Product User Manual

NRT, Offline and Data Record Vertical Ozone Profile and Tropospheric Ozone Column Products

EUMETSAT
AC SAF
ATMOSPHERIC COMPOSITION MONITORING

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Date	Issue	Pages affected	Description
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20191101	2.1.1	Sect 4.8	Added section explaining the continuous dissemination of data with failed flags in case of degraded L1b data.
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20200617	2.2.0	Sect 10.3	Instrument specific issues: added section related to use of certain rows of the G2C tropospheric column and vertical ozone profile product.
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20210209	2.3.0	Chapter 10, Table 12.1	Updates to 'Related product list'. Updates to instrument specific issues and the processor history.
20210421	2.4.0	Page 2; Chapter 12	Update of temporal coverage of O3M-112 in 'Related product list'. Updated text explaining that temporal changes listed in the processor history apply to NRT and Offline products, not to DR products.
20211001	2.5.0	Chapter 7; Section 12.1	First addition of the NetCDF product format definition for O3M-112 and other reprocessed products. Updated processor history.
20220225	2.5.1	Product list	Added version numbers for DR O3M-501 and O3M-550.
20221103	2.5.2	-	Small updates based on R2 Reprocessing RR.

Related product list

ID number	Product Descripion
O3M-38.1	NRT Ozone Profiles, high resolution (Metop-A)
O3M-47.1	NRT Ozone Profiles, high resolution (Metop-B)
O3M-311	NRT Ozone Profiles, high resolution (Metop-C)
O3M-39.1	Offline Ozone Profiles, high resolution (Metop-A)
O3M-48.1	Offline Ozone Profiles, high resolution (Metop-B)
O3M-312	Offline Ozone Profiles, high resolution (Metop-C)
O3M-112	Reprocessed Ozone Profiles in HR / R1 (based on R2 + NRT L1b) [2007–2018]
O3M-501	Reprocessed Ozone Profiles (based on R3 L1b + NRT L1b); Opera algorithm version: 2.10, software version: 2.11, output product format: 4.70.

O3M-550	Reprocessed Tropospheric Ozone (GOME-2A, B, C, based on O3M-501); Opera algorithm version: 2.10, software version: 2.11, output product format: 4.70.

Contents

Chapter 1

Introduction

1.1 Purpose of this document

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 Atmospheric Composition Monitoring (AC 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 AC SAF. This product user manual document does not go into much detail with regard to the algorithm or design of the software; For information on the algorithm, please refer to the Algorithm Theoretical Basis Document (ATBD) [*Tuinder et al.*, 2017].

1.3 Heritage

This algorithm and the software implementation was developed by KNMI (the Royal Netherlands Meteorological Institute) with contributions by ESA projects (such as CHEOPS-GOME and the Ozone Climate Change Initiative (O3-CCI)), and EUMETSAT projects (GOME-2-Tools, UVN-Tools) and the Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring (O3M SAF), renamed to Atmospheric Composition Monitoring SAF (AC SAF) as of March 2017 at the beginning of CDOP-3.

1.4 Glossary

1.4.1 Acronyms and abbreviations

Table 1.1: Acronyms and abbreviations

AAI	Absorbing Aerosol Index
ACSAF	Atmospheric Composition Monitoring SAF
ATBD	Algorithm Theoretical Basis Document
BOA	Bottom of Atmosphere
B & P	Bass and Paur [*Bass and Paur*, 1985]
BW	Birk and Wagner (2018)
CHEOPS	Climatology of Height-resolved Earth Ozone and Profiling Systems
CR	Coarse Resolution
CVF	Calibration/Validation Facility
DAK	Doubling-Adding KNMI
DFS	Degrees of Freedom for Signal
DPM	Detailed Processing Model
ECMWF	European Centre for Medium-range Weather Forecast
EPS	EUMETSAT Polar System
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(-1)	Global Ozone Monitoring Instrument (1) (on ERS-2)
GOME-2	Global Ozone Monitoring Instrument 2 (on Metop)
HDF	Hierarchical data Format
HR	High Resolution
IPA	Independent Pixel Approximation
IPA-Lamb	IPA- Lambertian
IPA-Scat	IPA- scattering layer
IR	Infrared
ISD	Interface Specification Document
KNMI	Royal Netherlands Meteorological Institute
LABOS	LAyer Based Orders of Scattering
LIDORT	LInearized Discrete Ordinate Radiative Transfer
LUT	Look Up Table
MDR	Measurement Data Record

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Table 1.1 – *Continued from previous page*

MetOP	Meteorological Operational satellite
MLL	McPeters, Labow, Logan
MSC	Main Science Channels
NHP	NRT High resolution ozone Profile
NOP	NRT Ozone Profile (in coarse resolution)
NRT	Near Real Time
NTO	NRT Total Ozone
O3MSAF	Satellite Application Facility on Ozone Monitoring
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
OPF	Output Product Format
PDU	Product Dissemination Unit
PGE	Product Generation Element
PMD	Polarisation Measurement Detectors
PSC	Polar Stratospheric Clouds
PUM	Product User Manual
RMS	Root Mean Square
RTM	Radiative Transfer Model
SAA	Solar Azimuth Angle
SAF	Satellite Application Facility
SAGE	Stratospheric Aerosol and Gas Experiment
SBUV	Solar Backscatter Ultra-Violet radiometer
SCIAMACHY	Scanning Imaging Absorption spectroMeter for Atmospheric CartograpHY
SRD	Software Requirements Document
StrOC	Stratospheric Ozone Column
SUM	Software User Manual
SW	Software
SZA	Solar Zenith Angle
TBA	To Be Added
TBC	To Be Confirmed
TBD	To Be Defined
TOA	Top Of Atmosphere

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Table 1.1 – *Continued from previous page*

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

1.5 Applicable and Reference Documents

1.5.1 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

1.5.2 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 [*Rodgers*, 2000]
RD5	Algorithm Theoretical Basis Document for Opera, version 2.0.1, dated 2018-11-15, or later version. [*Tuinder et al.*, 2017]

Chapter 2

Introduction to EUMETSAT Satellite Application Facility on Atmospheric Composition Monitoring (AC 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 the 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 an important activity for EUMETSAT and the world-wide scientific community.

2.2 Objectives

The main objectives of the AC SAF are to process, archive, validate and disseminate atmospheric composition products (O_3, NO_2, SO_2, OClO, HCHO, BrO, H_2O), aerosols and surface ultraviolet radiation utilising the satellites of EUMETSAT. The majority of the AC SAF products are based on data from the GOME-2 spectrometer and the IASI interferometer onboard Metop satellite series. Another important task of the AC SAF is the research and development in radiative transfer modelling and inversion methods for obtaining long-term, high-quality atmospheric composition products from the satellite measurements.

2.3 Product families

The AC SAF products are grouped into different families: total columns of trace gases, vertical profiles of trace gases, aerosol products and land surface products and UV dose products. An overview is given Table 2.1

Table 2.1: AC SAF Product families

Near real-time	Total Columns: O_3, NO_2, O_3Tropo, NO_2Tropo, SO_2
	Vertical Profiles: Vertical Ozone Profile
	UV Index
	Absorbing Aerosol Index, ash
Offline	Total Column: O_3, NO_2, O_3Tropo, NO_2Tropo, SO_2, BrO, H_2O, HCHO, OClO
	Vertical Profiles: Vertical Ozone Profile
	UV Index
	Absorbing Aerosol Index
Data Record	Total Column: O_3, NO_2, O_3Tropo, NO_2Tropo, SO_2, BrO, H_2O, HCHO, OClO
	Vertical Profiles: Vertical Ozone Profile
	UV Index
	Absorbing Aerosol Index
	Lambertian Equivalent Reflectivity

2.4 Product timeliness and dissemination

Data products are divided in a few categories depending on how quickly they are available to users. See Table 2.1:

- Near real-time products: these are available in less than three hours after measurement. These products are disseminated via EUMETCast (such as NHP, NTO, NAP), the GTS (also NHP, NTO) or the internet (like NUV).
- Offline products: these are available within two weeks from the measurement and they are archived at the AC SAF archives at the Finnish Meteorological Institute (such as OHP, OUV, ARP) and the German Aerospace Center (such as OTO and related total columns). The products can be ordered via the EUMETSAT Data Centre (EDC).
- Data records: these products are 'static' in the sense that they cover a certain period and are produced once and are not updated as more data comes in. These products can be superseded by more recent versions. The Data Record products can also be ordered via the EUMETSAT Data Centre (EDC).

Products with "pre-operational" or "operational" status are disseminated to users. The up-to-date status of all the AC SAF products and ordering info is available on the AC SAF website.

2.5 Further information

Information about the AC SAF project in general, its NRT, Offline or Data Record products and its services can be found on the AC SAF website: http://acsaf.org/

The AC SAF Helpdesk can be contacted via: helpdesk@acsaf.org

Chapter 3

Platforms and Instruments

3.1 Metop and GOME-2

3.1.1 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.

Currently three EPS Metop satellites (Metop-A (launched 2006), Metop-B (lauched 2012) and Metop-C (lauched 2018)) fly in a sun-synchronous polar orbit at an altitude of about 840 km, circling the planet 14-15 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 (depending on the position of the satellites in the orbital plane).

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

3.1.2 GOME-2

The Metop satellite carries a number of instruments including the Global Ozone Monitoring Experiment-2 (GOME-2). This instrument is designed to measure the total columns and vertical profiles of atmospheric trace gases, such as ozone, and the distribution of other key atmospheric constituents (such as aerosols). GOME-2 is a nadir viewing across-track scanning spectrometer with a maximum 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

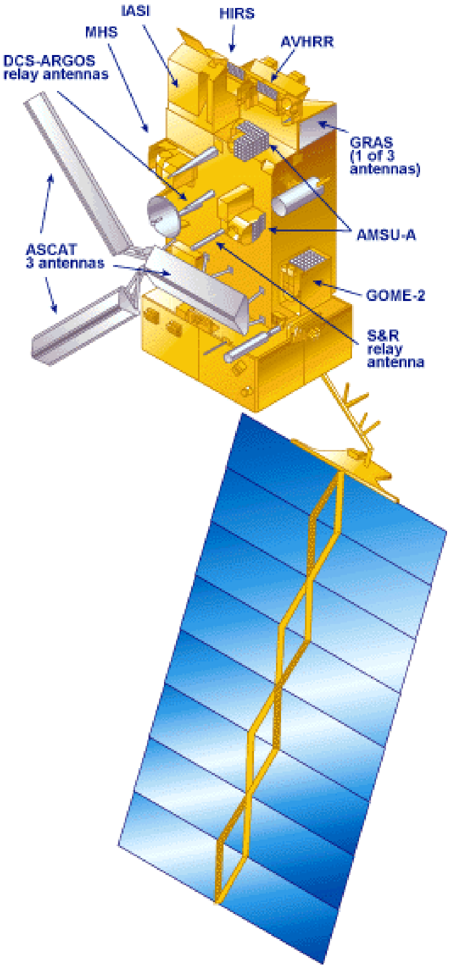

Figure 3.1: Metop

mechanism which scans across the satellite track with a maximum scan angle that can be varied, with three multi-spectral sets of samples (integration times) per scan. The ground pixel size of GOME-2 is usually 80 x 40 km^2 for the shortest integration times, but is usually 8 times larger for the detector measuring the shortest UV wavelengths (Band 1a), as was the case for its predecessor GOME-1.

Figure 3.2: GOME-2

Table 3.1: Default GOME-2 properties

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)

3.2 Other instruments

The ozone profile product generated by the Opera algorithm can be retrieved from other instruments as well, such as GOME-1, SCIAMCHY and OMI. This document may contain references and particular details from these instruments for legacy and comparison purposes.

Chapter 4

The Ozone Profile Retrieval 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 and 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 of GOME-1 and 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 example, for GOME-1 this means that two full scan mirror sweeps, each comprising of 4 ground pixels, must be averaged to reach the same surface footprint as the band 1a measurement in the set which has a 12 sec integration time. For GOME-2 this means that typically eight pixels of bands 1b-2b are averaged.

In short:

- GOME-1: 1 band 1a pixel (12 s) is combined with 8 band 1b-2b pixels (1.5 s)
- 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 0.001 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 AC SAF 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

The NRT ozone profile product in high resolution (NHP) has a nominal surface footprint of 40 x 80 km per ground pixel and has 24 pixels in the forward scan direction. The 8 back scan pixels are skipped (not retrieved and not stored).

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 AC SAF archive. Both the coarse and the high resolution NRT products are assembled separately into orbits. 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 0.001 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 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 500 hPa 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 (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 product (OHP) 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 product (historical, up to June 2017) 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.

4.8 Processing of degraded Level 1b data

The processor reads the Level-1 input data sequentially and makes an assessment on the data quality as it goes through the scans. If data is degraded or invalid or incomplete to the point where it is unusable (like when the error on the solar spectrum was set to zero during one of the GOME-2A Solar Gaps in 2018), then the L2 processor will flag this pixel, store it in the output, and move on to the next possible ground pixel / profile retrieval. This may lead to an L2 output product where all data is flagged but nevertheless disseminated to users.

4.9 Considerations for trend studies

With the upgrade to software version 2.x of the ozone profile product, an instrument dependent correction on the measured reflectance is applied to compensate for the degradation of the instrument (i.e. the consolidated changes in all the components in the optical path, including the detectors). The correction is based the difference between the measured reflectance and the simulated reflectance for similar situations where the ozone profile comes from an ozone climatology [*McPeters et al.*, 2013]. This means that the reflectance – on average – is brought back to the ozone amount and shapes in the reference climatology. This limits its use for trend studies of global ozone amounts.

Chapter 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.

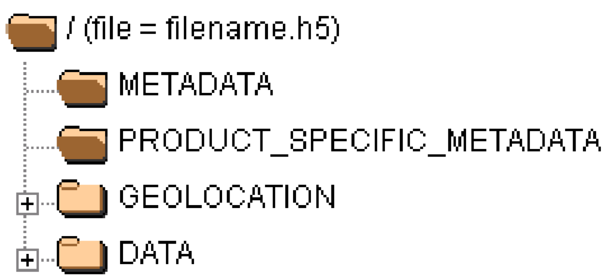

Figure 5.1: Structure of the HDF5 file.

The Metadata group contains parameters about the satellite instrument required by UMARF [AD3], such as metadata given in the AC SAF 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 below.

The geolocation information of each ground pixel can be found in Geolocation group. It contains all information such as corner and centre coordinates. See Figure 5.2 and Figure 5.3 for the definition of the seven points of the ground pixel.

The calculated results are stored in the Data group. It contains information about the quality of the retrieval,

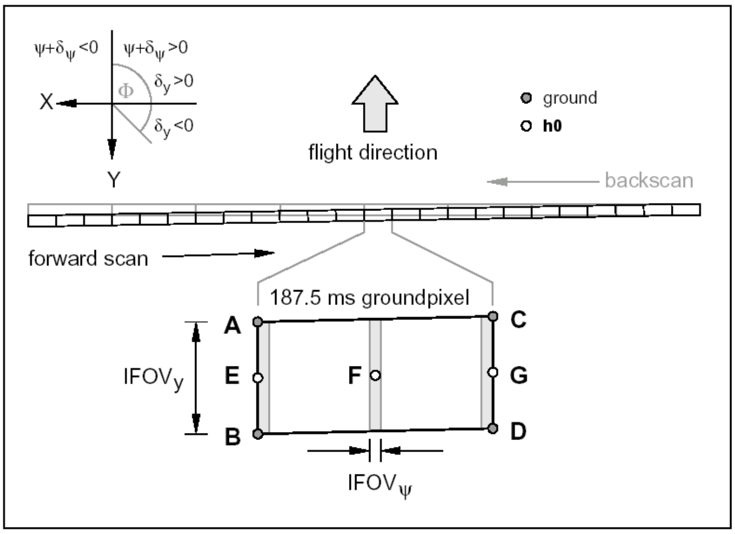

Figure 5.2: Ground pixel geometry (ref: [RD3])

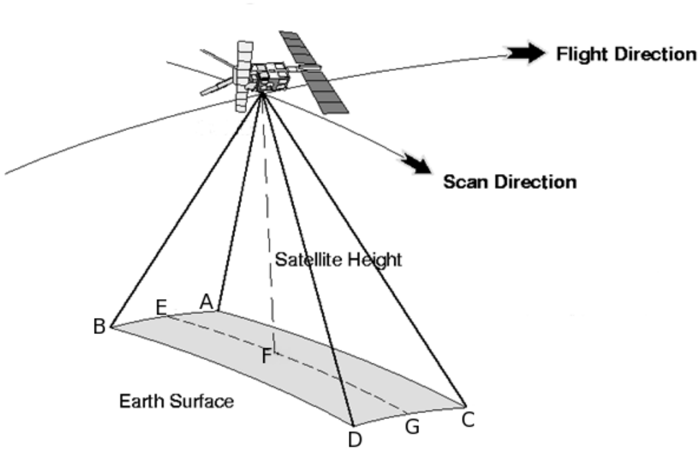

Figure 5.3: Ground pixel geometry (ref: [RD3])

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 5.4.

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 $\times$ MaxState. However, an individual retrieval may not use all of these MaxState elements. The real number of its retrieval parameters can be found

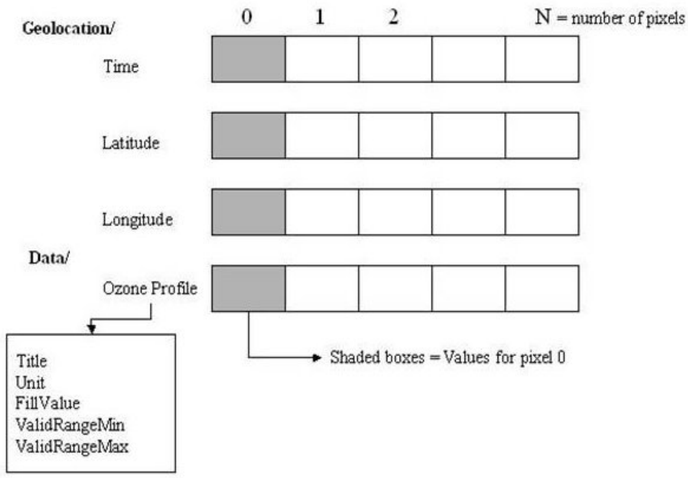

Figure 5.4: Organization of the pixel data in HDF5 file

in DATA/NState (hence NState $\leq$ MaxState). Finally, of all the Nstate parameters, NOutputlayers parameters are used for the ozone profile.

For products generated with output product format versions before 4.60, NProfiles was not present, and the size of IndexInScan or Time can be taken instead.

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 5.5).

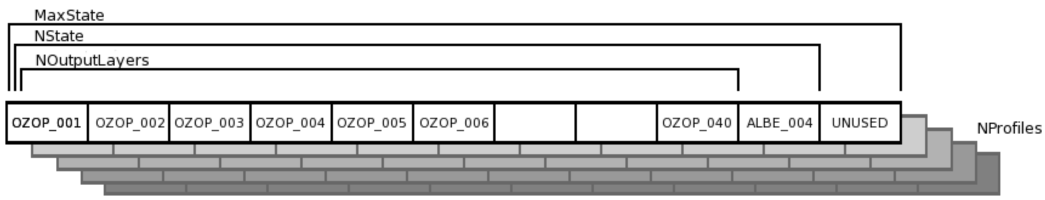

Figure 5.5: The definition of the state vector within the output product

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 5.1: 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 CCSDS 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 data.	O3KNM or other String
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.	2
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

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Table 5.1 – *Continued from previous page*

Attribute name	**Data Type**	**Description**	**Allowed values**
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 first complete scan start point (tbd), at start of dataset.)	-90 to 90
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

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Table 5.1 – *Continued from previous page*

Attribute name	**Data Type**	**Description**	**Allowed values**
MissingDataPercentage	int	Percentage of Earthshine MDR records skipped by L2 software due to time breaks or other data requirements, w.r.t total number of read Earthshine MDRs.	0 - 100
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	Float	Ascending Node Longitude	String containing a float.
ProductID	String	Product identifier, as per the AC SAF 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 re-processed product: 10.15770/EUM_SAF_O3M_0003
ConfigurationFileVersion	Float	Configuration file version	e.g. 2.00
Inclination	Float	Inclination of the orbit with respect to the Earth's axis of rotation	e.g.: 98.698
ProjectID	String	Project Identifier	e.g.: O3M, or other string
ShortProductName	String	Short Product Name	e.g.: NHP
RevisionID	String	Revision Identifier	e.g.: R2

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 5.2: Product Specific Metadata group contents.

Attribute name	**Level1 usage section** **Data Type**	**Description**
NWindows	Int	Number of spectral windows
WindowMin	Float array, rank 1	Minimum wavelength of windows [nm]; 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
Attribute name	**Atmosphere and Surface Model Section** 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)

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Table 5.2 – *Continued from previous page*

Attribute name	**Data Type**	**Description**
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)

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Table 5.2 – *Continued from previous page*

Attribute name	**Data Type**	**Description**
RTMFlags	Int array, rank 1, size 8	Radiative 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 are 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. UseConCritCost (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 on which output profile is given

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Table 5.2 – *Continued from previous page*

Attribute name	Data Type	Description
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
NProfiles	Float	Number of profiles in the product

5.1.3 Table Attibutes

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

Table 5.3: 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 5.2 and Figure 5.3.

Table 5.4: Geolocation group contents.

Dataset name	Data Type	Unit	Description
Time	String arr rank 1	-	UTC time in CCSDS format
EndUTCTime	String arr 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
Latitude_B	Float arr rank 1	degree	Latitude of corner B of the pixel

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Table 5.4 – *Continued from previous page*

Dataset name	**Data Type**	**Unit**	**Description**
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 rank 1	degree	Geodetic latitude of subsatellite point
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.

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Table 5.4 – *Continued from previous page*

Dataset name	Data Type	Unit	Description
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
ScannerAngle	Float arr, rank 1	degree	Angle of the scanner mirror
AnglesReferenceHeight	Float arr, rank 1	km	Height at which the angles are given

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 5.5: Data group contents, Quality section.

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 1. Non-nominal level 1 due to instrument degradation; DEGRADED_INST_MDR in Level1b [RD1]) 2. Non-nominal level 1 due to processing degradation; DEGRADED_PROC_MDR in Level1b [RD1] 3. Groundpixel is in SAA; F_SSA in Level1b / PCD_BASIC [RD1] 4. Sunfile of date missing: older sunfile used 5. Meteo forecast file missing: climatological meteo data used 6. Meteo forecast data missing: climatological meteo data used 7. Meteo forecast data invalid 8. Earthshine radiance data missing 9. Earthshine radiance data invalid 10. Solar irradiance data missing

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Table 5.5 – *Continued from previous page*

Dataset name	**Data Type**	**Unit**	**Description**
			11. Solar irradiance data invalid 12. Measurement data invalid 13. Auxiliary data invalid 14. Absorbing Aerosol Index data invalid 15. Failure in setup of the Forward Model Input 16. Failure in State vector definition setup 17. Sunglint flag 18. Cloud fraction forced to zero 19. Cloud Pressure Adjusted to Surface Pressure 10. Other error 21 - 32: 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. 1. Overall Convergence was reached (indicates successful retrieval) 2. Convergence reached on Cost 3. Convergence reached on State 4. Convergence not reached after maximum number of iterations 5. Out of bound retrieval values 6. Too high values for Chi Square 7. No retrieval done! (due to incorrect inputs or other reasons). 8 - 32: reserved for future use

Table 5.6: Data group contents, Auxiliary section.

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 NProfiles
AltitudeProfile	Float arr, rank 2	km	Altitudes of OutputPressureGrid above sea level, Dimension = (NOutputLayers + 1) x NProfiles
TemperatureProfile	Float arr, rank 2	K	Average temperature of layers, Dimension = NOutputLayers x NProfiles
CloudPressure	float arr, rank 1	hPa	Cloud top Pressure
CloudFraction	float arr, rank 1	-	Cloud fraction
CloudAlbedo	float arr, rank 1	-	Cloud albedo
SurfaceAlbedo	Float arr, rank 1	-	Surface albedo;

Table 5.7: Data group contents, State Vector Definition section.

State Vector Definition Section **Dataset 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 NProfiles (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 NProfiles (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 NProfiles (of which NState (i) elements are used for each retrieval 'i')

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Table 5.7 – *Continued from previous page*

Dataset name	Data Type	Unit	Description
AprioriValueSource	String arr, rank 2	N/A	Source of apriori value of state vector element (e.g. for O3: FK=Fortuin/Kelder [*Fortuin and Kelder*, 1998], ML=McPeters/Labow [*McPeters et al.*, 2007], ML2012=McPeters/Labow [*McPeters et al.*, 2013], TOMSv8,) Dimension = MaxState x NProfiles (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 NProfiles (of which NState (i) elements are used for each retrieval 'i')
AprioriCovarianceSource	String arr, rank 2	N/A	Source of apriori error covariance of (profile) state vector element (e.g., FixedCorrelation, ZeroCorrelation); Dimension = MaxState x NProfiles (of which NState (i) elements are used for each retrieval 'i')

Table 5.8: Data group contents, Retrieval Result Section.

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
CostChange	Float arr, rank 1	-	Cost change of the last iteration step
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 arr, rank 2	-	χ^2 (CostMeas per window) per window, Dimension = NWindows x NProfiles
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)

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Table 5.8 – *Continued from previous page*

Dataset name	**Data Type**	**Unit**	**Description**
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	-	Level index indicating the Tropopause selected from the TemperatureProfile and PV
TropopausePressure	Float arr, rank 1	hPa	Pressure of the tropopause level
TroposphericIntegratedProfile	Float arr, rank 1	DU	Tropospheric Integrated Vertical Ozone Profile from surface to the tropopause pressure (possibly partial top layer)
TroposphericIntegrated-ProfileError	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
StratosphericIntegrated-ProfileError	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 arr, rank 2	<StateUnit>	Retrieved values of State vector elements, transformed back to physical value using StateRel; Dimension = MaxState x NProfiles (of which NState (i) elements are used for each retrieval 'i')
StateRetrievedError	Float arr, rank 2	<StateUnit>	Errors of retrieved values of State vector elements, transformed back to physical value using StateRel; Dimension = MaxState x NProfiles (of which NState (i) elements are used for each retrieval 'i')
Apriori	Float arr, rank 2	<StateUnit>	Apriori values of State vector elements, transformed back to physical value using StateRel; Dimension = MaxState x NProfiles (of which NState (i) elements are used for each retrieval 'i')
AprioriError	Float arr, rank 2	<StateUnit>	Errors of apriori values of State vector elements, transformed back to physical value using StateRel; Dimension = MaxState x NProfiles (of which NState (i) elements are used for each retrieval 'i')

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Table 5.8 – *Continued from previous page*

Dataset name	**Data Type**	**Unit**	**Description**
AprioriErrorCovariance	Float arr, rank 3	<StateUnit>	Apriori Error Covariance Matrix ; Dimension = MaxState x MaxState x NProfiles (of which NState(i) x NState(i) x NProfiles elements are used foreach retrieval 'i')
ErrorCovarianceTotal	Float arr, rank 3	<StateUnit>	State Covariance Matrix, including smoothing error [RD4] ; Dimension = MaxState x MaxState x NProfiles (of which NState(i) x NState(i) x NProfiles 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 NProfiles (of which NState(i) x NState(i) x NProfiles elements are used foreach retrieval 'i')
AveragingKernel	Float arr, rank 3	-	Averaging Kernel Matrix [RD4]; Dimension = Dimension = MaxState x MaxState x NProfiles (of which NState(i) x NState(i) x NProfiles elements are used foreach retrieval 'i')
AltitudeProfile_Raw	Float arr, rank 2	Km	Altitude values associated with raw temperature profile
PressureProfile_Raw	Float arr, rank 2	hPa	Pressure values associated with raw temperature profile
TemperatureProfile_Raw	Float arr, rank 2	K	'Raw' Temperature profile, from the external data source. Usually in higher resolution than the temperature profile in the RTM model.
IntegratedVerticalProfile-SurfaceTo500hPa	Float arr, rank 1	DU	Integrated vertical ozone profile from the surface to the 500hPa pressure level
IntegratedVerticalProfile-ErrorSurfaceTo500hPa	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)

Table 5.9: Data group contents, Optional output (may not be present in your output product)

Optional Output Section Dataset name	Data Type	Unit	Description
FailReasonFlag	Int arr, rank 2	-	Indicator giving the reason that spectral pixels have been flagged. Undetermined = -9 OK = 0 L1b_Radiance = 1 L1b_RadianceErr = 2 L1b_Irradiance = 3 L1b_IrradianceErr = 4 Reflectance_LT_Zero = 5 SAA = 6 SunDivZero = 7 Blackout = 8 Unknown = 9 EarthshineErrorFlags = 10
Fraunhofer_Correction_Value	Float arr, rank 1	-	Spectral correction value based on a Fraunhofer line. Can be used as a reference for the spectral offset.
NWP_Model_O3_DU	Float arr, rank 2	-	Ozone profile from an NWP model
Wavelength	Float arr, rank 2	Nm	Wavelength of the spectral information
Measurement	Float arr, rank 2	-	Sun Normalised Reflectance (SNR) = Earthshine / Solar Irradiance
MeasurementErr	Float arr, rank 2	-	Error on the SNR
Simulation	Float arr, rank 2	-	Simulated SNR
SimulationErr	Float arr, rank 2	-	Error on the simulated SNR
SpectralMask	Float arr, rank 2	-	Array indicating which spectral pixels are taken into account in the OE inversion step

5.2 Data Types

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

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 GOME-2, these are foreseen as having the following layout for the HDF5 format files: S-O3M_GOME_OHP_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, and on Metop-C this number is M03. 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 OHP indicates the high resolution offline ozone profile product. Note that these three letters are replaced by NHP for the Near Real Time products.

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 archived historical coarse resolution offline ozone profile 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 (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.

Chapter 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 [*W.M.O.*, 1995] 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) 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 5.2 and 5.3 for the definition of the coordinates and angles of the ground pixel.

6.2 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
```

6.3 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 O3 DENSITY
 31  010002  HEIGHT
 . . .
100  007004  PRESSURE
101  007004  PRESSURE
102  015020  INTEGRATED O3 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 O3 DENSITY
. . .
205  015020  INTEGRATED O3 DENSITY
```

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

$$\begin{aligned} IntegratedOzoneDensity(i) &= DU\_per\_Layer(i) * \\ &\quad DUToCm2/CM2ToM2\ / \\ &\quad N_A * M_{O3}/1000.0 \quad [KG/M^2] \end{aligned} \tag{6.1}$$

Where:

- M_{O3} Molecular Mass Ozone in: grams / mole: M_{O3} = 47.9982
- N_A Avogadro's number: N/Mole: N_A = 6.02205E23
- Const in: Col[cm^2] = 2.69E16 * col[DU]: = number of molecules per cm^2
- DUToCm2 = 2.68668E16
- CM2ToM2 = 1.0E-4

6.4 File name conventions

File names of NHP product disseminated via EUMETCast are following the names of the input files. For GOME-2, these are foreseen as having the following layout for the BUFR format files:

- S-O3M_GOME_NHP_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 disseminated via the GTS 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.

6.5 File size estimate

6.5.1 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. The NHP high resolution BUFR file is smaller than 350Kb per 720 retrievals.

Chapter 7

Product format definition of the offline ozone profile product in NetCDF

7.1 Format

Below is a short description of the NetCDF output product. Given are the global attributes, the metadata attributes, the dimensions, and the data sets in the various groups. The details of the variables / data sets are can be looked up in Chapter 5 where the HDF5 product is described.

The NetCDF product is also linear in terms of profile sequence, similar to the HDF5 product. This means that for a normal PDU, there are 30 x 32 = 720 ground pixels. Due to compatibility with other products, the variable 'scanline' is the dimension running along the sequence of ground pixels.

As an example, a converted PDU is used here as an example, so the actual values are specific to that particular product file.

```
// global attributes:
:source = "S-O3M_GOME_NHP_02_M01_20210521121158Z_20210521121458Z_N_O_20210521132
:refrences = "http://www.acsaf.org";
:comment = "This product was produced by KNMI within the scope of the EUMETSAT/A
:Conventions = "CF-1.7";
:title = "ACSAF NHP data file.";
:institution = "EUMETSAT / ACSAF / KNMI";
:history = "ACSAF/KNMI";

group: METADATA
  // group attributes:
  :AscNodeCrossingTime = "2021-05-21T11:33:01.000";
  :AscNodeLongitude = "149.3280";
  :BaseAlgorithmVersion = "6.3";
  :ConfigurationFileVersion = "2.02";
  :DOI = "Unknown";
  :DegradedRecordCount = 0; // int
  :DegradedRecordPercentage = 0; // int
```

```
    :DispositionMode = "O";
    :GranuleType = "DP";
    :Inclination = 98.712f; // float
    :InstrumentID = "GOME";
    :InstrumentMode = "NORMAL_VIEW";
    :MissingDataCount = 0; // int
    :MissingDataPercentage = 0; // int
    :OrbitType = "LEO";
    :OverallQualityFlag = "NOK";
    :ParentProducts = "GOME_xxx_1B_M01_20210521121158Z_20210521121458Z_N_O_2021052
    :ProcessingCentre = "O3KNM";
    :ProcessingLevel = "02";
    :ProcessingMode = "N";
    :ProcessingTime = "2021-05-21T13:25:54.410";
    :ProductAlgorithmVersion = "2.02";
    :ProductFormatType = "NC/KNMI";
    :ProductFormatVersion = 1.0; // double
    :ProductID = "O3M-47.1";
    :ProductSoftwareVersion = "2.08";
    :ProductType = "O3MNHP";
    :ProjectID = "O3M";
    :QualityInformation = "Input_failure";
    :ReceivingCentre = "SVL";
    :ReferenceTime = "2021-05-21T12:11:58.000";
    :RevisionID = ".1";
    :SatelliteID = "M01";
    :SensingEndTime = "2021-05-21T12:14:58.000";
    :SensingStartTime = "2021-05-21T12:11:58.000";
    :ShortProductName = "NHP";
    :StartOrbitNumber = 45005; // int
    :SubSatellitePointEndLat = 30.568f; // float
    :SubSatellitePointEndLon = -36.013f; // float
    :SubSatellitePointStartLat = 41.071f; // float
    :SubSatellitePointStartLon = -32.793f; // float
    :datetime = "2021-05-21 12:11:58";
    :ProductFormatDate = 20210611L; // long

  group: PRODUCT_SPECIFIC_METADATA
    // group attributes:
    :AddedRadianceError = 0.01f; // float
    :AddedRadianceErrorCorrelationLength = -9999.0f; // float
    :AerosolSource = "NONE";
    :AlbedoSource = "LER";
    :AtmosphereFlags = 1; // int
    :CloudAlbedoSource = "Level1b";
    :CloudFractionSource = "Level1b";
    :CloudPressSource = "Level1b";
    :CloudUsage = "IPA-lamb";
```

```
    :CoAddingAlongTrack = -1; // int
    :CoAddingCrossTrack = -1; // int
    :ConCritCost = 0.02f; // float
    :ConCritState = 0.02f; // float
    :DefaultOutputGrid = 1000.0f; // float
    :DefaultPressureGrid = 1000.0f; // float
    :GroundPixelBinning = "Band1bPixel";
    :InversionFlags = 0; // int
    :InversionMethod = "Optimal Estimation";
    :MaxNIter = 10; // int
    :NAtmosLayers = 40; // int
    :NOutputLayers = 40; // int
    :NProfiles = 720; // int
    :NStokes = 1; // int
    :NStreams = 4; // int
    :NWindows = 3; // int
    :RTM = "LidortA&PolLUT";
    :RTMFlags = 1; // int
    :Raman = "NONE";
    :SphericalCorrection = "Solar Viewing";
    :SurfacePressureSource = "terrainheight_derived";
    :TemperatureSource = "PG";
    :TerrainElevationSource = "Level1b";
    :Tracegasses = "O3";
    :TracegassesSource = "ML+BR4";
    :WindowBand = "COADDED 1a  ";
    :WindowMax = 284.0f; // float
    :WindowMin = 265.0f; // float

dimensions:
  int time(time=1);
  int scanline(scanline=720);
  int ground_pixel(ground_pixel=1);
  double wavelength(wavelength=700);
  int corner(corner=4);
  int flagindex(flagindex=32);
  int level(level=41);
  int layer(layer=40);
  int level_raw(level_raw=140);
  int layer_raw(layer_raw=139);
  int statevector(statevector=42);
  int window(window=3);

variables:
  float latitude(time=1, scanline=720, ground_pixel=1);
  float longitude(time=1, scanline=720, ground_pixel=1);
  int delta_time(time=1, scanline=720);
```

```
double Cost(time=1, scanline=720, ground_pixel=1);
double CostChange(time=1, scanline=720, ground_pixel=1);
double CostMeas(time=1, scanline=720, ground_pixel=1);
double CostState(time=1, scanline=720, ground_pixel=1);
double DFS(time=1, scanline=720, ground_pixel=1);
double DFS_Profile(time=1, scanline=720, ground_pixel=1);
int NIter(time=1, scanline=720, ground_pixel=1);
int NMeasurements(time=1, scanline=720, ground_pixel=1);
int NState(time=1, scanline=720, ground_pixel=1);
double Fraunhofer_Correction_Value(time=1, scanline=720, ground_pixel=1);
double IntegratedVerticalProfile(time=1, scanline=720, ground_pixel=1);
double IntegratedVerticalProfileError(time=1, scanline=720, ground_pixel=1);
double IntegratedVerticalProfileSurfaceTo500hPa(time=1, scanline=720, ground_pix
double IntegratedVerticalProfileErrorSurfaceTo500hPa(time=1, scanline=720, groun
double StateUpdate(time=1, scanline=720, ground_pixel=1);
double StratosphericIntegratedProfile(time=1, scanline=720, ground_pixel=1);
double StratosphericIntegratedProfileError(time=1, scanline=720, ground_pixel=1)
int QualityInput(time=1, scanline=720, flagindex=32);
int QualityProcessing(time=1, scanline=720, flagindex=32);
double Wavelength(time=1, scanline=720, wavelength=700);
double Measurement(time=1, scanline=720, wavelength=700);
double MeasurementErr(time=1, scanline=720, wavelength=700);
double Simulation(time=1, scanline=720, wavelength=700);
double SimulationErr(time=1, scanline=720, wavelength=700);
int SpectralMask(time=1, scanline=720, wavelength=700);
int FailReasonFlag(time=1, scanline=720, wavelength=700);
double AltitudeProfile(time=1, scanline=720, level=41);
double OutputPressureGrid(time=1, scanline=720, level=41);
double AltitudeProfile_Raw(time=1, scanline=720, level_raw=140);
double PressureProfile_Raw(time=1, scanline=720, level_raw=140);
double TemperatureProfile(time=1, scanline=720, layer=40);
double NWP_Model_O3_DU(time=1, scanline=720, layer=40);
double TemperatureProfile_Raw(time=1, scanline=720, layer_raw=139);
double Apriori(time=1, scanline=720, statevector=42);
double AprioriError(time=1, scanline=720, statevector=42);
double StateRetrieved(time=1, scanline=720, statevector=42);
double StateRetrievedError(time=1, scanline=720, statevector=42);
String AprioriErrorSource(time=1, scanline=720, statevector=42);
String AprioriValueSource(time=1, scanline=720, statevector=42);
String AprioriCovarianceSource(time=1, scanline=720, statevector=42);
String StateDef(time=1, scanline=720, statevector=42);
String StateRel(time=1, scanline=720, statevector=42);
String StateUnit(time=1, scanline=720, statevector=42);
double ChiSq(time=1, scanline=720, window=3);
double AprioriErrorCovariance(time=1, scanline=720, statevector=42, statevector=
double AveragingKernel(time=1, scanline=720, statevector=42, statevector=42);
double ErrorCovarianceNoise(time=1, scanline=720, statevector=42, statevector=42
double ErrorCovarianceTotal(time=1, scanline=720, statevector=42, statevector=42
```

```
group: SUPPORT_DATA
  group: INPUT_DATA
    variables:
      double CloudAlbedo(time=1, scanline=720, ground_pixel=1);
      double CloudFraction(time=1, scanline=720, ground_pixel=1);
      double CloudPressure(time=1, scanline=720, ground_pixel=1);
      int TropopauseLevel(time=1, scanline=720, ground_pixel=1);
      double TropopausePressure(time=1, scanline=720, ground_pixel=1);
      double TropopausePressure_PV(time=1, scanline=720, ground_pixel=1);
      double TropopausePressure_Thermal_Raw(time=1, scanline=720, ground_pixel=1);
      double TroposphericIntegratedProfile(time=1, scanline=720, ground_pixel=1);
      double TroposphericIntegratedProfileError(time=1, scanline=720, ground_pixel
      double SurfaceAlbedo(time=1, scanline=720, ground_pixel=1);

  group: GEOLOCATIONS
    variables:
      float latitude_bounds(time=1, scanline=720, ground_pixel=1, corner=4);
      float longitude_bounds(time=1, scanline=720, ground_pixel=1, corner=4);
      double DeltaTimes(time=1, scanline=720, ground_pixel=1);
      String Time(time=1, scanline=720, ground_pixel=1);
      String EndUTCTime(time=1, scanline=720, ground_pixel=1);
      int NrOfPixelsInScan(time=1, scanline=720);
      int IndexInScan(time=1, scanline=720, ground_pixel=1);
      double SubSatellitePointLatitude(time=1, scanline=720, ground_pixel=1);
      double SubSatellitePointLongitude(time=1, scanline=720, ground_pixel=1);
      double ScannerAngle(time=1, scanline=720, ground_pixel=1);
      int ScanDirection(time=1, scanline=720, ground_pixel=1);
      double LineOfSightZenithAngle_E(time=1, scanline=720, ground_pixel=1);
      double LineOfSightAzimuthAngle_E(time=1, scanline=720, ground_pixel=1);
      double SolarZenithAngle_E(time=1, scanline=720, ground_pixel=1);
      double SolarAzimuthAngle_E(time=1, scanline=720, ground_pixel=1);
      double LineOfSightZenithAngle_F(time=1, scanline=720, ground_pixel=1);
      double LineOfSightAzimuthAngle_F(time=1, scanline=720, ground_pixel=1);
      double SolarZenithAngle_F(time=1, scanline=720, ground_pixel=1);
      double SolarAzimuthAngle_F(time=1, scanline=720, ground_pixel=1);
      double LineOfSightZenithAngle_G(time=1, scanline=720, ground_pixel=1);
      double LineOfSightAzimuthAngle_G(time=1, scanline=720, ground_pixel=1);
      double SolarZenithAngle_G(time=1, scanline=720, ground_pixel=1);
      double SolarAzimuthAngle_G(time=1, scanline=720, ground_pixel=1);
      double RelativeAzimuthAngle_Quadrature(time=1, scanline=720, ground_pixel=1)
      double SatelliteAltitude(time=1, scanline=720, ground_pixel=1);
      double EarthRadius(time=1, scanline=720, ground_pixel=1);
      double AnglesReferenceHeight(time=1, scanline=720, ground_pixel=1);
```

7.2 File name convention

File names of product are following the names of the input files. For GOME-2, these are foreseen as having the following layout for the HDF5 format files: S-O3M_GOME_OHP_02_AAA_SSSS_EEEE_W_Z_PPPP.nc Where AAA is the flight model number. On Metop-A this number is M02, on Metop-B this number is M01, and on Metop-C this number is M03. 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 OHP indicates the high resolution offline ozone profile product. Note that these three letters are replaced by NHP for the Near Real Time products.

7.3 File size estimate

7.3.1 Estimated size of NetCDF 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 NetCDF output file.

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

Chapter 8

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.

8.1 The Ozone Profile Product

8.1.1 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 period
- 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.

8.1.2 Data Group

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

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 and indicates the boundaries of the layers (therefore: the grid has N+1 values compared to the number of layers). 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).

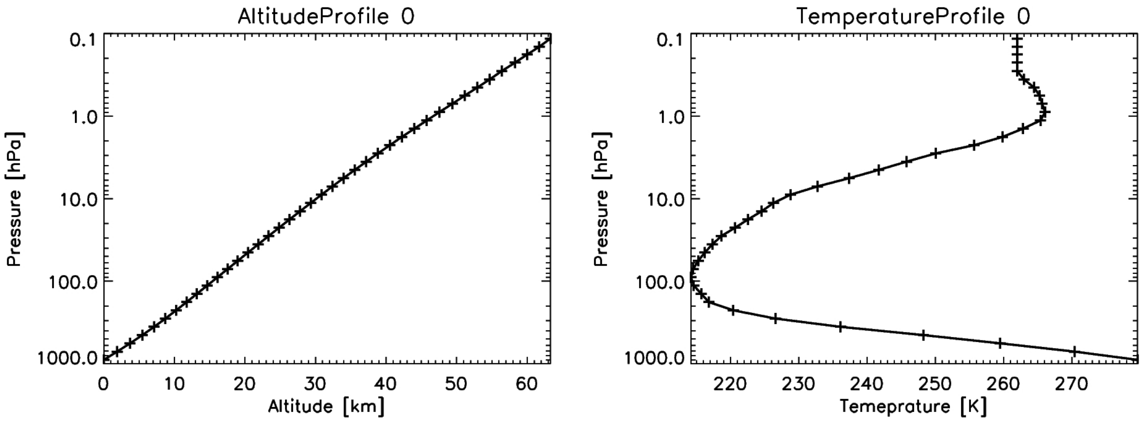

Figure 8.1: Relation between pressure and altitude and the temperature profile for an example retrieval.

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 climatologies or from previous retrievals. Initial cloud information comes from Level 1b for GOME-2 or from an internally implemented FRESCO cloud retrieval [*Koelemeijer et al.*, 2001] (such as 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.

Examples the vertical ozone profiles are shown in Figure 8.2 to Figure 8.4. In Figure 8.2 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 8.3 (A) and Figure 8.4 (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.

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.

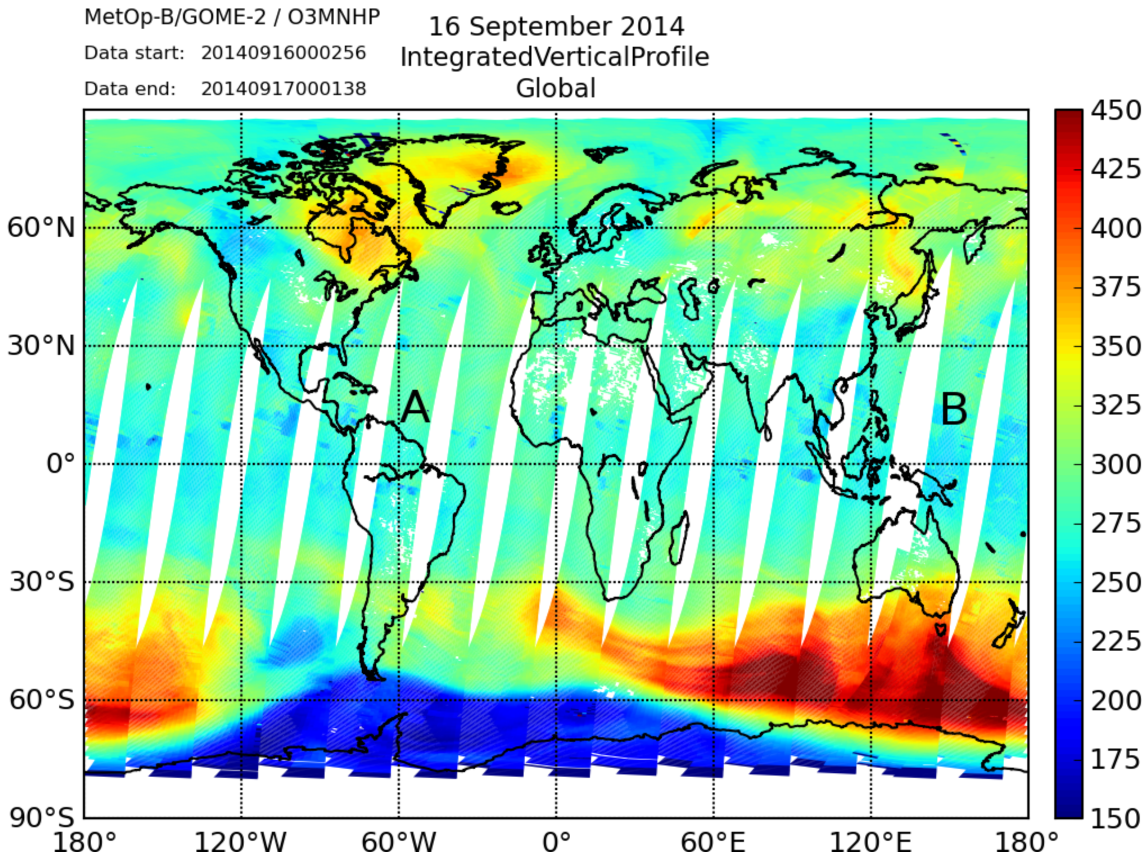

Figure 8.2: Total ozone column, calculated as the sum of the retrieved profile for September 16th 2014. Instrument: GOME-2B

The chosen climatology is indicated in these records. For ozone, the mnemonics FK indicates Fortuin and Kelder ([*Fortuin and Kelder*, 1998], ML indicates McPeters et al [*McPeters et al.*, 2007], 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 8.5.

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

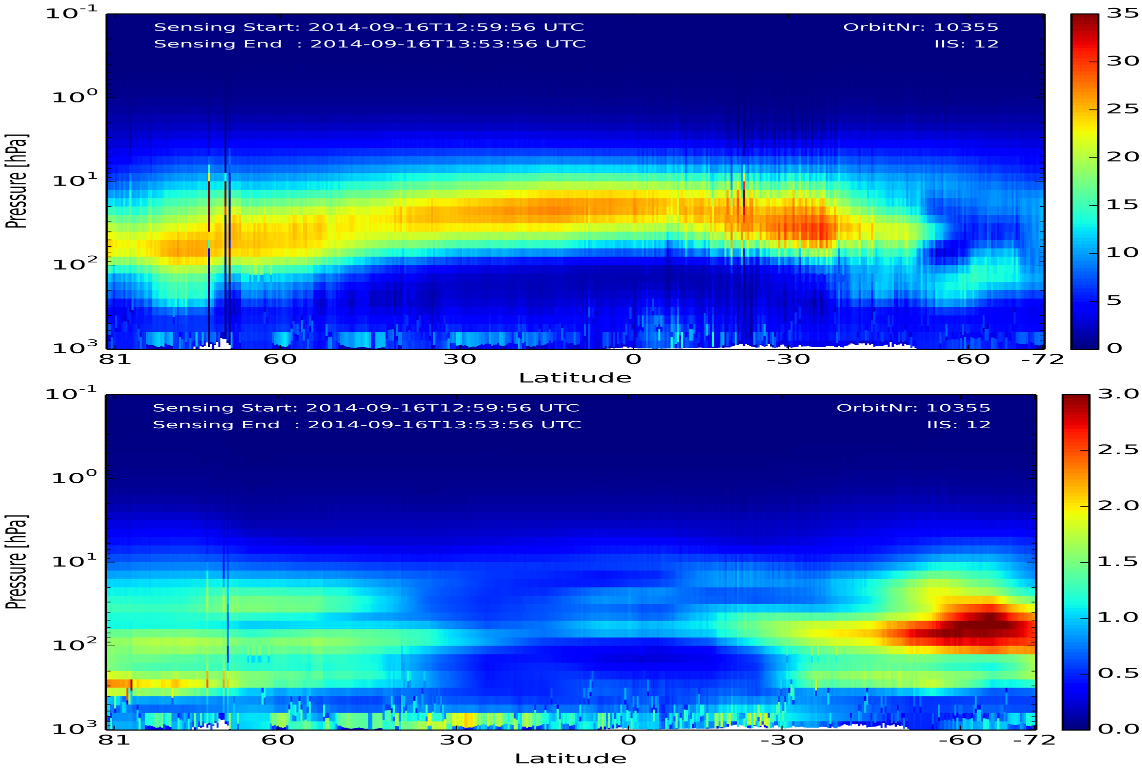

Figure 8.3: Retrieved ozone profile (top) and its retrieved error (bottom) for nadir swath in orbit 10355, indicated with letter (A). Instrument: GOME-2B

($\hat{x}$) to the true (x_{true}) and the a priori profile (x_a) according to:

$$\hat{x} - x_a = A(x_{true} - x_a) \tag{8.1}$$

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].

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 all 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). Further filtering (blacklisting) reduces the number of radiance elements even more. 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.

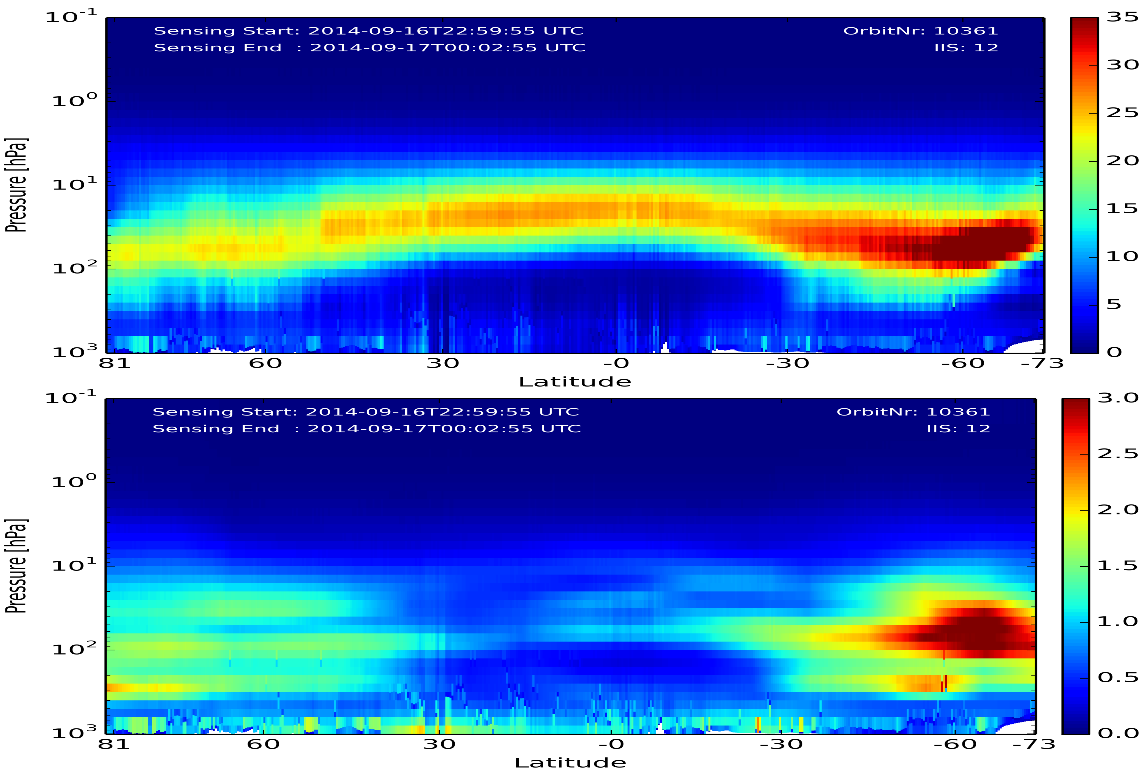

Figure 8.4: Retrieved ozone profile (top) and its retrieved error (bottom) for western swath of orbit 11361, indicated with letter (B). Instrument: GOME-2B

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 8.6. In this case, the Metop-B DFS ranges roughly between 3 to 4.5.

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.

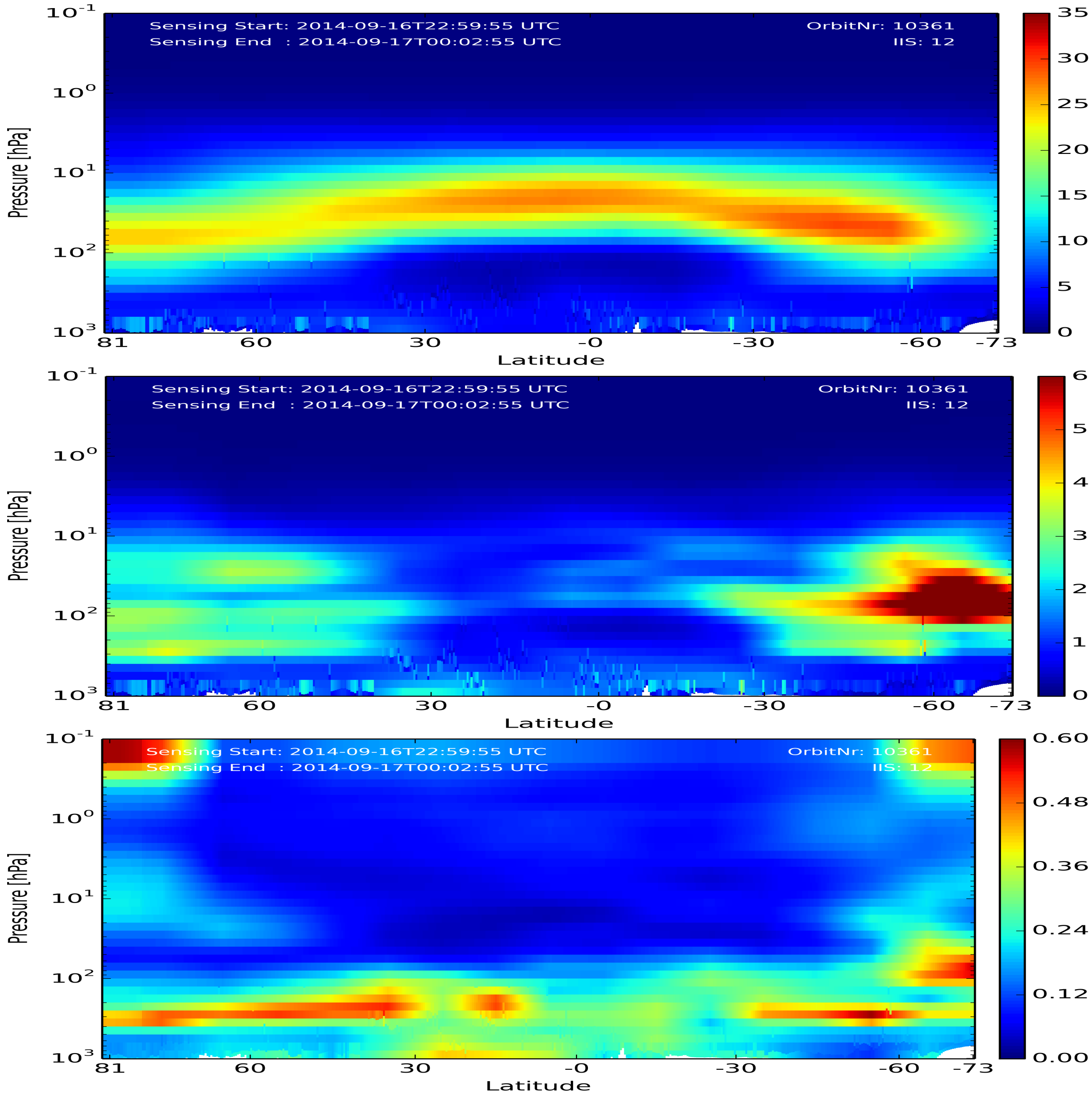

Figure 8.5: A priori ozone profile (top), its error (center) and relative error (bottom). The example refers to orbit 11361 (A) of GOME-2B

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 8.7, Figure 8.8 and Figure 8.9. 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.

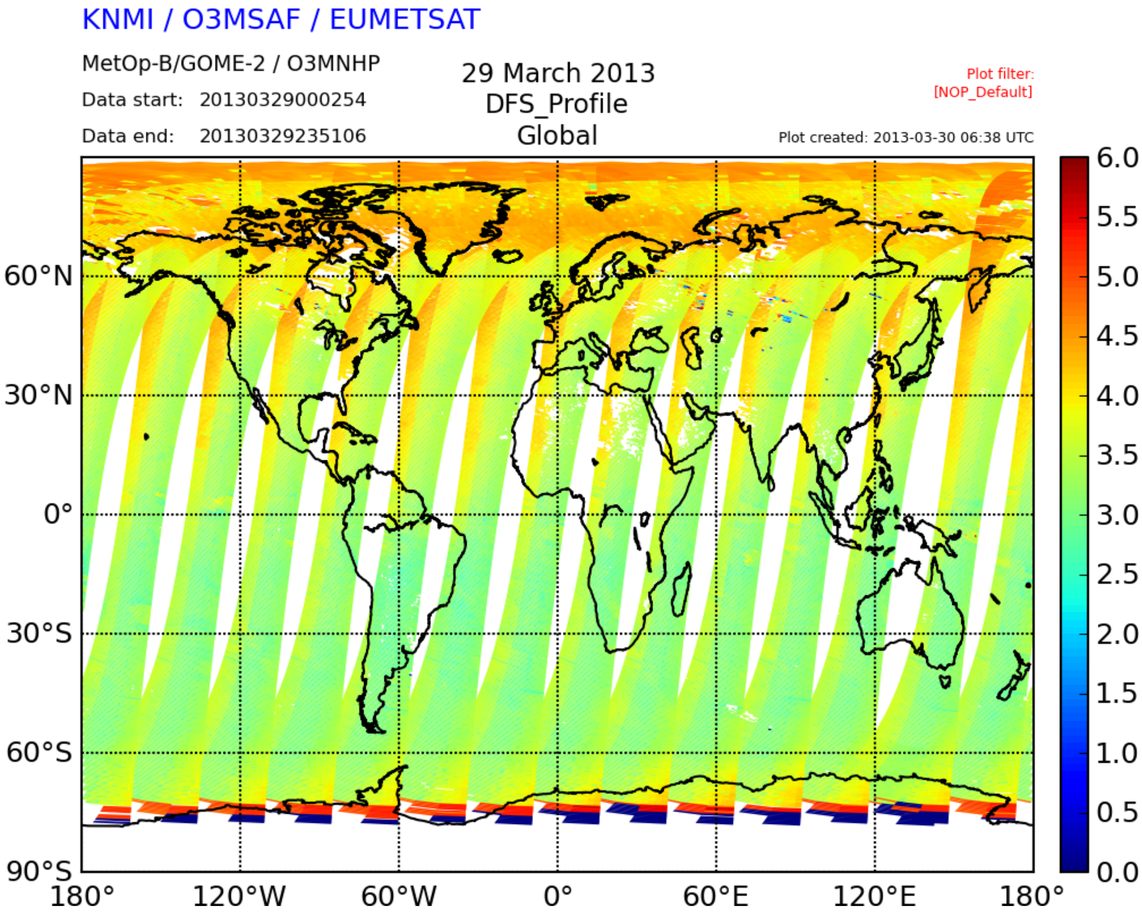

Figure 8.6: Degrees of Freedom for Signal for retrieved ozone profiles of GOME-2 on Metop-B on March 29th 2013.

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 8.2) is shown in Figure 8.10. 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.

The Tropospheric Ozone Column Product

An example of the Tropospheric Ozone Column Product (TrOC) and the partial column from the surface to 500 hPa, calculated from the vertical ozone profile, is given in Figure 8.11. From the south of Africa, the

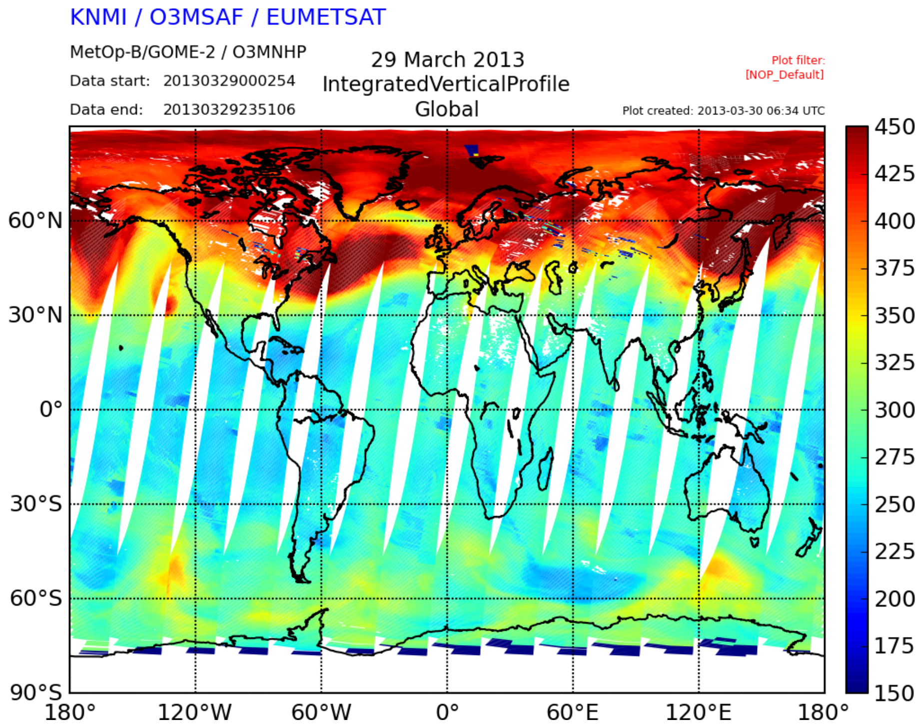

Figure 8.7: Integrated vertical ozone profile from GOME-2 on Metop-B, calculated as the sum of the retrieved profile on March 29th 2013.

increased tropospheric ozone is clearly visible. This ozone is related to extensive biomass burning in the region.

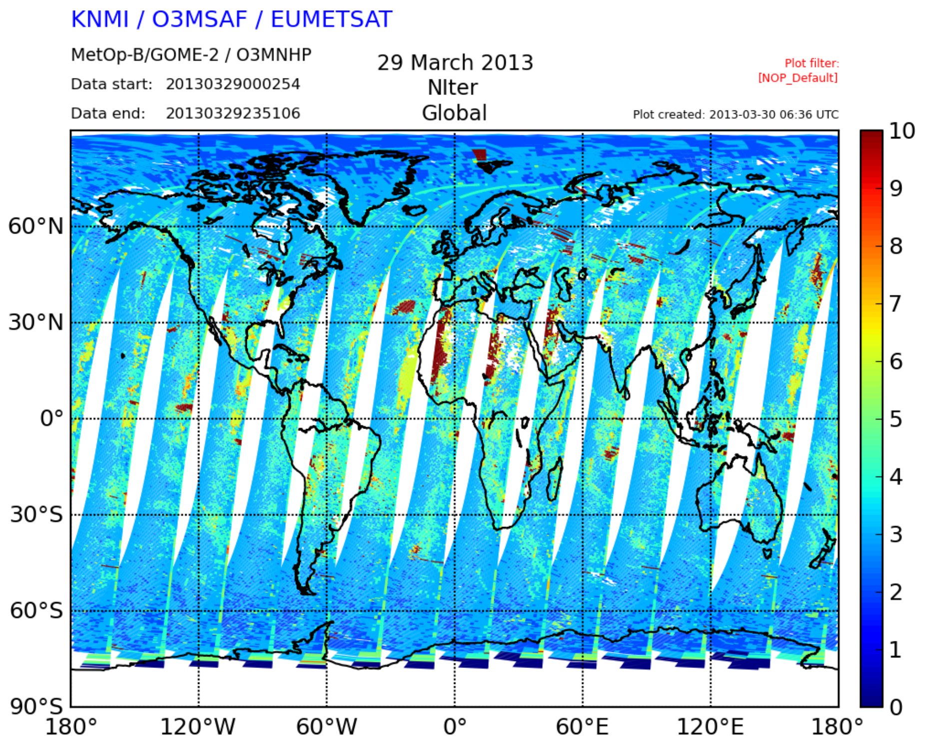

Figure 8.8: Number of iterations for each retrieval from GOME-2 on Metop-B on March 29th 2013. Brown pixels indicate non-converged profiles.

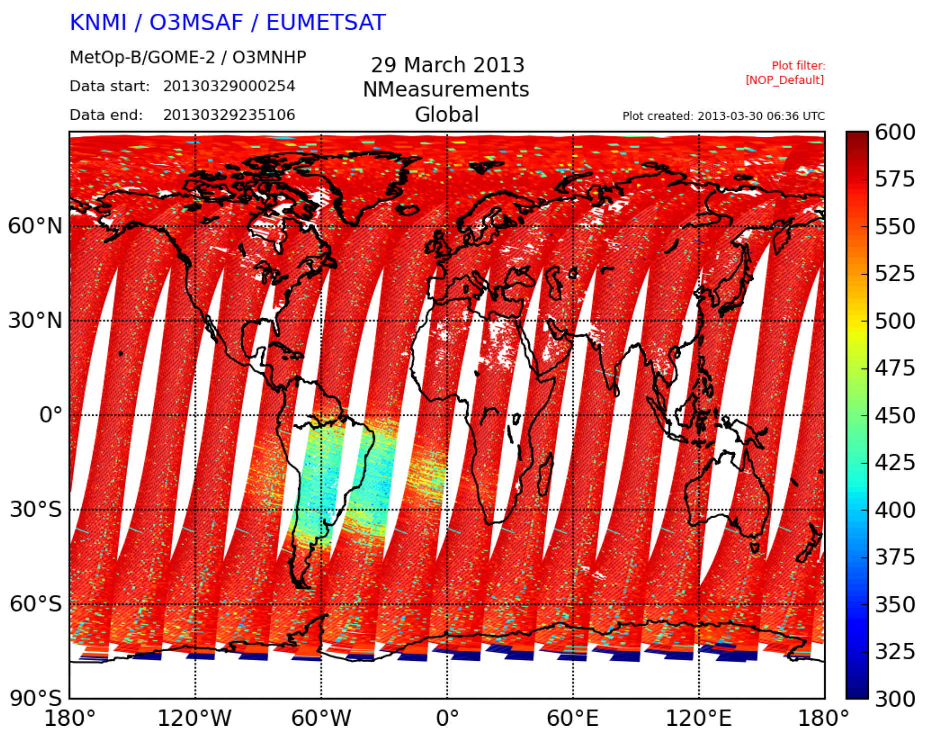

Figure 8.9: Number of spectral measurements of GOME-2 on Metop-B for each retrieved vertical ozone profile on March 29th 2013.

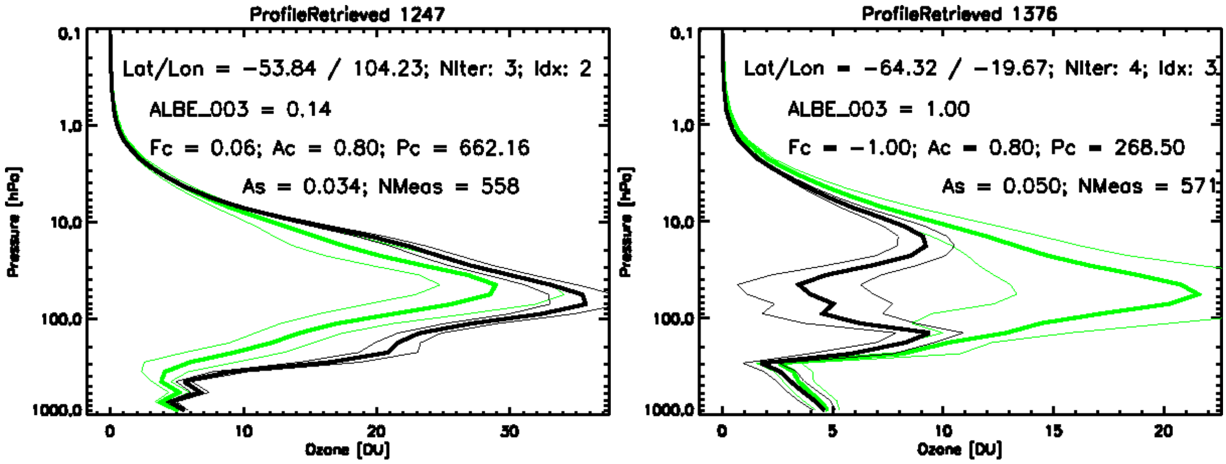

Figure 8.10: Retrieved ozone profiles (black), it's a priori (green) for retrieval in the ozone maximum in orbit 4679 (left), and in the ozone hole in orbit 4683 (right), indicated with the A and B. Instrument: GOME-2 on Metop-A.

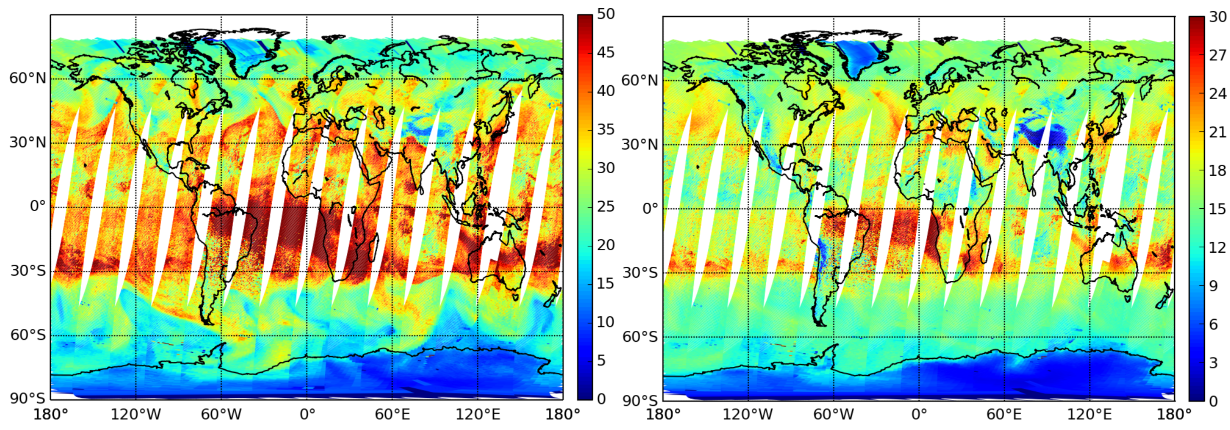

Figure 8.11: Tropospheric Ozone Column (left) and Surface to 500 hPa ozone (right) from GOME-2 on Metop-A on 2010-10-09.

Chapter 9

Accuracy of the ozone products

9.1 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.

9.2 Tropospheric Ozone Column: threshold, target and breakthrough accuracy

The AC SAF Product Requirements Document describes the accuracies as follows:

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

9.3 Main causes of error (uncertainty)

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. This degradation is corrected for products generated with software versions 2.x.x and higher (i.e.: products generated after November 2018).

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 19 degrees 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.

9.4 Regular monitoring of AC SAF product quality

The actual values of the accuracy of the product will be given in the SeSP document. Also, the AC SAF 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 AC SAF Validation Report on the ozone profile product.

Chapter 10

Instrument specific information

10.1 GOME-2A specific

- On 15th of July 2013, the GOME-2A swath width was reduced to half its previous width.
- Please be aware of ongoing instrument degradation.
- The operationally produced NRT and offline ozone profiles data between Dec 2018 and Mar 2019 was affected by the non-availability of the error values of the solar irradiance in the 'solar gap'.
- Please be aware that near the end of the mission, there is no longer a daily solar spectrum measurement. A solar irradiance model is used instead. This can lead to errors in the ratio / reflectance, and therefore to artificial changes in the ozone profile.

10.2 GOME-2B specific

- Please be aware of ongoing instrument degradation.

10.3 GOME-2C specific

Note: for version 6.3-2.02-2.07 and earlier, there appears to be a significant scan angle dependency present in the data. At this time, we recommend the users to only consider the center pixels (nrs 9 – 16) in the operational version of the product. After a degradation correction update, the product should be suitable again for the end user for the full swath. This will be communicated through the operations reports, available on the website of the AC SAF (`https://www.acsaf.org`).

Chapter 11

Further information

11.1 AC SAF website

Further up to date information and documentation on the ozone profile and tropospheric column products should be available from the AC SAF website: http://acsaf.org

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

11.2 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.

11.3 Acknowledgement instructions

When AC SAF 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 Atmospheric Composition (AC SAF)".

Chapter 12

History of software and product updates

Below is a list of changes made to the PPF (L1b version), the algorithm version (Alg.), the software version (Softw.) or configuration parameters. Other events are also recorded if significant.

This list of changes through time is relevant for data that was produced in NRT and the data stored Offline in the ACSAF archive. For Data Records, which are produced with one processor version, the history is of less importance (assuming that no errors are found at a later stage that affect the DR). Errata of DR products (if any) will listed on the ACSAF website on the product info page.

Table 12.1: Processor version change history

PPF	Alg.	Softw.	Sensing Start 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;

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Table 12.1 – *Continued from previous page*

PPF	Alg.	Softw.	Sensing Start Date	Remarks
				- 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:mm	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	20150625082655Z	Update of L1 processor.
6.1	1.12	1.34	20150914041756Z	Adding ScannerAngle to the product output file
6.1	1.12	1.35	20151116051459Z	Version increase as a result of a bug fix s to the AAI part of the code. No changes related to the ozone profiles.
6.1	1.12	1.37	20160623045354Z	Bugfix: - Correct the north-south orientation of the global temperature fields used in the operational vertical ozone profiles, due to differences in the orientation of the GRIB fields read in using the pygrib library (v1.8.4 vs v2.0.0). This bug existed since v1.32 (2015-02-23).; Increasing maximum allowed cloud albedo to 1.3 because the FRESCO values are occasionally 1.2+ in bright cloud conditions. ; - Increasing maximum allowed cloud fraction from 1.06 to 1.08 to get more fully clouded scenes to be used.;

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Table 12.1 – *Continued from previous page*

PPF	Alg.	Softw.	Sensing Start Date	Remarks
				- Fix of small negative cloud fraction values (now set to 0.0)
6.1	1.12	1.xx	2017	ReferenceTime changed to SensingStartTime. Does not affect the ozone profile product.
6.2	1.30	1.50	2018-08-13	Product maintenance update.
6.2	1.30	1.51	2018-08-20	Bugfix update
6.2	2.00	2.00	2018-11-19	Operational use of the degradadation correction
6.2	2.00	2.01	20181203061155Z	Bugfix: Albedo / LER interpolation of time was inverted
6.3	2.00	2.01	20181217094157Z	
6.3	2.01	2.02	20190114064154Z	Bugfix: Fix to handle the fill values in the irradiance error from the temporary Solar Model spectrum of GOME-2A.
6.3	2.02	2.03	20190211055356Z	Bugfix: Fix to handle infinity and NaN values across compilers in a uniform way.
6.3	2.02	2.06	20190715052358Z	Bugfix: Interpolation of the viewing zenith angle for the DLER calculation.
6.3	2.02	2.07	20200302054756Z	Shortening the time period over which the O3P degradation correction is calculated: 2016-current instead of the full mission period.
6.3	2.02	2.08	20200914055954Z	Upgrade of GOME-2C products to operational status, including degradation correction for the ozone profile and aerosol products; Use of DLER database derived from both GOME-2A and -B (previously just from -A); Preset snow/ice albedo of 0.8 for FRESCO cloud and weighting of Surface Albedo with AVHRR snow ice fraction.
6.3	2.1	2.1	20210603053257Z	Enables Solar Eclipse corrections in regions affected by the shadow of the moon. Application of this correction is signalled to the user by QualityInput flag nr 20, which is normally 0 and turns to 1 where applied on a scan level basis. This affects the NAR, NAP and AAH product (via the internal FRESCO retrieval).
7.0	2.1	2.1	20210608090300Z	Update to PPF v7.0

Chapter 13

Traceability of metadata to UMARF parameters

The UMARF metadata parameters [AD3] which are applicable to the AC SAF 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.

Table 13.1: UMARF trace table

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 AC 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 AC SAF archive; not included in the product file, provided to EDC by archive software
APNM	ProductType	
APPN	ParentProducts	
APXS	PixelSize	
ASTI	SatelliteID	
AVBA	BaseAlgorithmVersion	
AVPA	ProductAlgorithmVersion	
GDMD	(TBD)	Disposition Mode

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Table 13.1 – *Continued from previous page*

UMARF Short Name	Attribute Name	Notes
GGTP	GranuleType	
GNFV	ProductFormatVersion	
GNPF	ProductFormatType	
GNPO	N/A	Native Pixel Order; N/A for AC
GNSP	N/A	Number of Spectral Bands; N/A for AC
GORT	OrbitType	
GPLV	ProcessingLevel	
GPMD	ProcessingMode	
LLAE	SubSatellitePointEndLat	
LLAS	SubSatellitePointStartLat	
LLOE	SubSatellitePointEndLon	
LLOS	SubSatellitePointStartLon	
LMAP	N/A	Map Projection; N/A for AC
LONE	N/A	End Orbit Number; N/A for AC
LONS	StartOrbitNumber	
LSCD	SpatialCoverageModel	
LSCT	AscNodeCrossingTime	Ascending Node Crossing Date and Time ; N/A for AC
LSVT	AscNodeLongitude	Ascending Node Longitude
OCLA	N/A	Occultation Latitude (TBC) ; N/A for AC
OCLO	N/A	Occultation Longitude (TBC) ; N/A for AC
OCSA	N/A	Occultation Satellite ID (TBC) ; N/A for AC
OCTM	N/A	Occultation Date and Time (TBC) ; N/A for AC
PPDT	N/A	Processing Start Date and Time; N/A for AC
PPRC	ProcessingCentre	
PPST	ProcessingTime	Processing End Date and Time
QCCV	N/A	Cloud Coverage; N/A for AC
QDLC	MissingDataCount	
QDLP	MissingDataPercentage	
QDRC	DegradedRecordCount	
QDRP	DegradedRecordPercentage	
QQAI	QQAI	
QQOV	OverallQualityFlag	

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Table 13.1 – *Continued from previous page*

UMARF Short Name	Attribute Name	Notes
RRBT	N/A	Reception Start Date and Time; N/A for AC
RRCC	ReceivingCentre	
RRST	N/A	Ibid. End Date and Time; N/A for AC
SMOD	InstrumentMode	
SNIT	ReferenceTime	Equal to SensingStartTime after version 1.37. A reference time mainly used for selection of the product file in the EUMETSAT Data Centre.
SSBT	SensingStartTime	
SSST	SensingEndTime	
UDSP	DispositionFlag	
UUDT	N/A	Ingestion Date and Time; N/A for AC

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