vector elements. Usually the initial state vector comes from an ozone climatology and albedo database which is then also used for *a priori*. Convergence criteria based on the magnitude of the state update and the deviation between measurement and simulation are applied to decide on a possible next iteration.

A more in depth description of the algorithm can be found in the ATBD [RD 5].

4.3 Retrieval and vertical model grid

The ozone profile is retrieved on an almost fixed pressure grid consisting of usually 40 layers, logarithmically spaced between 1000 and 0.1 hPa. Almost, because the actual surface pressure replaces one or more levels below it and the level closest to the cloud top is replaced by the latter. The vertical grid on which all geophysical profiles are defined is equal to this grid.

4.4 Level 1 Input

The basic level 1B data consists of a calibrated solar spectrum and spectra of calibrated geolocated radiances; each spectrum comes with a wavelength grid, error estimates and status flags. In the geolocation record, solar and line-of-sight viewing angles are specified at the spacecraft, satellite height and earth radius are specified for the sub-satellite point, and for each nadir-view footprint the centre co-ordinates (surface latitude and longitude) are given.
The South Atlantic Anomaly (SAA) causes spikes in the spectrum, especially in Band 1a. These spectral pixels will not be taken into account in the ozone profile algorithm. The reduced number of useful wavelengths in the spectrum will decrease the amount of information as e.g. expressed in the DFS. Please refer to the ATBD to find more information on the methodology for the SAA filtering.

In a normal O3MSAF operational context, the Opera profile retrieval software will ingest Product Dissemination Units (PDU's) consisting of 3 minutes of measurements. These are disseminated via the EUMETCast system (see section 4.6).

4.5 Level 2 output

In normal operation, the software will produce two types of output: an NRT product in the HDF5 and in the BUFR format, and an offline product in the HDF5 format. In this section we will discuss the main characteristics of each of the products.

4.5.1 The Near Real Time Ozone Profile Products

There are two NRT ozone profile products: one in coarse resolution (**NOP**, 40 x 640 km) and one in high resolution (**NHP**, 40 x 80 km). The data format of the two products is the same, only the resolution of the footprint (projection) differs. The NOP usually has 3 forward scan pixels cross-track (East, Center, West, with the back scan not retrieved) and the NHP has 24 pixels in the forward scan direction with 8 back scan pixels skipped.

The NRT ozone profile products in BUFR format have a minimal content and are meant for fast distribution through limited bandwidth communication channels. The product (like the SBUV BUFR product) contains only:

- Instrument identification
- Date, time and geo-location per ground pixel
- Solar zenith angle, cloud cover and pressure
- The ozone partial columns for each layer and the associated error estimates.

The NRT ozone product in HDF5 has the same format as the offline product described below, just the granule size is limited to blocks of 3 minutes (PDUs).

4.5.2 The Offline Ozone Profile Product

The offline ozone profile products are in the HDF5 format. From the PDU-sized Level-2 files produced in NRT a full orbit is reconstructed for the archive. There is no further processing so the orbit contains the collection of NRT results. The orbit-sized product is what offline users will be able to obtain from the O3MSAF archive. Both the coarse and the high resolution NRT products are assembled separately into orbits. The coarse orbit product is called OOP and the high resolution product is called OHP.

The HDF5 product is the 'full' product. It contains the most complete set of output parameters:

- Instrument ID and characteristics
- Algorithm versions
- Production time stamp
- Fitting window information
- *A priori* and cloud data source information
- Radiative transfer model settings
- Date, time and geolocation for each ground pixel / retrieval
- Cloud fraction, cloud pressure and cloud albedo; Surface albedo and surface pressure
- Solar zenith/azimuth angle and line of sight zenith/azimuth angle for each retrieval

- Quality input flags, Quality processing flags
- Definition, units and source for the *a priori* and state vector
- Retrieved ozone profile and full error covariance matrices
- Averaging kernel and Degrees of Freedom for Signal (DFS)
- Number of iterations and number of spectral pixels used in the inversion.

The ozone profile is reported as partial columns, in Dobson Units, usually between 41 pressure levels logarithmically spaced between surface pressure and 0.1 hPa. For cloudy and partially cloudy scenes, the cloud pressure replaces the nearest pressure level.

The offline product will consist of a full orbit of data concatenated from the Product Dissemination Units (PDUs) at a later stage, while the NRT products will be produced directly from the individual PDUs and will be disseminated as soon as the PDU has been processed.

4.5.3 The Tropospheric Ozone Column Product (NRT and Offline)

Using integration of the vertical ozone profile, we can calculate various sub-columns spanning multiple model layers. Based on the NHP/NOP products, the full tropospheric vertical integrated profile (Tropospheric Ozone Column) is calculated from the surface to the tropopause (based on thermal and PV), as well as the surface to 500hPa column. Since these tropospheric sub-columns are so closely associated with the vertical ozone profile product, the tropospheric column values are included in the HDF format NRT and Offline products.

4.6 Delivery Time

The Near Real Time Ozone Profile products (NOP/NHP) will be delivered to the EUMETCast uplink station as soon as possible after completion of the processing. This means that the user will get BUFR data in PDU sized chunks within three hours after sensing. More information on the EUMETCast dissemination system can be found on the EUMETSAT website www.eumetsat.int via tabs [Access to Data / Delivery Mechanisms / EUMETCast] and [Publications, Technical and Scientific Documentation]

For the offline product a longer delivery time is allowed, to ensure that all PDU's have been processed and collected together in a full orbit file. The delivery time of the Offline Ozone Profile (OOP/OHP) product to the archive is within two weeks.

4.7 Geographical coverage and Granularity of the level 2 product

The geographical coverage of the ozone profile product is practically all of the sun-lit side of the earth. There are areas where the software has difficulty doing a retrieval: solar zenith angles larger than 85 degrees and above snow and ice.

The swaths of the GOME-2 instrument do not cover the earth completely every day at the equator, but at latitudes higher than 45 degrees there is a full coverage and there is possibility that the same surface area is viewed more than once a day.

For the coarse resolution it is necessary to combine information from Band 1a and Bands 1b and 2. These bands have different integration times. All band 1b and band 2 pixels within the Band 1a pixel are averaged to obtain the spectrum from which the ozone profile for the Band 1a ground pixel can be derived. The granularity of the default coarse resolution output product is the same as the Band 1a measurements.

For the high resolution product a retrieval is done for every band 1b pixel, which is combined with its encompassing band 1a measurement. The projection will be the smallest (B1b) pixel.

If other co-adding methods are applied the granularity will be closest to the smallest co-added footprint.

5. PRODUCT FORMAT DEFINITION OF THE NRT AND OFFLINE OZONE PROFILE PRODUCT IN HDF5

5.1 Format

The main format of the NRT and offline Level 2 ozone profile product file is HDF5 [RD2]. The data in the HDF5 file is organized in four groups: *Metadata*, *Product_Specific_Metadata, Geolocation* and *Data* (see Figure 1). The values in all groups are either taken from the level 1 [RD1] or other input data files, copied from the configuration file, or calculated by the program.

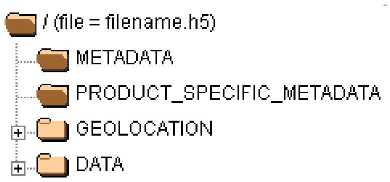


Figure 1: Structure of the HDF5 file.

The *Metadata* group contains parameters about the satellite instrument required by UMARF [AD3], such as metadata given in the O3MSAF software requirements [AD2], the scanning mode, the algorithm version and other general information about the product.

The *Product_Specific_Metadata* group is reserved for additional information specific to this product (*e.g.* parameters related to the algorithm) which has been used to generate the product.
All values in the Metadata and Product_Specific_Metadata groups are stored as attributes. Its content will be explained in Sections 5.1.1 and 5.1.2.

The geolocation information of each ground pixel can be found in *Geolocation* group. It contains all information such as corner and center coordinates. See Figure 2 and Figure 3 for the definition of the seven points of the ground pixel.

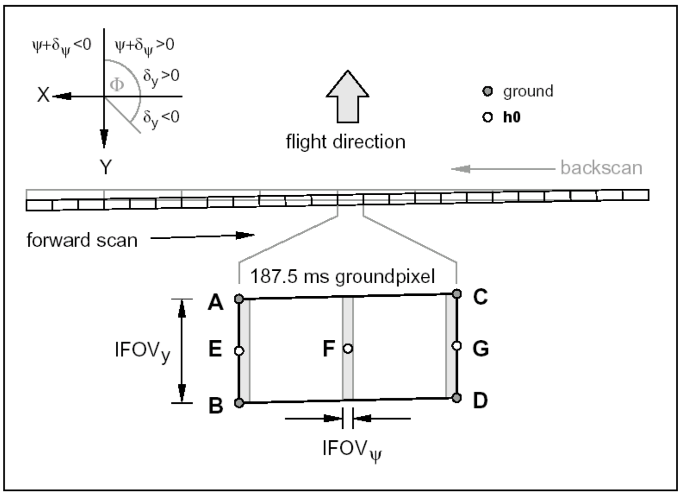


Figure 2: Ground pixel geometry (ref: [RD3])

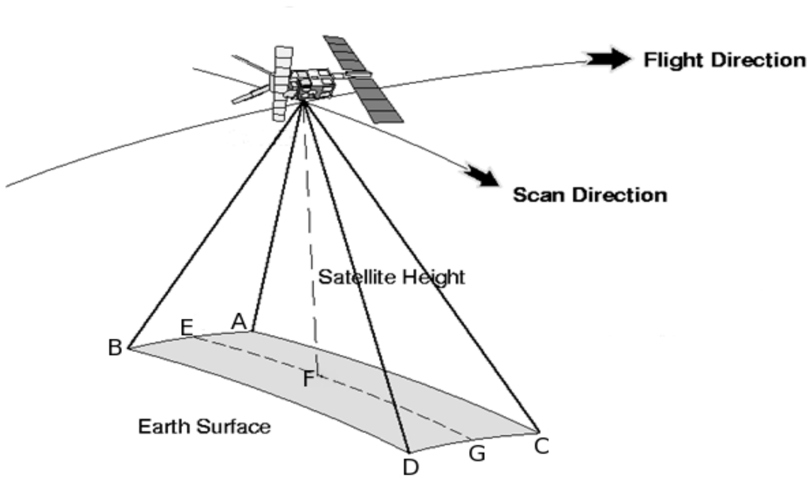


Figure 3: Ground pixel geometry (ref: [RD3])

The calculated results are stored in the *Data* group. It contains information about the quality of the retrieval, auxiliary information, the definition of the state vector and the retrieval results.

Because the output product contains information for series of pixels, all information in the Data and Geolocation group is organized in multi-dimensional arrays. The first dimension always corresponds to the total number of pixels which has been processed, hereafter referred to as *NProfiles*. The organization of the data is illustrated in Figure 4.

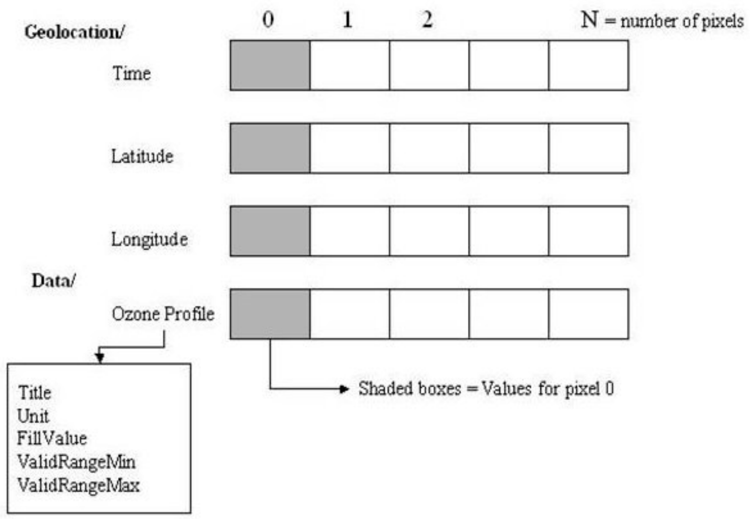


Figure 4: Organization of the pixel data in HDF5 file.

Each retrieval can have a different definition and length of its state vector. *MaxState* is defined as the length of the largest state vector for the entire collection of retrievals, so within the output product the information related to state vectors is contained in arrays with dimension *NProfiles* × *MaxState*. However, an individual retrieval may not use all of these MaxState elements. The real number of its retrieval parameters can be found in DATA/NState (hence *NState* ≤ *MaxState*). Finally, of all the *Nstate* parameters, *NOutputlayers* parameters are used for the ozone profile.
DATA/StateDef defines what each state vector element represents (e.g. layer *n* of the ozone profile, or the albedo of window 4), and which of them are unused (see Figure 5).

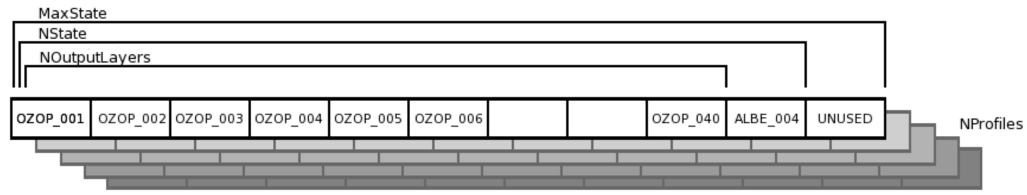


Figure 5: The definition of the state vector within the output product

If a value could not be calculated, a fill value is written to the array as a placeholder, indicating no data (in contrast to invalid data).
Each array has five attributes: Title, Unit, FillValue, ValidRangeMin and ValidRangeMax, which are used to describe the contents of the array.

A detailed description of the datasets and attributes in the Geolocation and Data groups can be found in Sections 5.1.4 and 5.1.5.

5.1.1 Metadata Group

The content of the Metadata group is shown in the following table. The allowed values for the parameters which are required by UMARF are consistent with the requirements given in [AD3]. The allowed values given in *italics* mean any value of the given type (e.g. *string* means that the attribute can contain any string, within the UMARF size limit).

Table 2. Metadata group contents.

Attribute name	Data Type	Description	*Allowed values*
SatelliteID	string	Platform identifier (mission and spacecraft the product originated from).	*Mnn*
OrbitType	string	Coverage of the product (global, local).	*LEO*
StartOrbitNumber	int	First of the two orbit numbers in the EPS product, valid at the start of sensing, i.e. at the beginning of a dump.	*int*
InstrumentID	string	Instrument which acquired the product.	GOME
InstrumentMode	string	Scanning mode of the instrument at the time of the acquisition.	NORTH_POLAR_VIEW, SOUTH_POLAR_VIEW, NARROW_VIEW, NORMAL_VIEW, STATIC_VIEW, UNKNOWN
SensingStartTime	String(23)	UTC date and time at acquisition start of the product.	*Date in CCDS format*
SensingEndTime	String(23)	UTC date and time at acquisition end of the product.	*Date in CCSDS format*
ReceivingCentre	string	Centre that received the data.	*String*
ProcessingCentre	string(5)	Centre that generated the	O3KNM *or other String*

		data.	
ProcessingMode	string(1)	Processing mode applied for generation of the product.	N(ominal), B(acklog), R(eprocessing), V(alidation)
ProcessingLevel	string(2)	Processing level applied for generation of the product.	02
ProcessingTime	String(23)	UTC date and time at processing end of the product.	*Date in CCSDS format*
BaseAlgorithmVersion	string(4)	Version of the algorithm which was used to generate the L1B or L2 EPS parent product, upon which the product is based.	*string*
ProductAlgorithmVersion	string(4)	Version of the algorithm that produced the product.	*string*
ParentProducts	string	Name of the parent products, upon which the product is based.	*string*
ProductType	string	Abbreviated name for the product type, or rather product category.	O3MOOP, O3MNOP, O3MNHP, O3MOHP
ProductFormatType	string	Data format of the product.	HDF5
ProductSoftwareVersion	string	Version number of the software that created this product.	string
ProductFormatVersion	string	Version number of the product format	*string*
SubSatellitePointStartLat	float	Latitude of the sub-satellite point at start of acquisition. (For EPS products: either the first measurement or	-90 to 90

		first complete scan start point **(tbd)**, at start of dataset.)	
SubSatellitePointStartLon	float	Longitude of the sub-satellite point at start of acquisition.	-180 to 180
SubSatellitePointEndLat	float	Latitude of the sub-satellite point at end of acquisition.	-90 to 90
SubSatellitePointEndLon	float	Longitude of the sub-satellite point at end of acquisition.	-180 to 180
OverallQualityFlag	string	Overall quality flag for the L2 product.	OK, NOK
QualityInformation	string	Several miscellaneous quality indicators for the L2 product.	*string*
DegradedRecordCount	int	Number of degraded and incomplete Earthshine MDRs detected by L2 software.	*int*
DegradedRecordPercentage	int	Percentage of degraded and incomplete MDRs detected by L2 software, w.r.t total number of read Earthshine MDRs.	0 - 100
MissingDataCount	int	Number of Earthshine MDR records skipped by L2 software due to time breaks or other data requirement failures.	*int*
MissingDataPercentage	int	Percentage of Earthshine MDR records skipped by L2 software due to time breaks or other data	0 - 100

		requirements, w.r.t total number of read Earthshine MDRs.	
GranuleType	string	Type description of the item.	DP (Data Product)
DispositionMode	string(1)	Disposition mode applied for generation of the product	O(perational), P(re-operational), D(emonstrational)
ReferenceTime	string	A reference time mainly used for the product file names. Time when the product is generated TBC	*Date in CCSDS format*
AscNodeCrossingTime	string	Ascending Node Crossing Date and Time	*Date in CCSDS format*
AscNodeLongitude	String (9)	Ascending Node Longitude	*String containing a float.*
ProductID	String	Product identifier, as per the O3MSAF Product Requirement Document	*O3M-XXX(.x) where XXX are digits*
DOI	String	Digital Object Identifier, issued by EUMETSAT for data set products	*e.g.: for the reprocessed OOP product:* *10.15770/EUM_SAF_O3M_0003*

5.1.2 Product_Specific_Metadata Group

The metadata definition specific for the ozone profiles is given in the following table. The parameters are stored as attributes of the Product_Specific_Metadata group.

Table 3. Product_Specific_Metadata group contents.

Level 1 Usage Section		
Attribute name	**Data Type**	**Description**
NWindows	Int	Number of spectral windows
WindowMin	Float array,	Minimum wavelength of windows [nm]

	rank 1	Dimension = NWindows
WindowMax	Float array, rank 1	Maximum wavelength of windows [nm] Dimension = Nwindows
WindowBand	String array, rank 1	Band in which windows Dimension = Nwindows
GroundPixelBinning	string	Binning of groundpixels (e.g. *Band1aPixel*, Band1bPixel)
AddedRadianceError	Float array, rank 1	Value of added relative error on measured earthshine radiance (to take calibration errors into account) [%], for each window Dimension = Nwindows
AddedRadianceError- CorrelationLength	Float array, rank 1	Correlation length of added relative error covariance [nm] for each window Dimension = Nwindows
CoAddingCrossTrack	Int	Number of ground pixels co-added cross track
CoAddingAlongTrack	Int	Number of ground pixels co-added along track
	Atmosphere and Surface Model Section	
Attribute name	**Data Type**	**Description**
NAtmosLayers	Int	Number of atmospheric layers
SurfacePressureSource	string	Source of surface pressure value (e.g. *MeteoForecast, ECMWF, terrainheight_derived*)
DefaultPressureGrid	Float array, rank 1	Default pressure grid [hPa]; Pressure at layer boundaries. May be different from retrieval input due to adjusted actual surface pressure and actual cloud top pressure for the retrieval. Dimension = NAtmosLayers + 1
TemperatureSource	string	Source of temperature data (e.g. *MeteoForecast, UKMO_climatology, fixed*)
TerrainElevationSource	string	Source of terrain elevation (e.g. *ETOPO, USGS [AD-4]*)
CloudUsage	string	Treatment of clouds (e.g. *Not, IPA-lamb, IPA-scat*)
CloudPressSource	string	Source of Cloud top pressure (e.g. *Level1, Fresco, Fixed*)
CloudFractionSource	string	Source of Cloud fraction (e.g. *Level1, Fresco, Fixed*)
CloudAlbedoSource	string	Source of Cloud albedo (e.g. *Level1, Fresco, Fixed, Fitted*)
AerosolSource	string	Source of aerosol data (e.g. *None, LOWTRAN, AERONETClim*)

AlbedoSource	string	Source of surface albedo data (e.g. *TOMSAlbedoDB, GOMEAlbedoDB, VALUE*)
Tracegasses	string	List of trace gasses included (e.g. *O3_NO2_SO2*)
TracegassesSource	string	Source of tracegas profile (e.g. *AFGL*)
AtmosphereFlags	Int array, rank 1, size 8.	Atmosphere Flags: Each flag occupies 1 integer position. Meaning of the Int values: 0 = false, 1 = true. 1. CloudPerWindow (Allow different cloud data for different spectral windows) 2. CloudPressureIncl (Cloud top pressure replaces closest grid point in PressureGrid) 3. AlbedoPerWindow(Allow different surface albedo for different spectral windows) 4.5.6.7.8. Not used
Radiative Transfer Section		
Attribute name	**Data Type**	**Description**
RTM	string	Radiative Transfer Model (e.g. *LIDORT, LIDORT&PolLUT, VLIDORT, LIRA*)
NStreams	Int	Number of Gaussian polar angles in RTM
NStokes	Int	Number of Stokes vector elements in RTM (1, 3 or 4). Only if RTM = *VLIDORT, LIRA)*
Raman	string	Treatment of Raman scattering (Ring effect) in RTM (e.g. *Not, SolarRingSpectrum, TelluricRingSpectrum, Solar&TelluricRingSpectrum, SingScatRaman*)
SphericalCorrection	String	Correction for atmospheric sphericity (e.g. *Not, Solar, Viewing, Solar&Viewing*)
RTMFlags	Int array, rank 1, size 8	Radiantive Transfer Model Flags: Each flag occupies 1 integer position. Meaning of the Int values: 0 = false, 1 = true. 1. Use spherical correction for solar irradiation 2. Use spherical correction for line of sight correction 3. Use Nakajima-Tanaka approximation (separate single scattering run) 4. Use coarse grid for multiple scattering run 5. Use delta-M method to improve results for peaked phase functions (for aerosols) 6. Use optimum wavelengths to calculate radiance field

		7. and 8. not used
Inversion Section		
Attribute name	**Data Type**	**Description**
InversionMethod	String	Inversion mothod (e.g. *OptimalEstimation, PhillipsTihkonov)*
MaxNIter	Int	Maximum number of iterations
ConCritCost	Float	Convergence criterium on cost function change [fraction of number of measurements] [RD4]
ConCritState	Float	Convergence criterium on state change [fraction of number of state vector elements] [RD4]
InversionFlags	Int array, rank 1, size 8	Inversion Flags: Each flag occupies 1 integer position. Meaning of the Int values: 0 = false, 1 = true. 1. UseConCritState (Use convergence criterium on cost function change) 2. UseConCritState (Use convergence criterium on state change) 3. 4. 5. 6. 7. 8. not used
Output Section		
Attribute name	**Data Type**	**Description**
NOutputLayers	Int	Number of layers onwhich output profile is given
DefaultOutputGrid	Float array, rank 1	Default output pressure grid [hPa]; may be adjusted using actual surface pressure and actual cloud top pressure Dimension = NOutputLayers + 1

5.1.3 Table Attibutes

Attributes attached to all datasets in the Geolocation group and Data group are shown in the table below.

Table 4. Attributes for the geolocation and data group datasets.

Attribute name	Data Type	Description
Title	string	Description of the dataset, e.g. "Solar noon UV index"
Unit	string	Unit of the values in the array, e.g. DU, second
FillValue	same as the dataset	Value in the array, in case actual data value is missing
ValidRangeMin	same as the dataset	Minimum allowed value for the data in the array
ValidRangeMax	same as the dataset	Maximum allowed value for the data in the array

5.1.4 Geolocation Group

The datasets in the Geolocation group are given in the following table. The data type and value of the Unit attribute are given for each dataset. The letters A - G in the description column refer to Figure 2 and Figure 3.

Table 5. Geolocation group contents.

Dataset name	Data type	Unit	Description
Time	String array rank 1	-	UTC time in CCSDS format
EndUTCTime	String array rank 1	-	UTC time in CCSDS format of the end of the integration period
LongitudeCenter	Float arr rank 1	degree	Longitude of the center of the ground pixel (F)
LatitudeCenter	Float arr rank 1	degree	Latitude of the center of the ground pixel (F)
Longitude_A	Float arr rank 1	degree	Longitude of corner A of the pixel
Latitude_A	Float arr rank 1	degree	Latitude of corner A of the pixel
Longitude_B	Float arr rank 1	degree	Longitude of corner B of the pixel

Dataset name	Data type	Unit	Description
Latitude_B	Float arr rank 1	degree	Latitude of corner B of the pixel
Longitude_C	Float arr rank 1	degree	Longitude of corner C of the pixel
Latitude_C	Float arr rank 1	degree	Latitude of corner C of the pixel
Longitude_D	Float arr rank 1	degree	Longitude of corner D of the pixel
Latitude_D	Float arr rank 1	degree	Latitude of corner D of the pixel
SolarZenithAngleE	Float arr rank 1	degree	Solar zenith angle at h0 point E of the ground pixel
SolarZenithAngleF	Float arr rank 1	degree	Solar zenith angle at H0 for point F of the ground pixel
SolarZenithAngleG	Float arr rank 1	degree	Solar zenith angle at H0 for point G of the ground pixel
SolarAzimuthAngleE	Float arr rank 1	degree	Solar azimuth angle at H0 for point E of the ground pixel
SolarAzimuthAngleF	Float arr rank 1	degree	Solar azimuth angle at H0 for point F of the ground pixel
SolarAzimuthAngleG	Float arr rank 1	degree	Solar azimuth angle at H0 for point G of the ground pixel
LineOfSightZenithAngleE	Float arr rank 1	degree	LineOfSight zenith angle at H0 for point E of the ground pixel
LineOfSightZenithAngleF	Float arr rank 1	degree	LineOfSight zenith angle at H0 for point F of the ground pixel
LineOfSightZenithAngleG	Float arr rank 1	degree	LineOfSight zenith angle at H0 for point G of the ground pixel
LineOfSightAzimuthAngleE	Float arr rank 1	degree	LineOfSight azimuth angle at H0 for point E of the ground pixel
LineOfSightAzimuthAngleF	Float arr rank 1	degree	LineOfSight azimuth angle at H0 for point F of the ground pixel
LineOfSightAzimuthAngleG	Float arr rank 1	degree	LineOfSight azimuth angle at H0 for point G of the ground pixel
RelativeAzimuthAngle_ Quadrature	Float arr rank 1	degree	Relative azimuth angles at H0 for the quadrature point(s)
SubSatellitePointLongitude	Float arr rank 1	degree	Geocentric longitude of subsatellite point
SubSatellitePointLatitude	Float arr	degree	Geodetic latitude of subsatellite point

Dataset name	Data type	Unit	Description
	rank 1		
SatelliteAltitude	Float arr rank 1	km	Geodetic altitude of satellite
EarthRadius	Float arr rank 1	km	Radius of the Earth
NrOfPixelsInScan	Int arr rank 1	N/A	Number of pixels within the scan line.
IndexInScan	Int arr rank 1	N/A	Index of the pixel within the scan line. This indicates whether the pixel is a forward scan pixel (indices 1 – 12 (1–24)) or backscan pixel (indices 13 – 16 (25 – 32)).
ScanDirection	Int arr rank 1	N/A	Scan direction of the mirror. Enumerated values: 0=Unknown, 1=Forward, 2=Backward, -9=FillValue

5.1.5 Data Group

The datasets in the Data group are given in Table 6. The data type and value of the Unit attribute are given for each dataset.

Attributes attached to all datasets in this group are the same as for the Geolocation group.

Table 6. Data group contents.

Quality Section			
Dataset name	**Data type**	**Unit**	**Description**
QualityInput	Int arr, rank 2, size 32	N/A	Quality flags for the input data. 0 = false, 1 = true 0: Non-nominal level 1 due to instrument degradation; DEGRADED_INST_MDR in Level1b [RD1]) 1: Non-nominal level 1 due to processing degradation; DEGRADED_PROC_MDR in Level1b [RD1] 2: Groundpixel is in SAA; F_SSA in Level1b/PCD_BASIC [RD1] 3: Sunfile of date missing: older sunfile used 4: Meteoforecast file missing: climatological meteo data used 5: Meteoforecast data missing: climatological meteo

			data used 6: Meteoforecast data invalid 7: Earthshine radiance data missing 8: Earthshine radiance data invalid 9: Solar irradiance data missing 10: Solar irradiance data invalid 11: Measurement data invalid 12: Auxiliary data invalid 13: Absorbing Aerosol Index data invalid 14: Failure in setup of the Forward Model Input 15: Failure in State vector definition setup 16: Sunglint flag 17: Cloud fraction forced to zero 18: Cloud Pressure Adjusted to Surface Pressure 19: Other error 20 – 31: reserved for future use
QualityProcessing	Int arr, rank 2, size 32	N/A	Quality flags for processing. 0 = false, 1 = true, -999 = No Retrieval done, -1 = value not initialized / not used. 0: Overall Convergence was reached (indicates successful retrieval) 1: Convergence reached on Cost 2: Convergence reached on State 3: Convergence not reached after maximum number of iterations 4: Out of bound retrieval values 5: Too high values for Chi Square 6: No retrieval done! (due to incorrect inputs or other reasons). 7 – 31: reserved for future use

Auxiliary Section			
Dataset name	**Data type**	**Unit**	**Description**
OutputPressureGrid	Float arr, rank 2	hPa	Pressure levels (of layer boundaries), on which retrieved profile is given [hPa]; possibly adjusted using actual surface pressure and actual cloud top pressure Dimension = (NoutputLayers + 1) x NProfile
AltitudeProfile	Float	km	Altitudes of OutputPressureGrid above sea level,

	arr, rank 2		Dimension = (NoutputLayers + 1) x NProfile
TemperatureProfile	Float arr, rank 2	K	Average temperature of layers, Dimension = NoutputLayers x NProfile
AAI	float arr, rank 1	-	Absorbing Aerosol Index
CloudPressure	float arr, rank 1	hPa	Cloud top Pressure
CloudFraction	float arr, rank 1	-	Cloud fraction
CloudAlbedo	float arr, rank 1	-	Cloud albedo
State Vector Definition Section			
Attribute name	**Data Type**	**Unit**	**Description**
Nstate	Int arr, rank 1	-	Number of State vector elements
StateDef	String arr, rank 2	N/A	Short description of state vector element, e.g. *OZOP_07 (ozone for layer7), ALBE_03 (surface albedo window 3), CLAL_03 (cloud albedo window 3); CEA0 (Calibration error Additive offset)* Dimension = MaxState x NProfile (of which NState (i) elements are used for each retrieval 'i')
StateUnit	String arr, rank 2	N/A	Unit of state vector element (e.g. *None, DU*) Dimension = MaxState x NProfile (of which NState (i) elements are used for each retrieval 'i')
StateRel	String arr, rank 2	N/A	Mathematical function relating state vector element to actual quantity (e.g. *ident*, *log*) Dimension = MaxState x NProfile (of which NState (i) elements are used for each retrieval 'i')
AprioriValueSource	String arr, rank 2	N/A	Source of apriori value of state vector element (e.g. for O3: FK=*Fortuin/Kelder*, ML=*McPeters/Labow*, *TOMSv8*,) Dimension = MaxState x NProfile (of which NState (i) elements are used for each retrieval 'i')
AprioriErrorSource	String arr, rank 2	N/A	Source of apriori error of state vector element (e.g. *O3FortuinLangematz, fixed absolute, fixed relative*) Dimension = MaxState x NProfile (of which NState (i) elements are used for each retrieval 'i')

AprioriCovarianceS	String arr, rank	N/A	Source of apriori error covariance of (profile) state vector

ource	2		element (e.g., *FixedCorrelation, ZeroCorrelation*) Dimension = MaxState x NProfile (of which NState (i) elements are used for each retrieval 'i')
Retrieval Result Section			
Dataset name	**Data type**	**Unit**	**Description**
NIter	Int arr, rank 1	-	Number of Iterations
Cost	Float arr, rank 1	-	Cost Function value at convergence = CostMeas + CostState
CostMeas	Float arr, rank 1	-	Part of cost function that measures deviation of simulated and measured spectrum: value at convergence
CostState	Float arr, rank 1	-	Part of cost function that measures deviation of state and apriori: value at convergence
ChiSq	Float array, rank 2	-	χ^2 (CostMeas per window) per window, Dimension = NWindows x NProfile
NMeasurements	Int arr, rank 1	-	Number of measurements (wavelengths) used in the retrieval
DFS	Float arr, rank 1	-	Degrees of Freedom for Signal [RD4]
DFS_Profile	Float arr, rank 1	-	Degrees of Freedom for Signal, limited to state vector elements corresponding to atmospheric profile (e.g. ozone)
IntegratedVerticalProfile	Float arr, rank 1	DU	Integrated Vertical Ozone Profile (Total Column)
IntegratedVerticalProfileError	Float arr, rank 1	DU	Error of the Integrated Vertical Ozone Profile
TropopauseLevel	Int arr, rank 1	-	Pressure level indicating the Tropopause selected from the TemperatureProfile
TroposphericIntegratedProfile	Float arr, rank 1	DU	Tropospheric Integrated Vertical Ozone Profile from surface to the tropopause pressure (possibly partial top layer)
TroposphericIntegratedProfileError	Float arr, rank 1	DU	Error on the Tropospheric Integrated Vertical Ozone Profile from surface to tropopause pressure (possibly partial top layer)
StratosphericIntegratedProfile	Float arr, rank 1	DU	Stratospheric Integrated Vertical Ozone Profile from the tropopause pressure (possibly partial bottom layer) to the top of the atmosphere
StratosphericIntegratedProfileError	Float arr, rank 1	DU	Error on the Stratospheric Integrated Vertical Ozone Profile from the tropopause pressure (possibly partial bottom layer) to the top of the

			atmosphere
StateRetrieved	Float array, rank 2	*<StateUnit>*	Retrieved values of State vector elements, transformed back to physical value using StateRel Dimension = MaxState x NProfile (of which NState (i) elements are used for each retrieval ‘i’)
StateRetrievedError	Float array, rank 2	*<StateUnit>*	Errors of retrieved values of State vector elements, transformed back to physical value using StateRel Dimension = MaxState x NProfile (of which NState (i) elements are used for each retrieval ‘i’)
Apriori	Float array, rank 2	*<StateUnit>*	Apriori values of State vector elements, transformed back to physical value using StateRel Dimension = MaxState x NProfile (of which NState (i) elements are used for each retrieval ‘i’)
AprioriError	Float array, rank 2	*<StateUnit>*	Errors of apriori values of State vector elements, transformed back to physical value using StateRel Dimension = MaxState x NProfile (of which NState (i) elements are used for each retrieval ‘i’)
AprioriErrorCovariance	Float arr, rank 3	*<StateUnit>*	Apriori Error Covariance Matrix Dimension = MaxState x MaxState x NProfile (of which NState(i) x NState(i) x NProfile elements are used foreach retrieval ‘i’)
ErrorCovarianceTotal	Float arr, rank 3	*<StateUnit>*	State Covariance Matrix, including smoothing error [RD4] Dimension = MaxState x MaxState x NProfile (of which NState(i) x NState(i) x NProfile elements are used foreach retrieval ‘i’)
ErrorCovarianceNoise	Float arr, rank 3	*<StateUnit>*	State Covariance Matrix, excluding smoothing error [RD4] Dimension = Dimension = MaxState x MaxState x NProfile (of which NState(i) x NState(i) x NProfile elements are used foreach retrieval ‘i’)
AveragingKernel	Float arr, rank 3	-	Averaging Kernel Matrix [RD4] Dimension = Dimension = MaxState x MaxState x NProfile (of which NState(i) x NState(i) x NProfile elements are used foreach retrieval ‘i’)
AltitudeProfile_Raw	Float arr, rank 2		Altitude values associated with raw temperature profile
PressureProfile_Raw	Float arr, rank 2		Pressure values associated with raw temperature profile

TemperatureProfile_Raw	Float arr, rank 2		'Raw' Temperature profile, from the external data source. Usually in higher resolution than the temperature profile in the RTM model.
~~TropopausePressure_Raw~~	~~Float arr, rank 1~~	~~-~~	~~TropopausePressure from raw temperature profile~~ Removed with OPF version 4.01
IntegratedVerticalProfileSurfaceTo500hPa	Float arr, rank 1	*DU*	Integrated vertical ozone profile from the surface to the 500hPa pressure level
IntegratedVerticalProfileErrorSurfaceTo500hPa	Float arr, rank 1	*DU*	Integrated vertical ozone profile error from the surface to the 500hPa pressure level, as a sum of the diagonal of the ErrorCovariance matrix
TropopausePressure_Thermal_Raw	Float arr, rank 1	*hPa*	Tropopause pressure from the raw temperature input (likely ECMWF)
TropopausePressure_PV	Float arr, rank 1	*hPa*	Tropopause pressure based on the potential vorticity (PV) from an NWP model (likely ECMWF)

5.2 Data Types

The data types to be used in the HDF5 files are given in the table below.

Table 7. Data types for the HDF5 files.

Data type	HDF5 predefined data type
char	H5T_NATIVE_CHAR
short int	H5T_STD_I16LE
int	H5T_STD_I32LE
float	H5T_IEEE_F32LE
double	H5T_IEEE_F64LE
String	H5T_NATIVE_CHAR

5.3 File name convention

File names of product are following the names of the input files. For GOME2, these are foreseen as having the following layout for the HDF5 format files:

S-O3M_GOME_OOP_02_AAA_SSSS_EEEE_W_Z_PPPP.hdf5

Where AAA is the flight model number. On MetOp-A this number is M02, On MetOp-B this number is M01. The SSSS is a placeholder for the SensingStartTime: (YYYYMMDDhhmmssZ); the EEEE is the placeholder for the SensingEndTime (also YYYYMMDDhhmmssZ), the PPPP is the processing time (also in the same format as SSSS and EEEE); The W indicates the Processing-Mode and Z indicates the Disposition-Mode of the file.

The OOP indicates the Offline Ozone Profile product. Note that these three letters are replaced by NOP for Near Real Time coarse resolution products. The high resolution ozone profile products codes are NHP and OHP for NRT and offline respectively.

5.4 File size estimate

5.4.1 Estimated size of HDF5 output product

The size of the output file can vary. The size is affected by different string lengths, the number of output layers that are used, the number of retrieved profiles, the addition of optional data sets to the file, and possibly the compression factor in the HDF5 output file.
The coarse resolution NOP output file in HDF5 is roughly 3.2Mb per 90 retrievals.
The coarse resolution OOP output file in HDF5 is about 37Mb per whole orbit.

The high resolution ozone profile data is about 37Mb per NHP file (PDU) and 257Mb per OHP orbit.

5.5 Relation of the Offline product w.r.t. the NRT product

The Offline Ozone Profile products (OOP, OHP) are files that cover an orbit starting from the ascending crossing of the equator (in the case of GOME-2 this is on the dark side of the earth). The offline product is put together by assembling all PDU sized HDF5 output files and concatenating them to one big file in the same format as described above. The offline product does not contain more information than the HDF5 files produced in NRT. In fact, some of the metadata values may be set to unknown if some of the input parameters of the original PDUs have had different values within one orbit.

6. PRODUCT FORMAT DEFINITION OF THE NRT OZONE PROFILE PRODUCT IN BUFR

6.1 Format

The Near Real Time (NRT) Level 2 ozone profile product file in BUFR is written with edition 4 conventions, following the WMO BUFR tables as implemented in the publicly available ECMWF BUFR software. The BUFR format follows the basic structure of descriptor number 310020, with the exception of the rescaling of the ozone data width and scale.

The geolocation information of each ground pixel is provided. The center coordinates (point F in fig 3/4) are given in BUFR descriptor number **301021**, and the information of the corner coordinates (points A, B, C, D) are in descriptor number **304034**. See Figure 3 and 4 for the definition of the coordinates of the ground pixel.

6.1.1 Unexpanded BUFR descriptors

DATA DESCRIPTORS (UNEXPANDED)

1 310022
2 301011
3 301013
4 301021
5 304034
6 112000
7 031001
8 201131
9 202129
10 007004
11 007004
12 202000
13 201000
14 201131
15 202133
16 015020
17 202000
18 201000
19 010002
20 224000
21 236000
22 101000
23 031001
24 031031
25 001031
26 001032
27 008023
28 101000
29 031001

30 224255

6.1.2 Expanded BUFR descriptors

Please note that the number of layers can differ per output product. The data element number only indicates the order.

DATA DESCRIPTORS (EXPANDED)

1 001007 SATELLITE IDENTIFIER
2 002019 SATELLITE INSTRUMENTS
3 001033 IDENTIFICATION OF ORIGINATING/GENERATING CENTRE
4 002172 PRODUCT TYPE FOR RETRIEVED ATMOSPHERIC GASES
5 004001 YEAR
6 004002 MONTH
7 004003 DAY
8 004004 HOUR
9 004005 MINUTE
10 004006 SECOND
11 005001 LATITUDE (HIGH ACCURACY)
12 006001 LONGITUDE (HIGH ACCURACY)
13 027001 LATITUDE (HIGH ACCURACY)
14 028001 LONGITUDE (HIGH ACCURACY)
15 027001 LATITUDE (HIGH ACCURACY)
16 028001 LONGITUDE (HIGH ACCURACY)
17 027001 LATITUDE (HIGH ACCURACY)
18 028001 LONGITUDE (HIGH ACCURACY)
19 027001 LATITUDE (HIGH ACCURACY)
20 028001 LONGITUDE (HIGH ACCURACY)
21 007022 SOLAR ELEVATION
22 005043 FIELD OF VIEW NUMBER
23 020010 CLOUD COVER (TOTAL)
24 020016 PRESSURE AT TOP OF CLOUD
25 033003 QUALITY INFORMATION
26 010040 NUMBER OF RETRIEVED LAYERS
27 031001 DELAYED DESCRIPTOR REPLICATION FACTOR
28 007004 PRESSURE
29 007004 PRESSURE
30 015020 INTEGRATED 03 DENSITY
31 010002 HEIGHT
. . .
100 007004 PRESSURE
101 007004 PRESSURE
102 015020 INTEGRATED 03 DENSITY
103 010002 HEIGHT
104 224000 FIRST ORDER STATISTICS FOLLOW
105 236000 BACKWARD REFERENCE BIT MAP
106 031001 DELAYED DESCRIPTOR REPLICATION FACTOR
107 031031 DATA PRESENT INDICATOR
. . .
182 031031 DATA PRESENT INDICATOR

183 001031 IDENTIFICATION OF ORIGINATING/GENERATING CENTRE
184 001032 GENERATING APPLICATION
185 008023 FIRST ORDER STATISTICS
186 031001 DELAYED DESCRIPTOR REPLICATION FACTOR
187 015020 INTEGRATED 03 DENSITY
. . .
205 015020 INTEGRATED 03 DENSITY

The following conversion is performed to go from DU per layer (in the HDF5 format) to kg/m^2 (in the BUFR format):

IntegratedOzoneDensity (LayerNr) =

DU_per_Payer (LayerNr) * DUToCm2 / CM2ToM2 / N_Avogadro *

Ozone_Mole_Mass / 1000.0 ! KG/M**2

Where:

Molecular Mass Ozone in: grams / mole: Ozone_Mole_Mass = 47.9982_SP

Avogadro's number: N/Mole: N_Avogadro = 6.02205E23

Const in: Col[cm2] = 2.69e16*col[DU]: = number of molecules per cm2

DUToCm2 = 2.68668E16

CM2ToM2 = 1.0E-4

6.2 File name conventions

File names of NOP product are following the names of the input files. For GOME2, these are foreseen as having the following layout for the BUFR format files:

S-O3M_GOME_NOP_02_AAA_SSSS_EEEE_W_Z_PPPP.bufr

Where AAA is the flight model number. On MetOp-A this number is M02. On MetOp-B this number is M01. The SSSS is a placeholder for the SensingStartTime: (YYYYMMDDhhmmssZ); the EEEE is the placeholder for the SensingEndTime (also YYYYMMDDhhmmssZ), the PPPP is the processing time (also in the same format as SSSS and EEEE); The W indicates the Processing-Mode and Z indicates the Disposition-Mode of the file.

The NHP product follows an alternative file name convention in line with the WMO guidelines on BUFR file names (See WMO document ET-IDM-III/Doc. 4(1) and EUMETSAT document EUM/OPS-EPS/TEN/07/0012).

W_NL-KNMI-DEBILT,<x>,<y>_C_EHDB_<s>_NHP_02_<d>_N_O_<n>_<q>.bin

Where <x> is SOUNDING+SATELLITE, <y> is METOPA+GOME2, <s> is the start time of the measurements, <d> is the end time of sensing, and <n> is the processing time. The indicator <q> also follows GTS standards and indicates upper air and sounding data including a geographical region and a version number.

6.3 File size estimate

6.3.1 Estimated size of BUFR formatted output file

The size of the output file can vary. The size is affected by the number of output layers that are used, the number of retrieved profiles, and possibly the compression factor in the BUFR output file.
On average, the NOP product in BUFR is smaller than 40Kb per 90 retrievals. The NHP high resolution BUFR file is smaller than 350Kb per 720 retrievals.

7. USING THE HDF5 OZONE PROFILE PRODUCT

The descriptions below are summaries and explanations of how the data stored in the output product can be used.

7.1 The Ozone Profile Product

7.1.1 Geolocation Group: Time, Geolocation, Angles

The following elements are stored in the Geolocation Group for each retrieval:

- the time at the end of the integration
- the latitude/longitude of the centre of the ground pixel
- the latitude/longitude of the ground pixel corners (A, B, C, D)
- the solar zenith angle, solar azimuth angle and the line of sight zenith angle and line of sight azimuth angle at the instrument specific reference height h0.

With these parameters users should be able to link the retrievals to other geo-referenced objects, or use the data for gridding.

7.1.2 Data Group

The Data group contains all non-geolocation information for each profile retrieval:

7.1.2.1 OutputPressureGrid, AltitudeProfile, TemperatureProfile

The model retrieval grid is adjusted for surface pressure and cloud pressure for each individual retrieval. The OutputPressureGrid is the grid used in the actual retrieval. The altitude profile is derived using the hydrostatic equation and the temperature profile (either from a zonally averaged, monthly mean temperature profile climatology or from weather forecasting analysis).

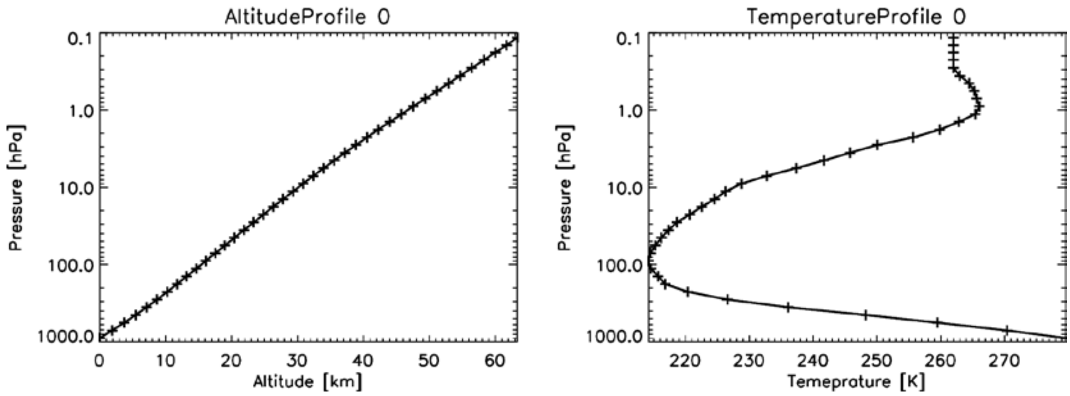


Figure 6: Relation between pressure and altitude and the temperature profile for an example retrieval.

7.1.2.2 StateDefinition, StateUnit, StateRetrieved, and the ozone profile

Because each profile retrieval can have a different number of fitting parameters with different units (e.g.: the number of layers can change, or the cloud or surface albedo can be fitted), there is a data structure called StateDefinition wherein each data value of the StateRetrieved array is described in mnemonics. The most important ones are:

- OZOP_NNN indicates ozone profile for layer NNN (counting from the bottom upwards).
- ALBE_MMM and CLAL_MMM indicate the surface albedo or the cloud albedo fit for window MMM. Only one of these parameters is fitted, not both.
- CEAO_MMM indicates an additional offset to fit window MMM. This is an optional fit parameter.

Initial values for ozone come from external climatology's or from previous retrievals. Initial cloud information comes from Level 1b for GOME-2 or from an internally implemented FRESCO cloud retrieval in the case of GOME-1. The offset has an initial value from the configuration file.

The units of the fit parameters are given in the StateUnit structure. The source of the state vector elements (in terms of origin of their values) can be taken from the AprioriValueSource structure, where for each element the source is given.

To extract the ozone profile from the retrieved state, one needs to look at the StateDefinition, find the elements that contain OZOP values. Then use the values in the same position of the StateRetrieved array.

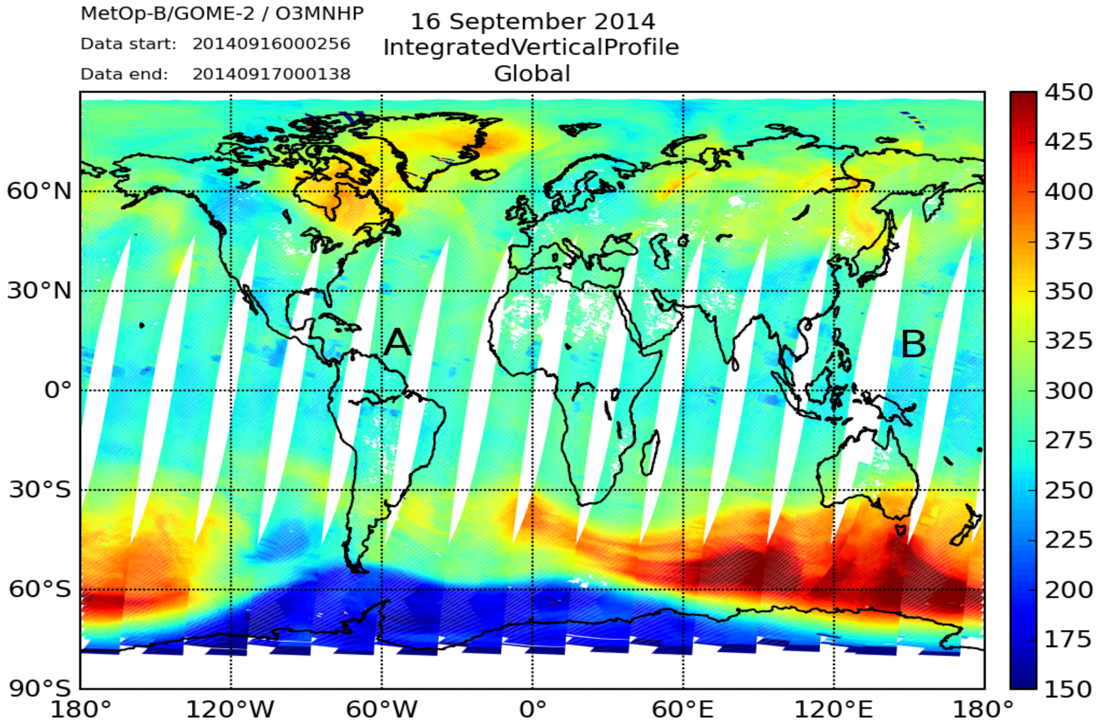


Figure 7: Total ozone column, calculated as the sum of the retrieved profile for September 16th 2014. Instrument: GOME-2B.

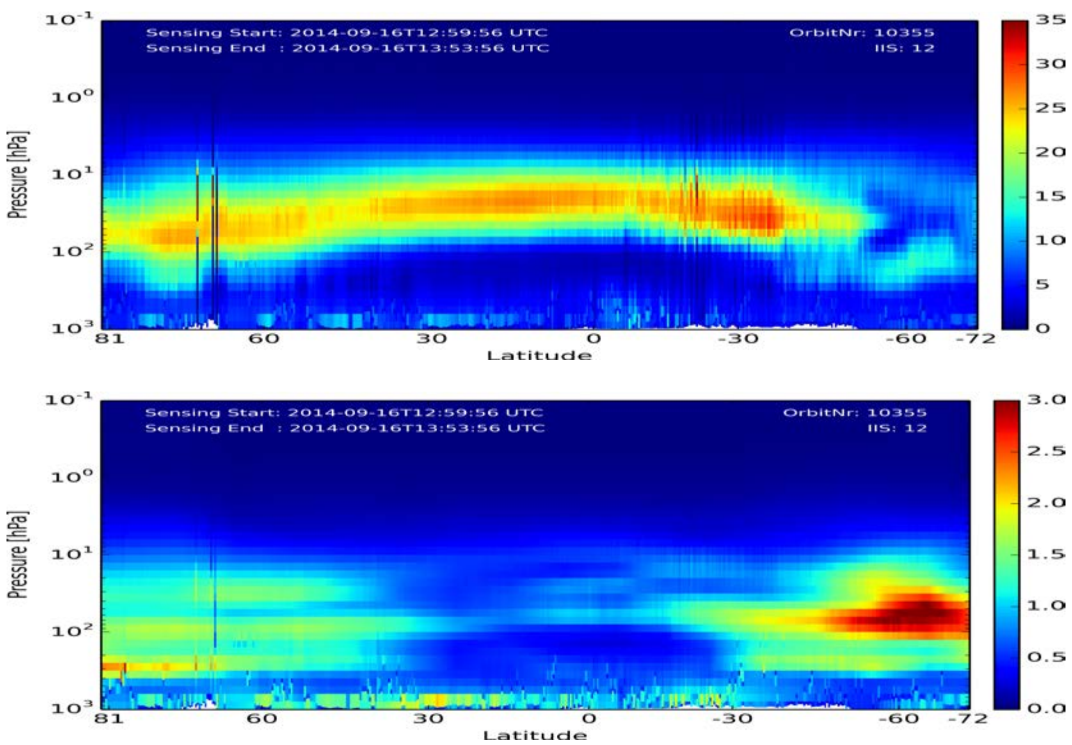


Figure 8: Retrieved ozone profile (top) and its retrieved error (bottom) for nadir swath in orbit 10355, indicated with letter (A). Instrument: GOME-2B.

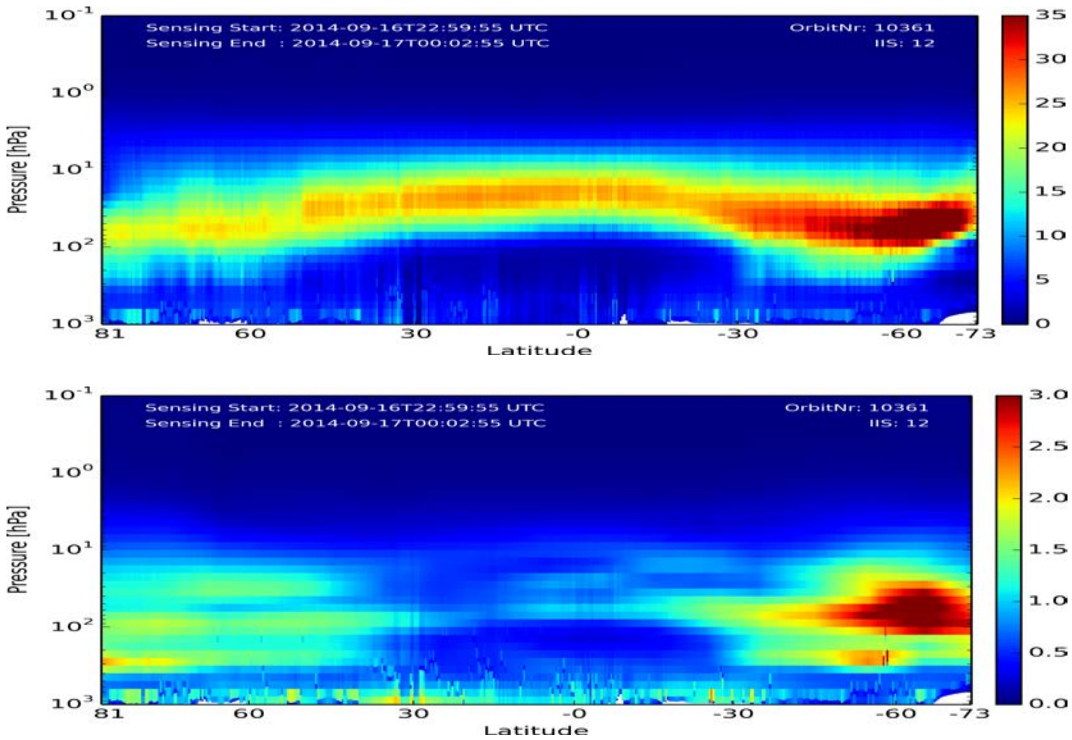


Figure 9: Retrieved ozone profile (top) and its retrieved error (bottom) for western swath of orbit 11361, indicated with letter (B). Instrument: GOME-2B.

Examples the vertical ozone profiles are shown in Figure 7 to Figure 9. In Figure 7 the vertical profiles of 16 Sept 2014 are integrated to a total column. The Antarctic ozone hole can be seen. In the figure, two orbits are indicated (A) and (B). The vertical ozone profiles and their retrieved errors for those orbits are shown in cross section (for the nadir position) in Figure 8 (A) and Figure 9 (B). In the cross section of orbit (A) the region with ozone depletion is seen on the right side of the figure where low ozone concentrations are present.

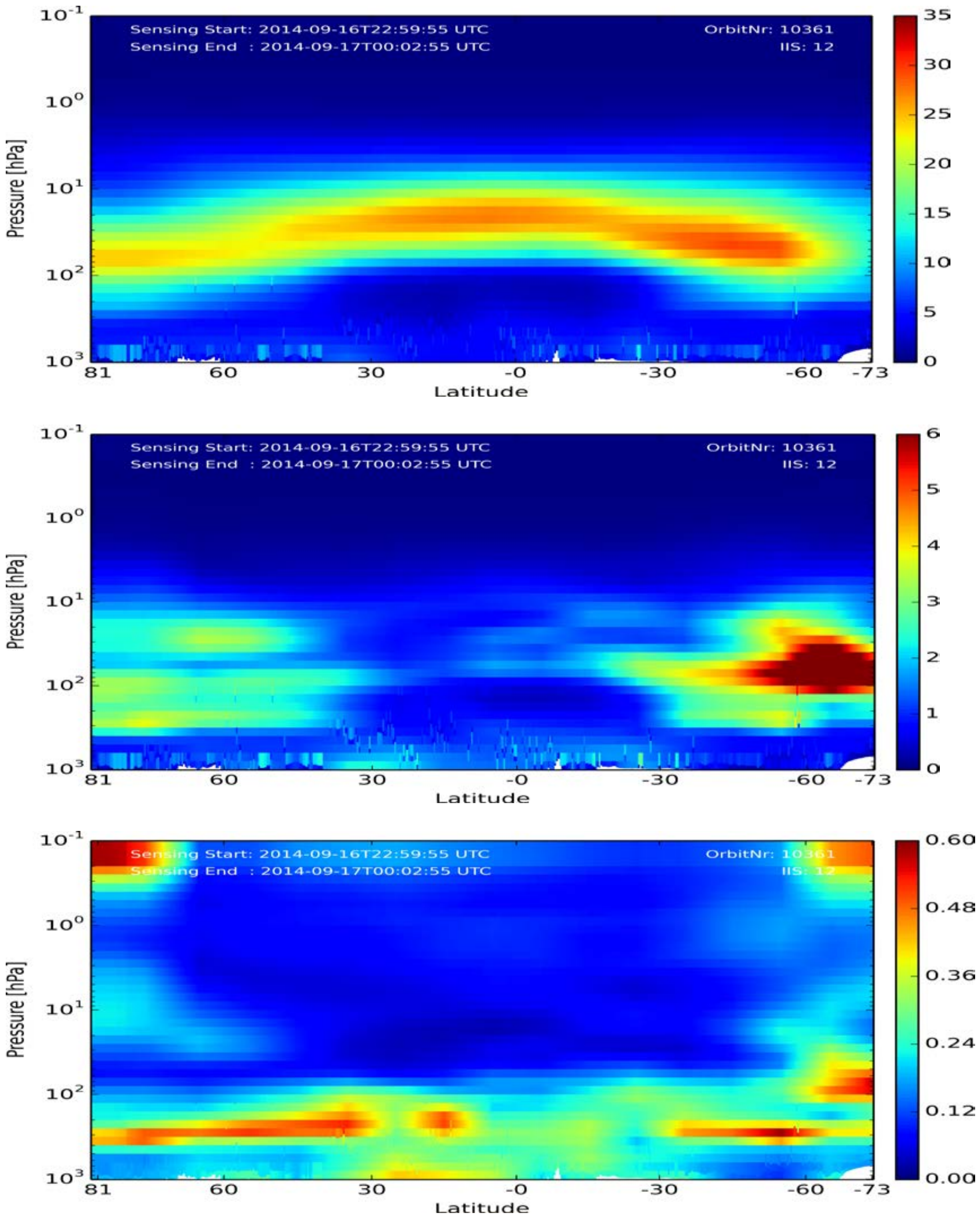


Figure 10: A priori ozone profile (top), its error (center) and relative error (bottom). The example refers to orbit 11361 (A) of GOME-2B.

7.1.2.3 The *a priori*

The *a priori* values follow the same definition and units as described in the StateDefinition and StateUnit. Please note that the source of the *a priori* values can be seen in AprioriValueSource and AprioriErrorSource. The chosen climatology is indicated in these records. For ozone, the mnemonics FK indicates Fortuin and Kelder, ML indicates McPeters et al, TOMSv8 is the TOMS version 8 climatology, and Sonde means that an external file was provided containing the *a priori* values. Please see the ATBD for full references. An example of the *a priori* ozone and its (relative) error is shown in Figure 10.

7.1.2.4 Averaging kernel

The averaging kernel of a certain layer indicates what other layers in the model have contributed to the information in this layer in a positive or negative way. When a user of a retrieved satellite based ozone profile product wants to compare the these profiles with profiles from other independent sources, such as a balloon ozone sounding or microwave soundings, this independent data needs to be treated in order to be compared properly. During the ascent, the ozone sensor on the balloon has a fast response time to changes in the ozone content of the air. Therefore, the vertical resolution of a balloon sounding is in the order of a few tens of meters, while the retrieved profile from satellite instruments typically have a vertical resolution of a few km. Since the balloon has such a high vertical resolution, this data needs to be binned into the layers of the retrieved profile. Then the Averaging Kernel needs to be applied to the binned sonde data, together with the a priori profile, in order to simulate the true profile as if it were retrieved. The averaging kernel (A) relates the retrieved profile ($\hat{x}$) to the true (x_{true}) and the a priori profile (x_a) according to:

$$\hat{x} - x_a = A(x_{true} - x_a) \quad (1.)$$

Use of an Averaging Kernel smoothes a high resolution balloon profile. A more complete description of the averaging kernels is given in the ATBD.[RD5].

7.1.2.5 NMeasurements, NIter

For each retrieval, the number of spectral radiance values used in the optimal estimation inversion is given in the NMeasurements structure. If one would use radiances from Band 1a, 1b, and 2b from 265-330 nm, the number of spectral elements is around 680. If the SAA filter is on, then the number of band 1a radiances drops in the South Atlantic Anomaly area, and usually drops to 350 (all spectral elements above 290 nm).

The number of iterations used to reach convergence is stored for each profile in the NIter structure. A zero or negative value means no retrieval has been attempted. A value at the cut-off (10 iterations) usually means that no convergence was reached (check quality flags). Profiles that have an NIter value of 10 are saved in the offline product, but should not be used for further processing, be it either validation, assimilation or otherwise. Some of the non-converged pixels are due to a “ping-pong” effect in the retrieval solution: the OE inversion jumps between two or more equally suitable solutions.

7.1.2.6 Degrees of Freedom for Signal (DFS)

The DFS indicates the number of independent pieces of information in the retrieved profile and is related to the amount of information the retrieved profile has gained from the spectral measurement. The DFS value is calculated as the sum of the diagonal elements of the averaging kernel matrix. A low DFS means that the retrieval is not very sensitive to the spectral measurement and that a considerable amount of information has come from the *a priori*. The DFS is seasonal, latitude and viewing angle dependent due to the changes in light path and *a priori* profile information. An example of the DFS values of a typical day of ozone profile retrievals is shown in Figure 11. In this case, the Metop-B DFS ranges roughly between 3 to 4.5.

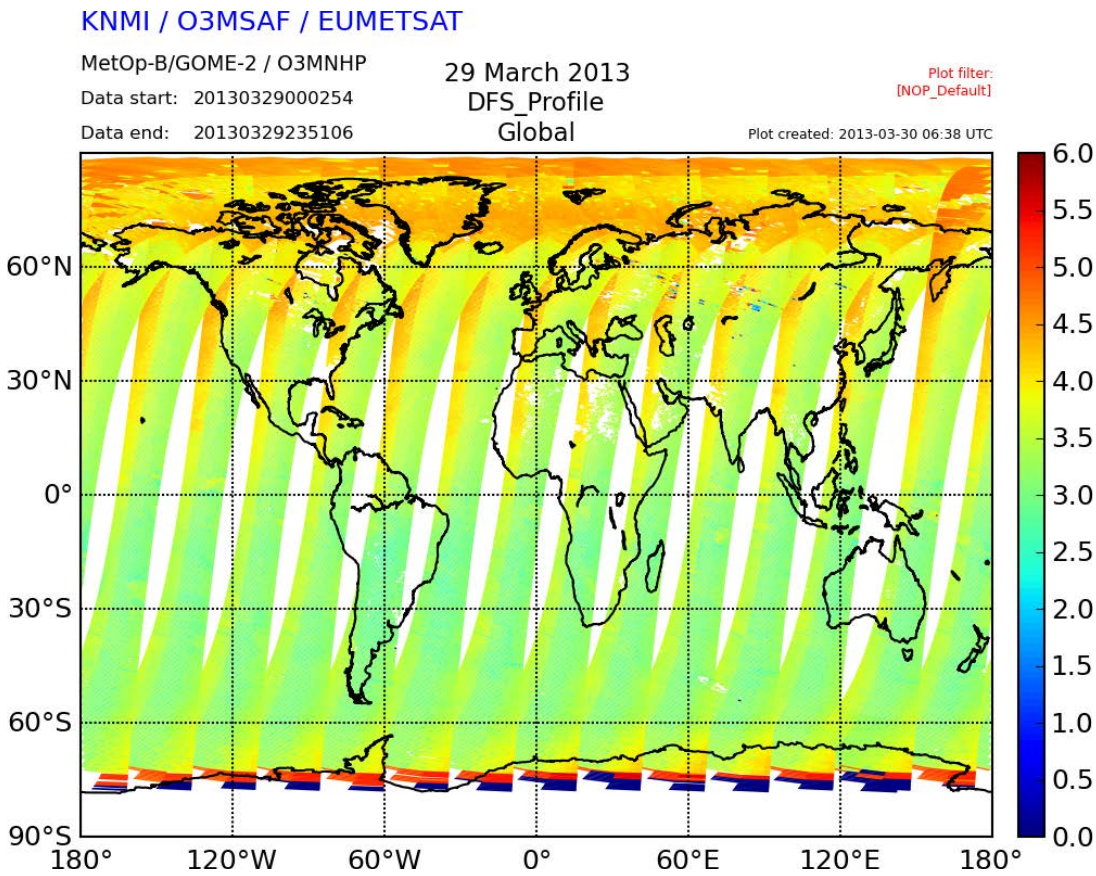


Figure 11: Degrees of Freedom for Signal for retrieved ozone profiles of GOME-2 on Metop-B on March 29th 2013.

7.1.2.7 Quality flags

Quality flags are very important indicators for the correctness of both the input and the retrieved ozone profile. There are two quality flag groups: QualityInput and QualityProcessing. In the input flags the types of failures are set: missing data (geometry-wise or spectral-wise), or out of range/invalid values. In the input quality flags there is a flag for sunglint and whether the cloud fraction has been forced to zero in case of negative albedo fits. The quality input flags datagroup does not contain all of the Level 1B flags but merely a subset that was deemed relevant. In the processing quality flags we can find the flag that indicates whether the retrieval has converged or whether there are out-of-bound retrieval values.

7.1.3 Visualisation examples of global fields

Examples of the global distribution of ozone, the number of iterations to reach convergence in the retrieval and the number of spectral measurements used in the retrieval are shown in Figure 12, Figure 13 and Figure 14. The brown pixels in the 'NIter' plot indicate pixels that hve not reached convergence. The plot with the number of spectral measurements shows the South Atlantic Anomaly where in the UV some measurements are filtered out due to a spike detection method.

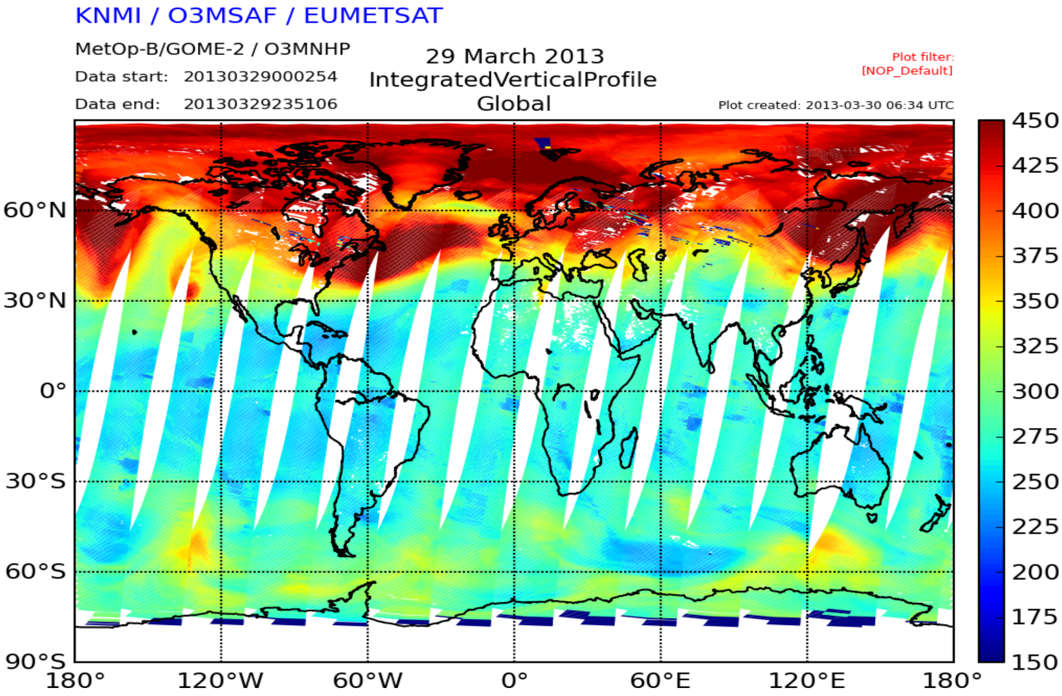


Figure 12: Integrated vertical ozone profile from GOME-2 on Metop-B, calculated as the sum of the retrieved profile on March 29th 2013.

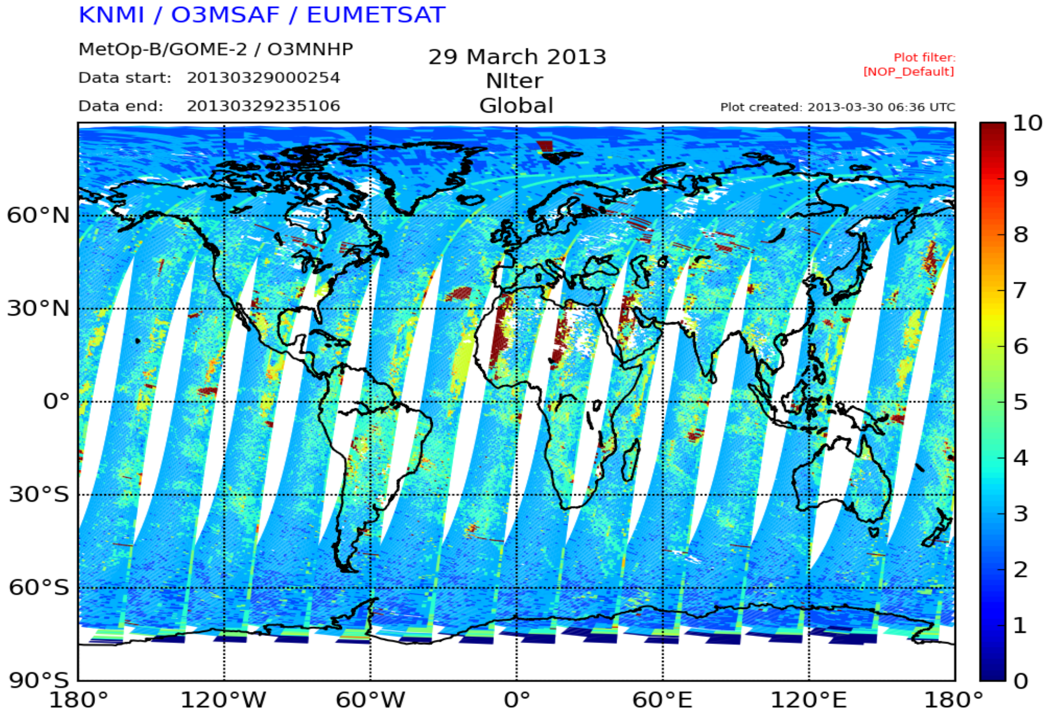


Figure 13: Number of iterations for each retrieval from GOME-2 on Metop-B on March 29th 2013. Brown pixels indicate non-converged profiles.

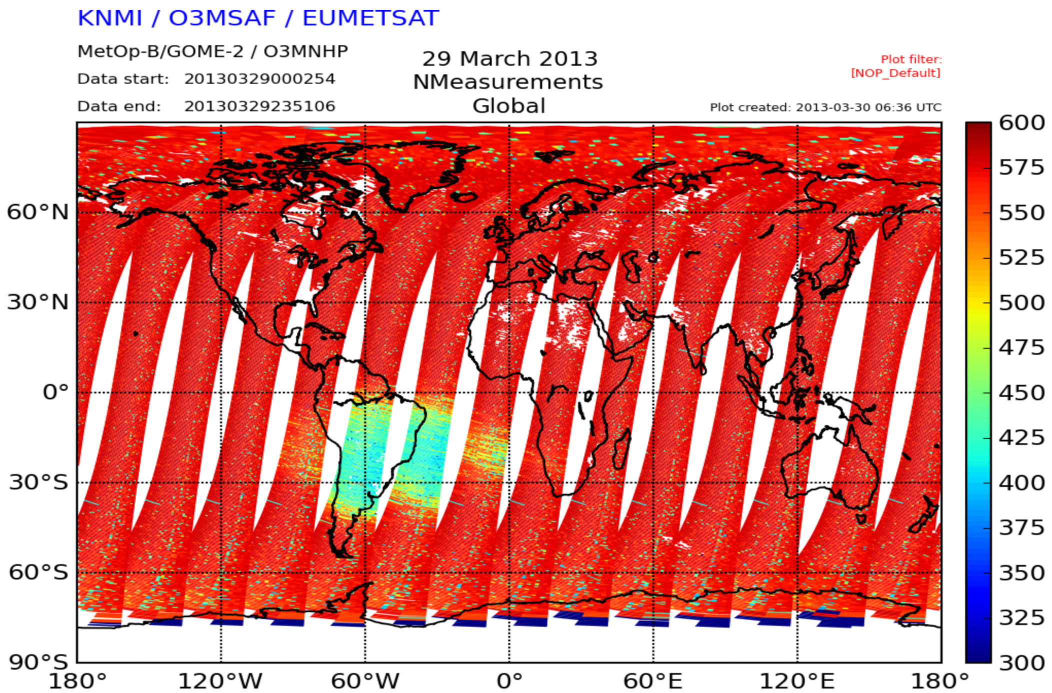


Figure 14: Number of spectral measurements of GOME-2 on Metop-B for each retrieved vertical ozone profile on March 29th 2013.

7.2 The Near Real Time Ozone Profile Product

The Near Real Time Ozone Profile product formats used in dissemination via EUMETCast are the HDF5 and the BUFR file format. The BUFR file contains the bare minimum of data for small bandwidth dissemination channels. The product contains per profile a geo-location, the date and time of the measurement, and the ozone profile and error on the number of model layers used in the retrieval. At the moment of writing, the complete covariance matrix of the retrieval is not included but planned for a future update when the *standard* BUFR table software from ECMWF supports the concept of averaging kernels and the concept of spatial covariance of a value.

If the user needs complete averaging kernels or more information, please refer to the product in HDF5 format (which is also disseminated in NRT as PDU-size blocks). An example of two vertical profiles from two different orbits (see Figure 7) is shown below in Figure 15. On the left a ‘normal’ profile is shown. On the right ozone depletion is taking place and reduces the ozone content significantly between 200 and 10 hPa..

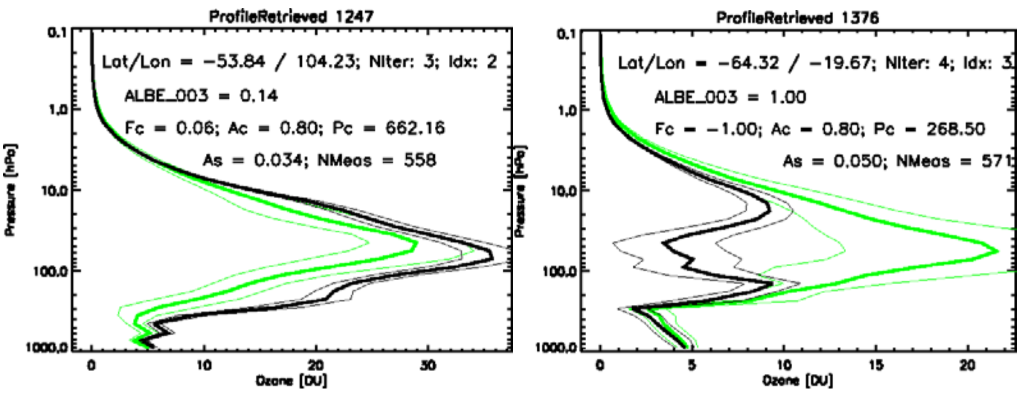


Figure 15: Retrieved ozone profiles (black), it’s a priori (green) for retrieval in the ozone maximum in orbit 4679 (left), and in the ozone hole in orbit 4683 (right), indicated with the A and B. Instrument: GOME-2 on Metop-A.

7.3 The Tropospheric Ozone Column Product

An example of the Tropospheric Ozone Column Product (TrOC) and the partial column from the surface to 500hPa, calculated from the vertical ozone profile, is given in Figure 16. From the south of Africa, the increased tropospheric ozone is clearly visible. This ozone is related to extensive biomass burning in the region. Some

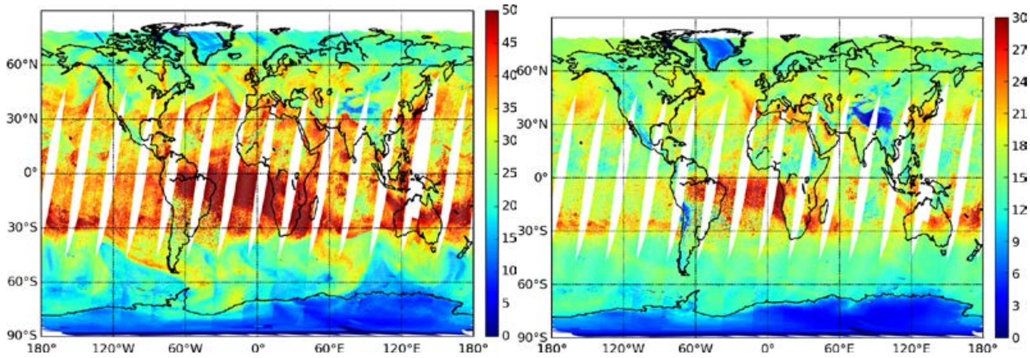


Figure 16: Tropospheric Ozone Column (left) and Surface to 500hPa ozone (right) from GOME-2 on Metop-A on 2010-10-09.

8. ACCURACY OF THE OZONE PRODUCTS

8.1 Vertical Ozone Profile: threshold, target and breakthrough accuracy

In the product requirements document, there are a few numbers set for the accuracy. The first set is the threshold, defined as the lowest accuracy of the product that would be useful to the end user.

The threshold accuracy specified for the NRT and offline product is:

- 70% in the troposphere
- 30% in the stratosphere

The second set of numbers is the target accuracy of the ozone profiles (both offline and near real time) are, averaged over a set of retrievals. This is the development goal during the CDOP phase.

The target accuracy specified for the NRT and offline product is:

- 30% in the troposphere
- 15% in the stratosphere

The third set of numbers is the breakthrough accuracy:

- 25% in the troposphere
- 10% in the stratosphere

The breakthrough accuracy is the estimated highest accuracy.

8.2 Tropospheric Ozone Column: threshold, target and breakthrough accuracy

The O3MSAF Product Requirements Document describes the accuracies as follows:

- Threshold accuracy: 50%
- Target accuracy: 20%
- Breakthrough accuracy: 15%

8.3 Main causes of error (inaccuracy)

The achieved accuracy depends strongly on the level1 data quality, the accuracy of the forward model and the auxiliary data sources such as cross sections, *a priori* and the vertical temperature profile.

The radiometric calibration in the L1b data converts an electrical charge into a physical quantity (W/m^2/sr) and assigns wavelengths to the radiance values. This needs to be accurate, because a soft calibration afterwards can only rectify some limited issues. The GOME-2 instrument (both on Metop-A and Metop-B) shows a strong degradation of the light reaching the detector. The exact cause is partially unknown but the scan mirror, the light path and the detectors (both the FPA and the PMD) are all possible causes. The loss of throughput causes the signal to noise ratio to decrease with time. Due to an inhomogeneous degradation of the Earth radiance and the Solar irradiance the reflectance (ratio of Earth / Sun) has changed over time. This causes a drift in the ozone profile at various levels.

The forward model uses a limited number of streams in its internal calculations to span the up and downward going energy flux. More streams will divide the sphere into smaller parts and usually is more accurate, at a cost of computational speed. In the current version of the algorithm 4 streams are used.

In the international ozone community there is a recurring discussion on the best ozone cross sections to use in modelling. Inaccurate cross sections give rise to anomalous peaks and troughs in the fit residue if the effect is small in spectral domain, or give rise to changes in the shape of the ozone profile in the fitting of broad band structures. The ozone cross absorption is temperature dependent which means that a vertical temperature profile for the full vertical domain needs to be reasonable accurate.

The *a priori* ozone profile regularises the profile, but it also limits the freedom of the retrieval to deviate from it. In cases of large gradients (e.g.: in mid-latitudes in the spring time) the climatological ozone profile (based on a latitudinal zonal mean) may be far off the actual situation. In these cases the retrieval algorithm has difficulty finding a solution, which usually leads a ‘non-converged’ profile.

When the vertical profile is integrated into partial sub-columns, the column vertical boundaries are the most important for the value. In case of the tropospheric sub-column, there are different choices for the tropopause definition. In the transition zone between 19degrees and 26 degrees, where the tropopause height linearly shifts from the thermal definition to the PV definition, errors can occur if the local atmospheric state differs too much from either definition.

8.4 Regular monitoring of O3MSAF product quality

The actual values of the accuracy of the product will be given in the SeSP document. Also, the O3MSAF constantly monitors the product quality and performs regular validations with balloon sondes, lidar and microwave instruments with data from sources all over the world. The results of the validation is in the O3MSAF Validation Report on the ozone profile product.

9. FURTHER INFORMATION

9.1 O3MSAF website

Further up to date information and documentation on the ozone profile and tropospheric column products should be available from the O3MSAF website: http://o3msaf.fmi.fi

Requests for data and questions with regards to O3MSAF products should be directed to the user services. Contact information is also available on the website mentioned above.

9.2 User Notification Service

EUMETSAT maintains a User Notification Service (UNS) that disseminates instantaneous messages relating to the platform (Metop-A), the GOME-2 instrument and derived L1 and L2 products, and weekly notifications of upcoming ground segment and SAF related scheduled maintenance activities. The SAF recommends that Near Real Time users subscribe to this notification service (at least the instrument related and weekly notifications). This ensures also that the SAF has a channel to notify users of upcoming changes in the L2 format and or quality of the products.

9.3 Acknowledgement instructions

When O3MSAF data is used for operational or scientific purposes, the source of this data should be acknowledged.

For example: "The data of the GOME-2 vertical ozone profiles are provided by KNMI in the framework of the EUMETSAT Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring (O3M SAF)".

10. HISTORY OF SOFTWARE AND PRODUCT UPDATES.

Below is a list of changes made to software or configuration parameters. Other events are also recorded if significant.

PPF version	Algorithm version	Software version	Date	Remarks
4.0	0.99	1.14	20080626 10:56	
4.0	0.99	1.15	20080711 10:35	
4.0	1.00	1.19	20081209 12:59	
			20081210	B1a/B1b wavelength shift from 307 to 283 nm
4.1	1.00	1.16	20090107 13:47	
4.2	1.00	1.16	20090407 07:38	
4.2*	1.00	1.16	200906xx	SAA correction in L1b
4.3	1.00	1.16	20090818 11:47	
4.3	1.0	1.16	20090907--	Throughput test
4.3	1.01	1.20	20091109 08:08	
4.4	1.01	1.20	20100121 13:02	
4.4	1.01	1.21	20100128 08:50	
4.4	1.01	1.22	20100302 07:44	Allow incomplete spectral averaging for coarse resolution pixels
4.4	1.10	1.23	20100429 07:14	Format version 3.7. - Pressure profile changed. Top three layers are different: PRESSURE_Old = ... 0.20 0.16 0.13 0.10 PRESSURE_New = ... 0.20 0.10 0.01 0.001 - CEA0 Offset fitted als fixed value * 1.0E+9 photons - Coupling of CEA0 fitted in Window-1 to Window-2 AAI: Added SunGlintFilter and ScatteringAngle to the output product

4.5	1.10	1.23	20100909 11:38	
5.0	1.10	1.24	20110105 12:51	Ability to read PFS v12 L1b data.
5.1	1.10	1.24	20110302 11:39	
5.2	1.10	1.24	20110906 11:50	
5.3	1.10	1.25	20120124 10:14	
5.3	1.10	1.25	20120130 07:11	Tropospheric and Stratospheric columns, Temperature profiles from ECMWF via pygrib, gsl1.15: extrapolation of Temperature to TOA and BOA, HDF4 phase out. OPF v3.9
5.3	1.10	1.26	20120807 06:20	Change in noise floor. High Resolution naming to NHP and OHP
5.3	1.11	1.28	20130513 04:32	Spectral peak filter (mainly for South Atlantic Anomaly), file name convention change for WMO style BUFR files
6.0	1.11	1.28	20140617 11:56	Update of L1 processor
6.0	1.12	1.32	20150223 10:17	Upgrade of L2 processor. OPF version 4.01. Use of temperature and potential vorticity as an indicator for the tropopause. Lower limit of valid temperature range from 150K down to 100K. Cloud Fraction max to 1.06 due to regular FRESCO overshoots in L1b. Internal naming of spectral windows Band-->COADDED in case of (averaging to) B1a footprint. Bugfixes: array inversion in temperature field.
6.0	1.12	1.33	20150528 hh:m	Upgrade of L2 software. Addition of ProductID and DOI identifiers in MetaData. This software upgrade does not affect the ozone profile product.
6.1	1.12	1.33	20150625 hh:mm	Update of L1 processor.

11. TRACEABILITY OF METADATA TO UMARF PARAMETERS

The UMARF metadata parameters [AD3] which are applicable to the O3MSAF products are stored in the HDF5 file as attributes in the Metadata group. The tracing of UMARF parameters to the attributes in the product file is shown in the following table. The attributes can have only values which are allowed by UMARF.

UMARF Short Name	Attribute Name	Notes
AARF	N/A	Archive Facility; not included in the product file, provided to UMARF by archive software
ABID	N/A	Spectral Band IDs; N/A for this O3M product
AENV	SourceEnvironment	
AIID	InstrumentID	
APAS	N/A	Product Actual Size; not included in the product file, provided to UMARF by archive software
APNA	N/A	Unique product identifier used in the O3M SAF archive; not included in the product file, provided to UMARF by archive software
APNM	ProductType	
APPN	ParentProducts	
APXS	PixelSize	
ASTI	SatelliteID	
AVBA	BaseAlgorithmVersion	
AVPA	ProductAlgorithmVersion	
GDMD	(TBD)	Disposition Mode
GGTP	GranuleType	
GNFV	ProductFormatVersion	
GNPF	ProductFormatType	
GNPO	N/A	Native Pixel Order; N/A for O3M
GNSP	N/A	Number of Spectral Bands; N/A for O3M
GORT	OrbitType	
GPLV	ProcessingLevel	
GPMD	ProcessingMode	

UMARF Short Name	Attribute Name	Notes
LLAE	SubSatellitePointEndLat	
LLAS	SubSatellitePointStartLat	
LLOE	SubSatellitePointEndLon	
LLOS	SubSatellitePointStartLon	
LMAP	N/A	Map Projection; N/A for O3M
LONE	N/A	End Orbit Number; N/A for O3M
LONS	StartOrbitNumber	
LSCD	SpatialCoverageModel	
LSVT	AscNodeCrossingTime	Ascending Node Crossing Date and Time ; N/A for O3M
LSVT	AscNodeLongitude	Ascending Node Longitude
OCLA	N/A	Occultation Latitude (TBC) ; N/A for O3M
OCLO	N/A	Occultation Longitude (TBC) ; N/A for O3M
OCSA	N/A	Occultation Satellite ID (TBC) ; N/A for O3M
OCTM	N/A	Occultation Date and Time (TBC) ; N/A for O3M
PPDT	N/A	Processing Start Date and Time; N/A for O3M
PPRC	ProcessingCentre	
PPST	ProcessingTime	Processing End Date and Time
QCCV	N/A	Cloud Coverage; N/A for O3M
QDLC	MissingDataCount	
QDLP	MissingDataPercentage	
QDRC	DegradedRecordCount	
QDRP	DegradedRecordPercentage	
QQAI	QQAI	
QQOV	OverallQualityFlag	
RRBT	N/A	Reception Start Date and Time; N/A for O3M
RRCC	ReceivingCentre	
RRST	N/A	*Ibid.* End Date and Time; N/A for O3M
SMOD	InstrumentMode	
SNIT	ReferenceTime	A reference time mainly used for the product file names.
SSBT	SensingStartTime	

UMARF Short Name	**Attribute Name**	**Notes**
SSST	SensingEndTime	
UDSP	DispositionFlag	
UUDT	N/A	Ingestion Date and Time; N/A for O3M

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