Algorithm Theoretical Basis Document

for the Gridded L3 products of O_3 profile, AAI, AAH and SIF

EUMETSAT AC SAF
ATMOSPHERIC COMPOSITION MONITORING

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CHANGE RECORD SHEET

Date	Issue	Pages affected	Description
20200915	0.0.1-0.0.x	All	First draft.
20210420	0.1.x-0.2.x	Example plots	First public release.
20211104	0.3.0	Example plots	Updates after RR/PCR review.
20230804	0.4.0	Example plots	Updates to current plotting format

Related product list

ID number	Product Description
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

Chapter 1

Introduction

1.1 Purpose of this document

This document is the Algorithm Theoretical Baseline Document for those ACSAF L3 Gridded products that are derived from the ACSAF 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 presents the general algorithmic procedure of the gridding process, and provides detail about its implementation.

1.2 Scope

Because the L2 products that are used as input for the gridded L3 products, this document is limited in its scope to strictly describing the details of the gridding process, the calculation of the standard deviation and the standard error where error values were present in the L2 product. Workflow details that are deemed relevant for the individual product families are also provided on a per product basis, e.g. filtering.

In the Product User Manual the product content (in the L3 product output file) is described.

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
ACSAF	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) [**?**]

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_3 and NO_2, total SO_2, total BrO, total HCHO, total H_2O) 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 OClO

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

Twitter: https://twitter.com/Atmospheric_SAF

Chapter 3

Gridding data

3.1 The L3 gridding process

The process of ’gridding’ the data from Level-2 to Level-3 consists of a couple of steps. Based on a grid definition, the the ground pixel of each retrieved data point is projected onto the fixed grid, and assigned a sub-cell index. After the sub-cell indices of the L2 ground pixels are known, the data can be combined in the grid, after which the data can be averaged and the error can be calculated. These steps are described in the sections below.

3.1.1 Grid definition

The creation of each L3 grid starts with a ’grid definition’ which describes, on a per-variable basis, the following features:

- the variable name in the L3 product
- the parameter in the L2 file to average
- the vertical and horizontal dimensions in terms of extent in the latitude and longitude direction and the number of grid cells in the latitude and longitude direction
- the vertical dimension in terms of pressure range, the number of grid cells in the vertical direction and their boundaries
- the time period over which is averaged

3.1.2 Projecting and binning

Due to the slanted trajectory of most satellite orbits, the projection of satellite ground pixels is almost never a one-to-one match with the regularly oriented north-south and east-west L3 grid cells. Most of the time parts of the satellite ground pixels are partially covering multiple cells when projected onto the regular grid. In order to contribute information to each of the the partially covered grid cells, the following steps are taken:

- the original ground pixel is split up into sub-pixels (divided x times in the along flight direction and y times in the cross track direction)
- those sub-pixels are then projected and binned onto the regular grid (i.e. the grid cell indices are obtained)
- the data value is added to the grid cells indicated by the sub-pixel indices.

The division into sub-pixels is perfomed taking into account the Earth's shape and we interpolate along great circles.

Figure 3.1 shows schematically how the projection and binning is done. The black lines indicate the boundaries of the grid cells, and the blue lines indicate the GOME-2 ground pixel and a set of sub-cell divisions. In red the projection of the sub-cell centre is indicated. This sub-cell centre is ultimately used for attribution to the grid box cell.

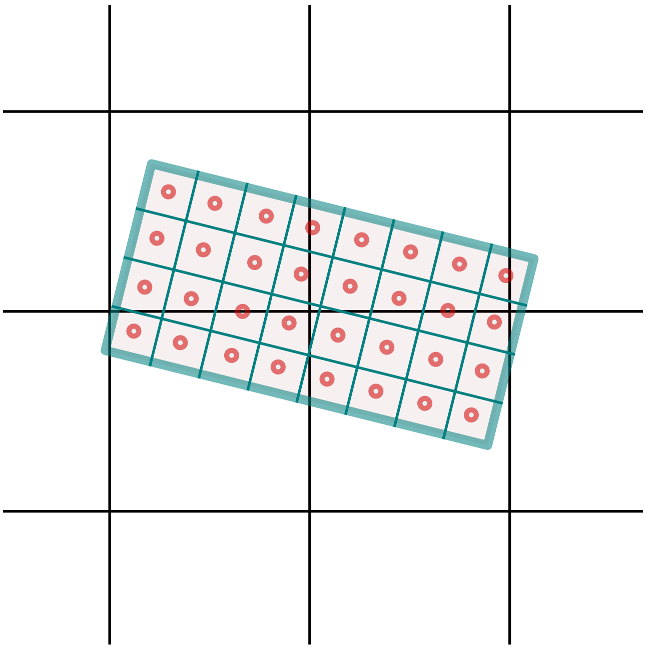

Figure 3.1: Projection of a satellite ground pixel footprint onto a regular grid and dividing it into sub-pixels.

3.1.3 Calculated parameters

In the L3 product we provide the arithmetic mean, the population standard deviation of the arithmetic mean, the weighted mean (weighted by the error values of the parameter, if available), and the standard error of the weighted mean.

The arithmetic mean value in a grid cell is calculated as follows:

$$Arithmetic\ Mean = \frac{\sum_{n=1}^{N} x_i}{N} \tag{3.1}$$

where x_i is the individual data point and N is the number of data points. In order to calculate the arithmetic mean, the number of data points in a grid cell and the sum of the data values in that grid cell need to be stored in the output.

The population standard deviation value in a grid cell is calculated as follows:

$$\sigma = \sqrt{\frac{\sum (x-\bar{x})^2}{N}} \tag{3.2}$$

$$\sigma = \sqrt{\left(\frac{1}{N}\sum_{n=1}^{N} x_i^2\right) - \left(\frac{1}{N}\sum_{n=1}^{N} x_i\right)^2} \tag{3.3}$$

$$\sigma = \frac{\sqrt{N\left(\sum_{n=1}^{N} x_i^2\right) - \left(\sum_{n=1}^{N} x_i\right)^2}}{N} \tag{3.4}$$

where σ is the population standard deviation. In order to calculate the standard deviation, the sum of the squared data values ($\sum_{n=1}^{N} x_i^2$) needs to be stored, in addition to the sum of the values (already stored).

If the weight of the weighted mean is taken as 1/variance = 1/($error_i^2$), then the weighted mean and the standard error can be written as:

$$Weighted\ Mean = \frac{\sum_{n=1}^{N}\left(x_i/(error_i^2\right)}{\sum_{n=1}^{N}\left(1/(error_i^2\right)} \tag{3.5}$$

$$Standard\ Error = \frac{1}{\sum_{n=1}^{N}\left(1/(error_i^2\right)} \tag{3.6}$$

If one keeps track of two sums:

$$SumValDivSqErr = \sum_{n=1}^{N}\left(x_i/(error_i^2\right) \tag{3.7}$$

$$SumOneDivSqErr = \sum_{n=1}^{N}\left(1/(error_i^2\right) \tag{3.8}$$

then the weighted mean and the standard error can be written as:

$$Weighted\ Mean = \frac{SumValDivSqErr}{SumOneDivSqErr} \tag{3.9}$$

$$Standard\ Error = \sqrt{\frac{1}{SumOneDivSqErr}} \tag{3.10}$$

For parameters where there is no error available, the error value is taken to be unity (i.e.: 1.0).

3.1.4 Parameters stored in the daily and monthly output

In the L3 product we store the following parameters per grid cell:

- 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 (Eq. 3.7)
- SumOneDivSqError (Eq. 3.8)

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

- the arithmetic mean (Eq. 3.1)
- the standard deviation (Eq. 3.2)
- the weighted mean (Eq. 3.9)
- the weighted mean error (Eq. 3.10)

Chapter 4

Gridded products

4.1 Potential use of gridded L3 products

Information on the global two- and three-dimensional distribution of atmospheric constituents, such as aerosol and ozone is in great demand. Time series of these parameters are consolidated as thematic climate data records (TCDRs) and often span years or even decades. These data records are important to monitor local and global trends in order to detect changes in atmospheric parameters. Some of these changes may be attributed to climate change.

Often users prefer Level-3 data on a regular grid over raw ground pixel based Level-2 data. These products are useful to the climate modelling community, because of their easy data access and limited data size. The ACSAF provides those L3 grids on a daily and monthly basis to help users use ACSAF data in their global transport models and other scientific studies.

For example, long time series of L3 ozone can be used to understand the trends in the depletion and expected recovery of stratospheric ozone of the Antarctic ozone hole. The L3 data can also be used to study global transport patterns of ozone and occurrences of ozone holes over the northern Arctic, like in 2019.

The global distribution of aerosol and aerosol height can be used in an assessment of the Earth's radiation balance. The transport of aerosol, such as desert dust and volcanic plumes can be studied, and assessments can be made how much dust is deposited in various areas. Well known is for example the effect that desert dust nutrients from the Sahara bring to the Amazonian forest across the Atlantic Ocean due to long range transport as an elevated aerosol layer.

4.2 Product specific details

In the process of data selection, there are some general filtering options, and some product specific filtering options and methods applied when projecting and binning the data. These are discussed in the next subsections. We will also provide a very short description of the original Level-2 product and refer the reader to the respective ATBD and PUM documents listed in the reference documents list in section 1.5. Just to provide an impression of the data in averaged form, one plot per product is also provided. The user is referred to the respective PUMs and the validation reports for information on product usage and product quality.

4.2.1 General filter options

The general filtering options applied for all products are listed here:

- 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.
- Solar eclipses are removed as much as possible

4.2.2 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.

Because the vertical layering of each retrieved vertical ozone profile is different based on surface pressure, terrain height and cloud height, there is no one-on-one correspondence with the pre-defined vertical layering of the 3D grid.

To handle this in the gridding process, the vertical profile is converted into a profile of columns that start at the surface and end at the particular level. That new profile of sums can then be interpolated to the 3D grid boundaries and then brought back to layer sub-columns by subtraction of the sum-value of the lower boundary from the sum-value of the upper boundary.

Ozone profile filter options

- Only converged retrievals are averaged

Gridded ozone profiles

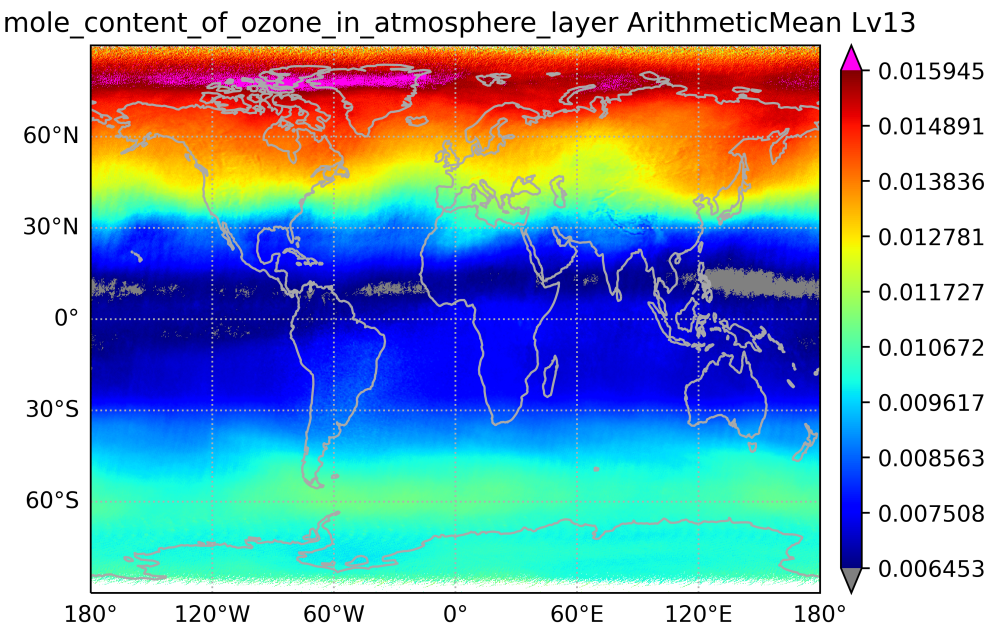

Figure 4.1: Example of GOME-2C monthly averaged ozone [mole / m2] for a layer around 45 hPa for March 2023.

4.2.3 Tropospheric Ozone

The tropospheric ozone is calculated from the full vertical L2 ozone profile (for more details see: 'ATBD for the NRT and Offline and Data Record Vertical Ozone Profile and Tropospheric Ozone Column Products'). 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.

Tropospheric ozone filter options

- Only converged retrievals are averaged

Gridded tropospheric ozone column

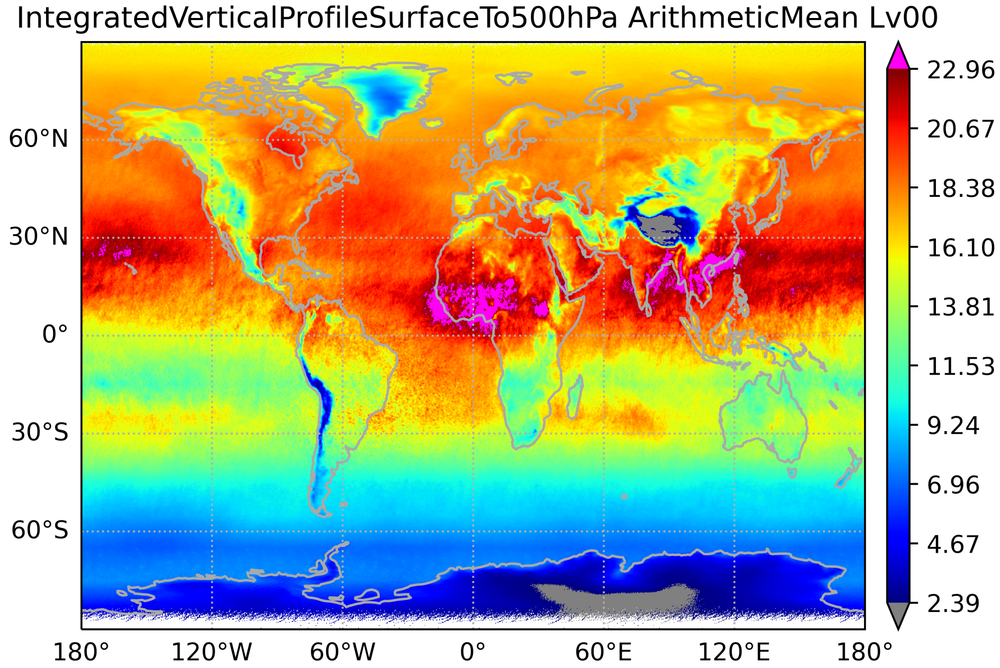

Figure 4.2: Example of GOME-2C monthly averaged tropospheric ozone [DU] from the surface to 500hPa for March 2023.

4.2.4 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.

AAI filter options

- Sunglint pixels are removed

Gridded Absorbing Aerosol Index

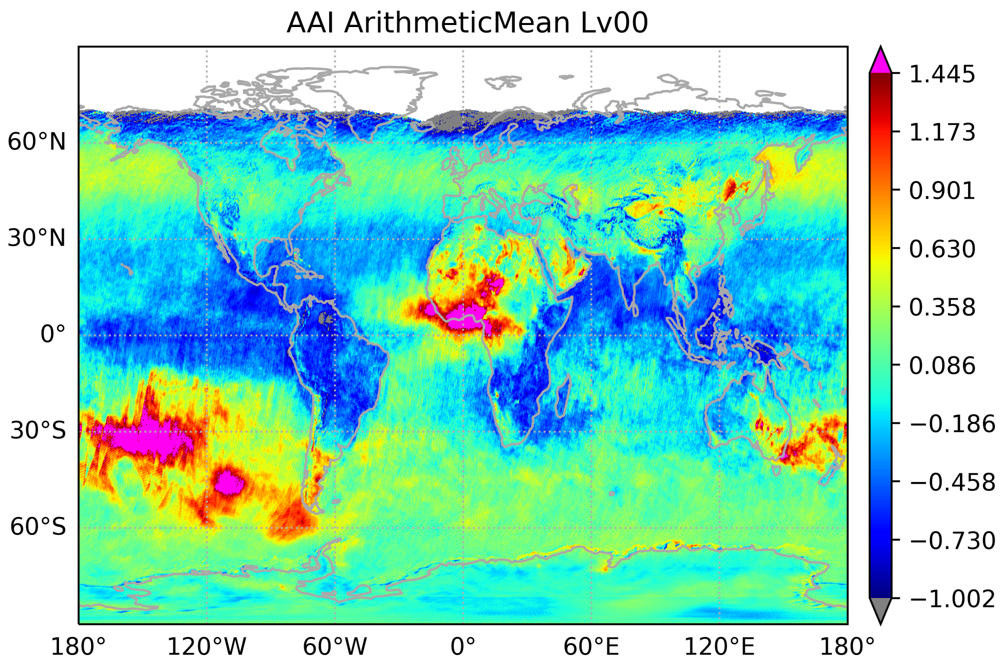

Figure 4.3: Example of GOME-2C monthly maximum AAI (PMD) values for January 2020, during the Australian Wildfires that started at the end of Dec 2019.

4.2.5 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.

AAH filter options

- Sunglint pixels are removed
- AAH are only included if the AAI is above 4.0

Gridded Absorbing Aerosol Height

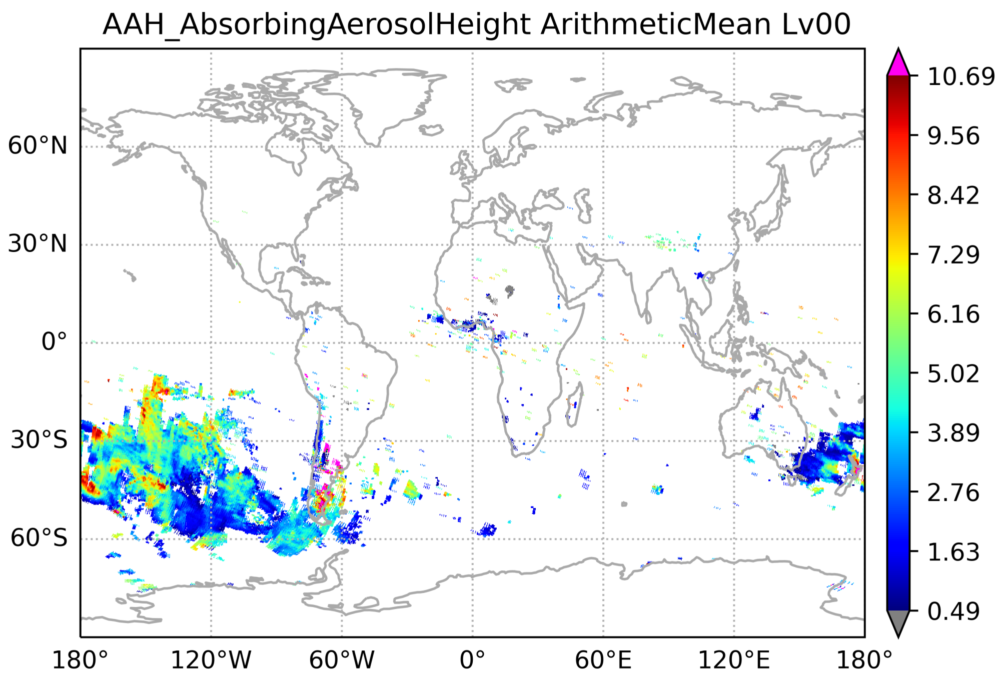

Figure 4.4: Gridded GOME-2C Absorbing Aerosol Height in January 2020, during the Australian wildfires, and the transport of aerosol afterwards in easterly direction.

4.2.6 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 ($\sim$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.

SIF filter options

We follow the recommendations from [*van Schaik et al.*, 2020] and the suggestions done by the review board.

- Only pixels with a cloud fraction < 0.2 are used
- Only pixels with a cloud fraction > -1.0 are used (no snow/ice)
- Only pixels with a cloud pressure > 0.0 are used (QA check)
- Only pixels with a single scattering angle > $0.1 \times \pi$ are used
- Only pixels with a surface albedo > 0.08 are used (i.e.: land)
- Only pixels with a residual autocorrelation value > 0.2 are used
- Only pixels with a surface height that is not zero are used, to avoid sea (-ice).

Gridded Sun Induced Fluorescence

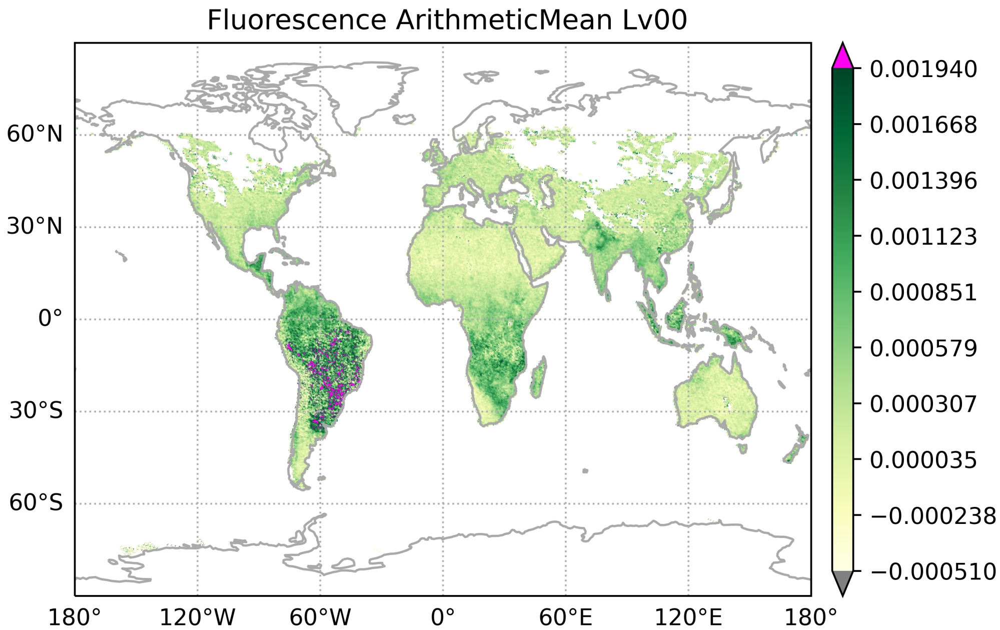

Figure 4.5: Example of GOME-2C monthly averaged fluorescence for January 2020.

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