

**Product User Manual**  
  
**for the Gridded L3 products**  
**of O<sub>3</sub> profile, AAI, AAH and SIF**



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<b>Author(s):</b>	O.N.E. Tuinder

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## CHANGE RECORD SHEET

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20220105	0.0.0-0.0.x	All	First draft.
20230804	0.1.x-0.9.x	All	First public release.
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### Related product list

<b>ID number</b>	<b>Product Description</b>
O3M-313	L3 daily gridded Ozone Profile
O3M-314	L3 monthly gridded Ozone Profile
O3M-367	L3 daily gridded Absorbing Aerosol Index from PMDs
O3M-370	L3 monthly gridded Absorbing Aerosol Index from PMDs
O3M-368	L3 daily gridded Absorbing Aerosol Height
O3M-371	L3 monthly gridded Absorbing Aerosol Height
O3M-411	L3 monthly SIF product
O3M-398	L3 monthly averaged tropospheric O3

# Contents

<b>1</b>	<b>Introduction</b>	<b>5</b>
1.1	Purpose of this document . . . . .	5
1.2	Scope . . . . .	5
1.3	Heritage . . . . .	5
1.4	Glossary . . . . .	6
1.4.1	Acronyms and abbreviations . . . . .	6
1.5	References . . . . .	8
<b>2</b>	<b>Introduction to EUMETSAT Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF)</b>	<b>9</b>
2.1	Background . . . . .	9
2.2	Objectives . . . . .	9
2.3	Product categories, timeliness and dissemination . . . . .	9
2.4	Further information . . . . .	10
<b>3</b>	<b>The GOME-2 Gridded L3 data product</b>	<b>11</b>
3.1	Product filename convention . . . . .	11
3.2	Product structure . . . . .	12
3.3	Parameter data sets stored in the gridded L3 output . . . . .	12
3.4	Product format . . . . .	13
<b>4</b>	<b>Product Examples</b>	<b>16</b>
4.1	Product specific details . . . . .	16
4.1.1	General filter options . . . . .	16
4.1.2	Ozone profiles . . . . .	17
4.1.3	Tropospheric Ozone . . . . .	18

4.1.4	Absorbing Aerosol Index . . . . .	19
4.1.5	Absorbing Aerosol Height . . . . .	20
4.1.6	Sun Induced Fluorescence . . . . .	21
4.2	Erratums . . . . .	22
4.2.1	Erratum Gridded Tropospheric Ozone . . . . .	22

<b>Bibliography</b>		<b>23</b>
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# Chapter 1

## Introduction

### 1.1 Purpose of this document

This document is the Product User Manual for those AC SAF L3 Gridded products that are derived from the Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF) L2 products that are produced at (or on behalf of) KNMI. These are the vertical ozone profile (O3P), the absorbing aerosol index (AAI) and absorbing aerosol height (AAH), and the sun induced fluorescence (SIF) products.

This document first provides information on product content, its structure, and provides guidance to the user on how to use the gridded Level-3 data product.

### 1.2 Scope

This PUM provides information on the non-time-critical and offline gridded L3 products of the AC SAF. These gridded products can contain data from one day only (daily), from the full month (monthly), or from any other time period (like weekly or 10 days). This product user manual document does not go into 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.*, 2021].

### 1.3 Heritage

This algorithm and the software implementation was developed by KNMI (the Royal Netherlands Meteorological Institute) and is based on experience from earlier work in national and international projects. For example: ESA projects (e.g.: O3-CCI), and EUMETSAT's Atmospheric Composition Monitoring SAF (AC SAF).

## 1.4 Glossary

### 1.4.1 Acronyms and abbreviations

Table 1.1: Acronyms and abbreviations

AAI	Absorbing Aerosol Index
AC SAF	Atmospheric Composition Monitoring SAF
ATBD	Algorithm Theoretical Basis Document
DFS	Degrees of Freedom for Signal
ECMWF	European Centre for Medium-range Weather Forecast
EPS	EUMETSAT Polar System
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
IR	Infrared
KNMI	Royal Netherlands Meteorological Institute
LUT	Look Up Table
L2	Level-2 data
L3	Level-3 data
MLL	McPeters, Labow, Logan
MSC	Main Science Channels
NHP	NRT High resolution ozone Profile
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
OPERA	Ozone Profile Retrieval Algorithm
OPF	Output Product Format

*Continued on next page*

Table 1.1 – *Continued from previous page*

PMD	Polarisation Measurement Detectors
PSC	Polar Stratospheric Clouds
PUM	Product User Manual
RMS	Root Mean Square
RTM	Radiative Transfer Model
SAA	South Atlantic Anomaly
SAF	Satellite Application Facility
SRD	Software Requirements Document
StrOC	Stratospheric Ozone Column
SUM	Software User Manual
SW	Software
SZA	Solar Zenith Angle
TOA	Top Of Atmosphere
TOMS	Total Ozone Mapping Spectrometer
TrOC	Tropospheric Ozone Column
UV	Ultra Violet
VIS	Visible

## 1.5 References

### **Vertical ozone profiles:**

- RD1 Algorithm Theoretical Baseline Document (ATBD) for the NRT and Offline and Data Record Vertical Ozone Profile and Tropospheric Ozone Column Products (O3MSAF/KNMI/ATBD/001, dd 2019, v2.0.2) [Tuinder *et al.*, 2017]
- RD2 Product User Manual (PUM) for the NRT and Offline and Data Record Vertical Ozone Profile and Tropospheric Ozone Column Products (O3MSAF/KNMI/PUM/001, dd 2019, v2.1.2) [Tuinder, 2017]

### **Absorbing Aerosol Index:**

- RD3 Algorithm Theoretical Baseline Document (ATBD) for the NRT, Offline and Data Record Aerosol Aerosol Index Products (O3MSAF/KNMI/ATBD/002, dd 2019, v2.61) [Tuinder *et al.*, 2019]
- RD4 Product User Manual (PUM) for the NRT, Offline and Data Record Aerosol Aerosol Index Products (O3MSAF/KNMI/PUM/002, dd 2020, v1.91) [Tuinder and Tilstra, 2020]

### **Absorbing Aerosol Height:**

- RD5 Algorithm Theoretical Baseline Document (ATBD) for the GOME-2 Aerosol Aerosol Height (SAF/AC/KNMI/ATBD/005, dd 2019, v1.4) [Tilstra *et al.*, 2019]
- RD6 Product User Manual (PUM) for the GOME-2 Aerosol Aerosol Height (SAF/AC/KNMI/PUM/006, dd 2020, v1.0) [Tilstra *et al.*, 2020]

### **Sun-Induced Fluorescence:**

- RD7 Algorithm Theoretical Baseline Document (ATBD) for the GOME-2 Sun-Induced Fluorescence of Terrestrial Ecosystem Retrieval - SIFTER (SAF/AC/KNMI/ATBD/007, dd 2020, v1.0) [Kooreman *et al.*, 2020]
- RD8 Product User Manual (PUM) for the GOME-2 NRT, Offline and Data Record Sun-Induced Fluorescence Products (SAF/AC/KNMI/PUM/008, dd 2021, v1.0 draft) [?]

### **Gridded L3 ATBD:**

- RD9 Algorithm Theoretical Baseline Document (ATBD) for the Gridded L3 products (SAF/AC/KNMI/ATBD/009, dd 2021, v1.0) [Tuinder *et al.*, 2021]

## Chapter 2

# Introduction to EUMETSAT Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF)

### 2.1 Background

The monitoring of atmospheric chemistry is essential due to several human caused changes in the atmosphere, like global warming, loss of stratospheric ozone, increasing UV radiation, and pollution. Furthermore, the monitoring is used to react to the threats caused by the natural hazards as well as follow the effects of the international protocols.

Therefore, monitoring the chemical composition and radiation of the atmosphere is a very important duty for EUMETSAT and the target is to provide information for policy makers, scientists and general public.

### 2.2 Objectives

The main objectives of the AC SAF is to process, archive, validate and disseminate atmospheric composition products ( $O_3$ ,  $NO_2$ ,  $SO_2$ , BrO, HCHO,  $H_2O$ , OClO, CO,  $NH_3$ ), aerosol products and surface ultraviolet radiation products utilising the satellites of EUMETSAT. The majority of the AC SAF products are based on data from the GOME-2 and IASI instruments onboard Metop satellites. Another important task besides the near real-time (NRT) and offline data dissemination is the provision of long-term, high-quality atmospheric composition products resulting from reprocessing activities.

### 2.3 Product categories, timeliness and dissemination

NRT products are available in less than three hours after measurement. These products are disseminated via EUMETCast, WMO GTS or internet.

- Near real-time trace gas columns (total and tropospheric  $O_3$  and  $NO_2$ , total  $SO_2$ , total HCHO, CO) and high-resolution ozone profiles

- Near real-time absorbing aerosol indexes from main science channels and polarization measurement detectors
- Near real-time UV indexes, clear-sky and cloud-corrected

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

- Offline trace gas columns (total and tropospheric O<sub>3</sub> and NO<sub>2</sub>, total SO<sub>2</sub>, total BrO, total HCHO, total H<sub>2</sub>O) and high-resolution ozone profiles
- Offline absorbing aerosol indexes from main science channels and polarization measurement detectors
- Offline surface UV, daily doses and daily maximum values with several weighting functions

Data records are available after reprocessing activities from the EUMETSAT Data Centre and/or the AC SAF archives.

- Data records generated in reprocessing
- Lambertian-equivalent reflectivity
- Total OCIO

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

## **2.4 Further information**

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

AC SAF Helpdesk: [helpdesk@acsaf.org](mailto:helpdesk@acsaf.org)

Twitter: [https://twitter.com/Atmospheric\\_SAF](https://twitter.com/Atmospheric_SAF)

## Chapter 3

# The GOME-2 Gridded L3 data product

### 3.1 Product filename convention

The filenames of the Gridded L3 product follow the standard naming convention in the ACSAF:

Example:

```
S-O3M_GOME_NAR_03_M01_20200124000254Z_20200125000254Z_N_O_20220104165756Z.nc
```

which consists of the following elements

```
S-O3M_GOME_AAA_BB_CCC_DDDDDDDDDDDDDZ_EEEEEEEEEEEEEEZ_F_G_HHHHHHHHHHHHHZ.nc
```

where

- S-O3M: prefix related to the O3MSAF / ACSAF
- GOME: the instrument: GOME-2
- AAA: product type
- BB: product level
- CCC: platform
- DDDDDDDDDDDDDZ: start sensing time
- EEEEEEEEEEEEEEZ: stop sensing time
- F: processing mode
- G: disposition mode
- HHHHHHHHHHHHHZ: production time
- nc: indicator for NetCDF

## 3.2 Product structure

The product structure is as follows:

- Product metadata as attributes of the main file
- Parameter group(s)
  - Dimensions
  - Parameter data sets in the group

Parameter groups are bundles of data sets associated with a particular variable, for example: AAI, total ozone column, number of iterations, cloud fraction, etc.

## 3.3 Parameter data sets stored in the gridded L3 output

In the L3 product the following sets values are stored per grid cell for each parameter group:

- the number of sub-pixels seen
- the minimum value of all data point values
- the maximum value of all data point values
- the sum of the data point values
- the sum of the square of each of the data point values
- SumValDivSqError
- SumOneDivSqError

The values above allow us to derive, per grid cell:

- the arithmetic mean
- the standard deviation
- the weighted mean
- the weighted mean error

### 3.4 Product format

The product format is described below in more detail. First we describe the global attributes in Table 3.1, then we describe the dimensions in Table 3.4, and then we describe the parameter sets in Table 3.3 with their attributes in Table 3.2.

Table 3.1: Global attributes

Attribute name	Data Type	Description	Example values
Origin	string	Production facility	KNMI, NL
Author	string	Author	<name>
Contact	string	contact address	<address> at <domain>
ProductSoftwareVersion	string	Product Software Version	2.00
ProductSoftwareVersionDate	string	Product Software Version Date	20230412
ProductFormatVersion	string	Product Format Version	2.00
ProductFormatVersionDate	string	Product Format Version Date	20230412
ProcessingTime	string	Processing Time	2023-04-19T14:15:17.000
SensingStartTime	string	Sensing Start Time	2023-01-01T00:02:55.000
SensingEndTime	string	Sensing End Time	2023-03-27T00:02:54.000
BaseAlgorithmVersion	string	Base Algorithm Version	7.0
ParentProductAlgorithmVersion	string	Parent Product Algorithm Version	1.40
ParentProductSoftwareVersion	string	Parent Product Software Version	2.11
InstrumentID	string	Instrument ID	GOME
SatelliteID	string	Satellite ID	M03
ReferenceTime	string	Reference Time	2023-03-26T00:08:54.000
ProcessingMode	string	Processing Mode	N
DispositionMode	string	Disposition Mode	O
ProcessingLevel	string	Processing Level	03
StartOrbitNumber	integer	Start Orbit Number	22731
ShortProductName	string	Short Product Name	NAR
ProductType	string	Product Type	O3MNAR
ProjectID	string	Project ID	O3M
RevisionID	string	Revision ID	R2
DOI	string	DOI	...
FileCreationDate	string	Production facility	2022-01-04 18:29:50.060735
GridVarNames	string	Production facility	AAI, PMD_CloudFraction, AAH_AbsorbingAerosolHeight

Table 3.2: Parameter group attributes

<b>Attribute name</b>	<b>Data Type</b>	<b>Description</b>	<b>Example values</b>
LongName	string	LongName	NValues, Arithmetic Mean, etc
standard_name	string	Standard name	atmosphere_mole_content_of_ozone, absorbing_aerosol_index, etc
description	string	Description of the parameter	"Number of values seen in this cell"
units	string	units	'-', or hPa, etc

Table 3.3: Group datasets per parameter

Dataset name	Data Type	Description	Size
ArithmeticMean	float	Arithmetic mean	(NLat, NLon, NPres, NTimes)
MaxValue	float	Maximum value	(NLat, NLon, NPres, NTimes)
MinValue	float	Minimum value	(NLat, NLon, NPres, NTimes)
NValues	int	Number of values seen in cell	(NLat, NLon, NPres, NTimes)
StandardDeviation	float	Standard deviation	(NLat, NLon, NPres, NTimes)
SumOneDivSqError	float	Sum of $1 / \text{error}^2$	(NLat, NLon, NPres, NTimes)
SumSqValues	float	Sum of $\text{value}^2$	(NLat, NLon, NPres, NTimes)
SumValDivSqError	float	Sum of $\text{value} / \text{error}^2$	(NLat, NLon, NPres, NTimes)
SumValues	float	Sum of values	(NLat, NLon, NPres, NTimes)
WeightedMean	float	Weighted mean	(NLat, NLon, NPres, NTimes)
WeightedMeanError	float	Weighted mean error	(NLat, NLon, NPres, NTimes)

Table 3.4: Dimensions

Attribute name	Data Type	Description	Allowed values
dimensions			
dim: time	int	time	$N=t$
dim: timeborders	int	time range	$N=t+1$
dim: latitude	int	gridbox central latitude	$N=i$ , e.g.: 720
dim: latitudeborders	int	gridbox latitude borders	$N=i+1$ , e.g.: 721
dim: longitude	int	gridbox central longitude	$N=j$ , e.g.: 1440
dim: longitudeborders	int	gridbox longitude borders	$N=j+1$ , e.g.: 1441
dim: pressure	int	gridbox central pressure	$N=p$
dim: pressureborders	int	gridbox pressure borders	$N=p+1$
variables			
time	float	Time past midnight	–
timeborders	float	Time range	–
latitude	float	grid box center latitude	Latitude in degrees north
longitude	float	grid box center longitude	Longitude in degrees east
latitudeborders	float	grid box latitude borders	Latitude in degrees north
longitudeborders	float	grid box longitude borders	Longitude in degrees east
pressure	float	Pressure	Pressure in hPa
pressureborders	float	Pressure	Pressure in hPa

# Chapter 4

## Product Examples

### 4.1 Product specific details

During the Level-2 data ingestion and processing, there are some general filtering options, and some product specific filtering options and methods are applied during projecting and binning the data. These are documented in the ATBD (see section 1.5). In the next sections we provide a very short description of the original Level-2 product. For more specific information on the L2 product usage and product quality we refer the reader to the respective Level-2 ATBD and PUM documents listed in the reference documents list in section 1.5.

#### 4.1.1 General filter options

In general, the following filtering options applied for all products:

- Only 'forward scan' pixels are used
- Anomalous retrievals are filtered out as much as possible (e.g. throughput tests, etc)
- Only nadir pointing retrievals are used
- Only southbound (descending node) data are used for averaging, in order to avoid matching too different solar zenith angles onto the same grid cell

### 4.1.2 Ozone profiles

The vertical ozone profile consists of a value for the ozone column partial column for each layer in a multi-layered atmosphere. The absorption cross section of ozone decreases steeply with wavelength between 260 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 265–340 nm contains information on the vertical ozone profile.

The vertical layering of each retrieved level-2 vertical ozone profile is different based on surface pressure, terrain height and cloud height. This is mapped onto the pre-defined vertical layering of the 3D grid.

The ozone profiles are given as 'mole content of ozone in atmosphere layer', conform the CF standard names with SI units  $\text{mole m}^{-2}$ . To save space and avoid duplication, the 3D ozone field in Dobson Units is omitted, and users that would like to have the ozone in this unit are recommended to use the conversion factor:  $446.2 \cdot 10^{-6} \text{ mole DU}^{-1}$

#### Gridded ozone profiles

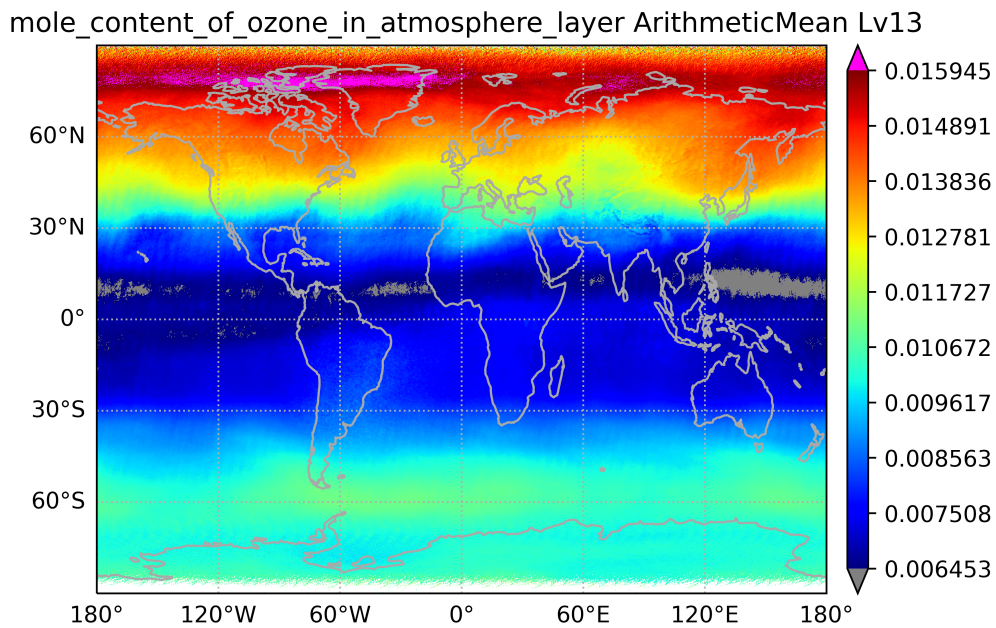


Figure 4.1: Example of GOME-2C monthly averaged ozone [mole / m<sup>2</sup>] for a layer around 45 hPa for March 2023.

### 4.1.3 Tropospheric Ozone

The tropospheric ozone is calculated (as a sum) from the full vertical L2 ozone profile. There are two variations:

- The vertically integrated profile from the surface to the tropopause
- The vertically integrated profile from the surface to 500hPa

In the example below we show the 'Surface to 500hPa' version, which gives a better indication of potential ozone episodes at ground level. The example plot below shows the increased ozone as outflow of western Africa, likely as a result of biomass burning.

The total column values, are given as IntegratedVerticalProfile in DU (Dobson Units) and as 'atmosphere mole content of ozone' in  $\text{mole m}^{-2}$ . The tropospheric column values, are given as TroposphericIntegratedProfile and IntegratedVerticalProfileSurfaceTo500hPa in DU (Dobson Units) and as 'tropospheric\_mole\_content\_of\_ozone' and 'surface\_to\_500hpa\_mole\_content\_of\_ozone' in  $\text{mole m}^{-2}$ . The conversion factor between the two is  $446.2 \cdot 10^{-6} \text{ mole DU}^{-1}$

#### Gridded tropospheric ozone column

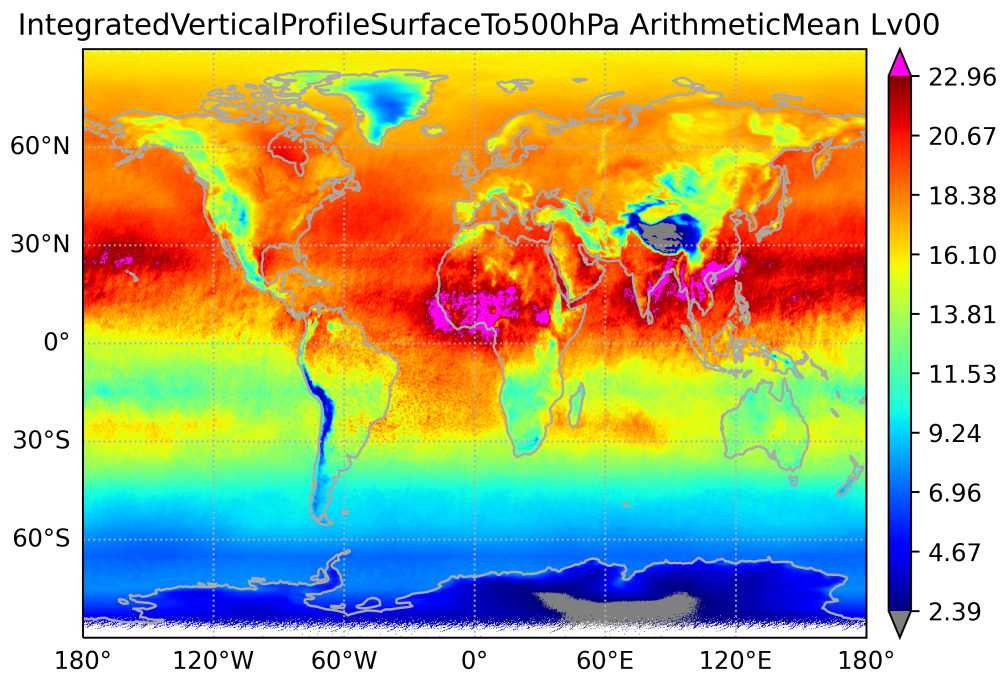


Figure 4.2: Example of GOME-2C monthly averaged tropospheric ozone [DU] from the surface to 500hPa for March 2023.

#### 4.1.4 Absorbing Aerosol Index

The Absorbing Aerosol Index indicates the presence of aerosols in the atmosphere. It separates the spectral contrast at two ultraviolet (UV) wavelengths caused by aerosol scattering and absorption from that of other effects, including molecular Rayleigh scattering, surface reflection, and gaseous absorption.

#### Gridded Absorbing Aerosol Index

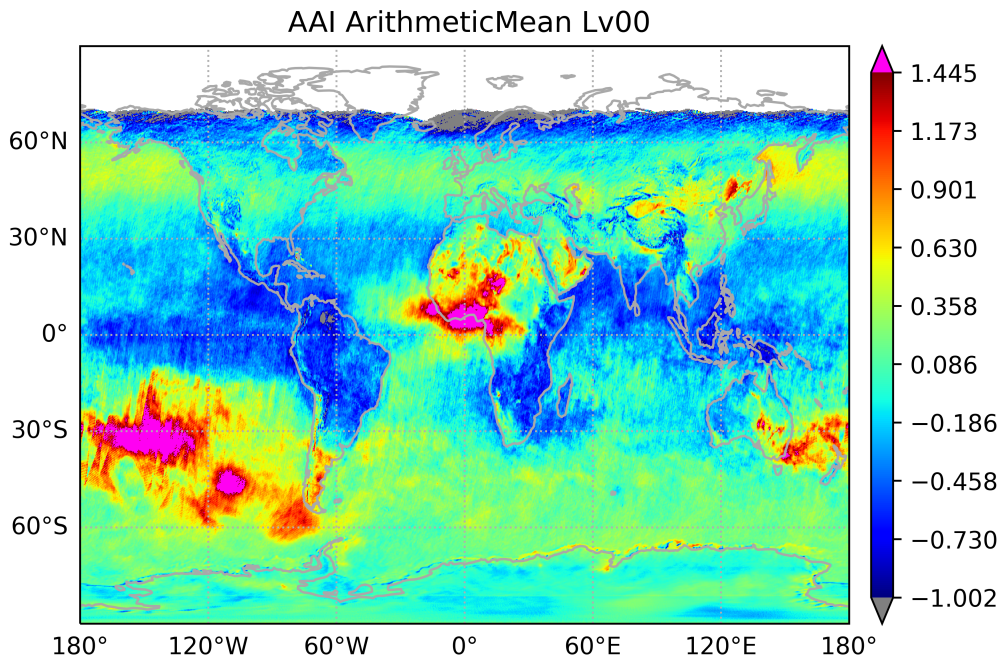


Figure 4.3: Example of GOME-2C monthly maximum AAI (PMD) values for January 2020, during the Australian Wildfires that started at the end of Dec 2019.

### 4.1.5 Absorbing Aerosol Height

The GOME-2 AAH is represents the absorbing aerosol layer height using two approaches. In the first approach the aerosol/cloud layer height is retrieved along with effective aerosol/cloud cover fraction. The aerosol layer albedo is set to a fixed value of 0.8, which is an appropriate value for clouds and also a functional value for thick aerosol layers. In the second approach, the scene albedo and scene height are derived by assuming the aerosol/cloud fraction to be equal to one. Large aerosol plumes often cover several GOME-2 pixels. Thus, it seems reasonable to assume an aerosol/cloud cover fraction of one in these situations. The scene height can be very different than the aerosol/cloud height. In the AAH algorithm, the aerosol/cloud height, scene height and surface height are converted to aerosol/cloud pressure, scene pressure and surface pressure using the standard Mid-Latitude Summer (MLS) atmosphere. Therefore, in the AAH products the terms “height” and “pressure” are interchangeable.

#### Gridded Absorbing Aerosol Height

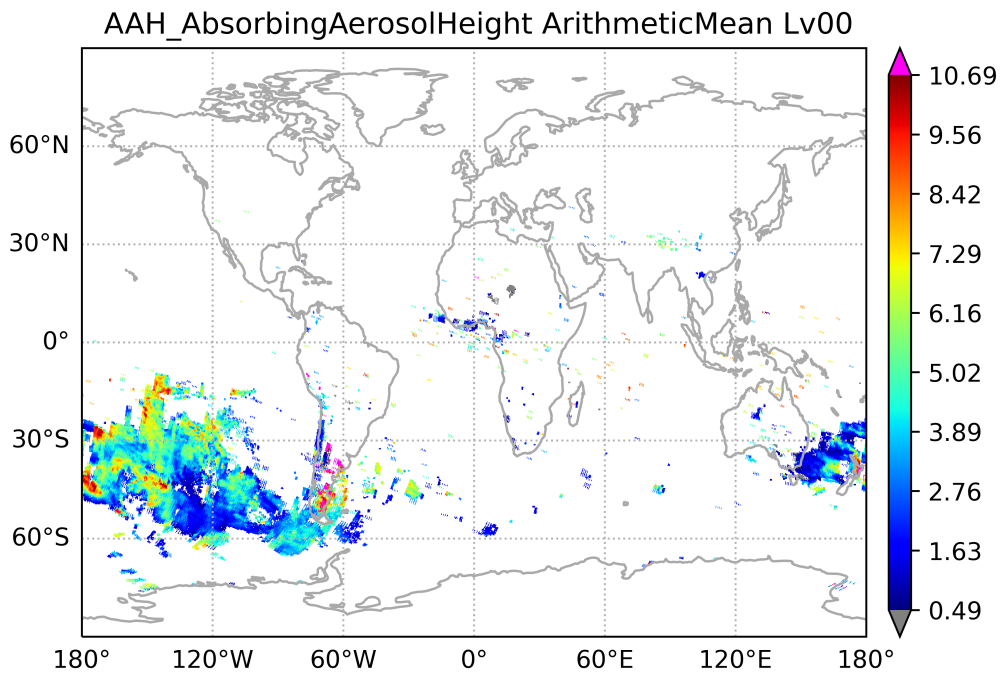


Figure 4.4: Gridded GOME-2A Absorbing Aerosol Height in January 2020, during the Australian wildfires, and the transport of aerosol afterwards in easterly direction.

### 4.1.6 Sun Induced Fluorescence

Remotely sensed vegetation fluorescence is a promising global proxy for gross primary productivity of plants. During photosynthesis, sunlight is absorbed by chlorophyll pigments in leaves and converted into chemical energy. Approximately 80% of the harvested energy is used for photosynthesis. Most of the rest is dissipated non-radiatively as heat and a small fraction (~1%) is emitted at longer wavelengths as fluorescence. This Sun-Induced Fluorescence (SIF) has a spectrally smooth signature with peaks at 683 (red fluorescence) and 737 nm (far-red fluorescence). Chlorophyll itself re-absorbs fluorescence within the canopy at wavelengths below 700 nm. The red SIF emission peak can be measured from space, but this product focuses on retrieving the far-red SIF emission peak.

#### Gridded Sun Induced Fluorescence

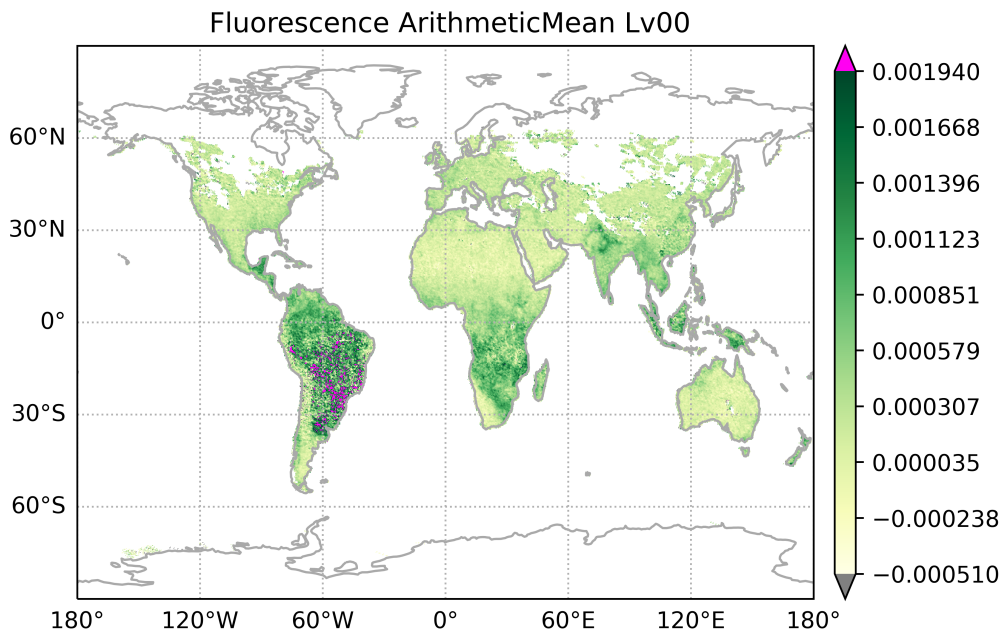


Figure 4.5: Example of GOME-2C monthly averaged fluorescence for January 2020.

## **4.2 Erratums**

### **4.2.1 Erratum Gridded Tropospheric Ozone**

Due to a small spelling mistake, the grid for troposphere mole content of ozone and the grid for surface to 500 hPa mole content of ozone were not filled correctly during initial processing. The ArithmeticMean values have been reconstructed from the corresponding parameters with Dobson Units, but those values where deconvolution was not possible are left empty. This will be fixed during the next full reprocessing in the 2025-2026 timeframe.

The tropospheric ozone identifier is TRO, but in the first release of the product some fields may have remaining identifiers referring to the original NHP product on which the TRO was built. This will also be fixed with the next full reprocessing.

# Bibliography

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# List of Figures

4.1	Example of GOME-2C monthly averaged ozone [mole / m <sup>2</sup> ] for a layer around 45 hPa for March 2023. . . . .	17
4.2	Example of GOME-2C monthly averaged tropospheric ozone [DU] from the surface to 500hPa for March 2023. . . . .	18
4.3	Example of GOME-2C monthly maximum AAI (PMD) values for January 2020, during the Australian Wildfires that started at the end of Dec 2019. . . . .	19
4.4	Gridded GOME-2A Absorbing Aerosol Height in January 2020, during the Australian wildfires, and the transport of aerosol afterwards in easterly direction. . . . .	20
4.5	Example of GOME-2C monthly averaged fluorescence for January 2020. . . . .	21

# List of Tables

1.1	Acronyms and abbreviations . . . . .	6
3.1	Global attributes . . . . .	13
3.2	Parameter group attributes . . . . .	14
3.3	Group datasets per parameter . . . . .	15
3.4	Dimensions . . . . .	15