Product User Manual

for the NRT, Offline and Data Record Absorbing Aerosol Index Products

EUMETSAT
AC SAF
ATMOSPHERIC COMPOSITION MONITORING

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20190408	1.90	All	First new issue
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		Chapter 6	Updated product quality conclusions (item 4 and 5).
		Section 1.5	Update of references
20210517	1.92b	Table 5.5	Added Solar Eclipse Corrections applied flag

Related product list

ID number	Instrument	Product Descripion
O3M-61.1	GOME-2A	NRT AAI from MSC
O3M-71.1	GOME-2B	NRT AAI from MSC
O3M-14.1	GOME-2A	Offline AAI from MSC
O3M-70.1	GOME-2B	Offline AAI from MSC
O3M-62.1	GOME-2A	NRT AAI from PMD
O3M-72.1	GOME-2B	NRT AAI from PMD
O3M-362	GOME-2C	NRT AAI from PMD
O3M-63.1	GOME-2A	Offline AAI from PMD
O3M-73.1	GOME-2B	Offline AAI from PMD
O3M-363	GOME-2C	Offline AAI from PMD
O3M-113	GOME-2A	Reprocessed AAI from MSC
O3M-179	GOME-2B	Reprocessed AAI from MSC
O3M-178	GOME-2A	Reprocessed AAI from PMD
O3M-180	GOME-2B	Reprocessed AAI from PMD

Contents

Chapter 1

Introduction

1.1 Purpose of this document

This document is the Product User Manual for the Offline ARS aerosol products retrieved within the context of the Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF). This document first presents some background information and a brief description of the retrieval algorithm. Next, the document provides information and guidance to the user on how to use and interpret the data product.

1.2 Scope

This PUM provides information on the ARS product of the AC SAF. This document does not go into much detail with regards to the algorithm or design of the software; please refer to the Algorithm Theoretical Basis Document (ATBD) for that information.

As the instruments go through phases of degradation, the product quality is affected. This Product User Manual does not describe the product quality beyond an initial demonstration of the output. For monitoring the product quality of the aerosol products, the reader is referred to the AC SAF Validation Report on the Aerosol products: (SAF/O3M/KNMI/VR/001).

1.3 Heritage

This algorithm was developed at KNMI (the Royal Netherlands Meteorological Institute) in the PhD thesis work of Martin de Graaf [*de Graaf et al.*, 2005] and was implemented in the Opera software for ozone profile retrieval.

This development was continued by 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
B & P	Bass and Paur
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
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
MLL	McPeters, Labow, Logan
MSC	Main Science Channels
NHP	NRT High resolution ozone Profile

Continued on next page

Table 1.1 – *Continued from previous page*

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
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
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
TOA	Top Of Atmosphere
TOMS	Total Ozone Mapping Spectrometer
TrOC	Tropospheric Ozone Column
UV	Ultra Violet
VIS	Visible

1.5 References

RD1	Algorithm Theoretical Basis Document for the NRT, Offline and Data Record Absorbing Aerosol Index Products, version 2.61, dd 2019-09-26.
RD2	Algorithm Theoretical Basis Document for the GOME-2 Absorbing Aerosol Height, SAF/AC/KNMI/ATBD/005, issue 1.4, 2 April 2019
RD3	De Graaf, M., P. Stammes, O. Torres, and R. B. A. Koelemeijer (2005), Absorbing Aerosol Index: Sensitivity analysis, application to GOME and comparison with TOMS, J. Geophys. Res., 110, D01201, doi:10.1029/2004JD005178.
RD4	O3MSAF Validation Report of the Absorbing Aerosol Index products, SAF/O3M/KNMI/VR/001, issue 3/2013, 2013-06-11.
RD5	ACSAF Validation Report of the NRT and Offline GOME-2C Absorbing Aerosol Index product, SAF/AC/KNMI/VR/007, issue 1/2019, 2019-10-09.
RD6	ACSAF Validation report on the Absorbing Aerosol Height products, SAF/AC/RMI-AUTH/VR/001, issue 1.0 / 2020-03-31.

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 in 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

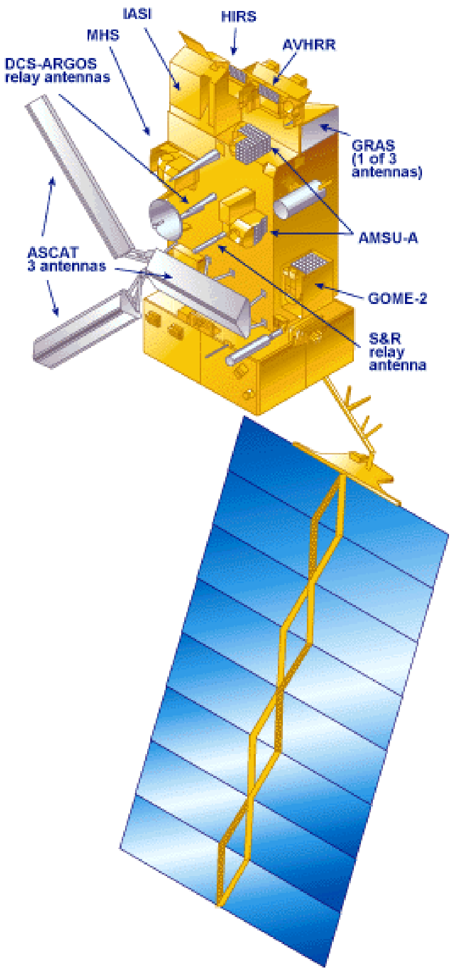

Figure 3.1: Metop

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.

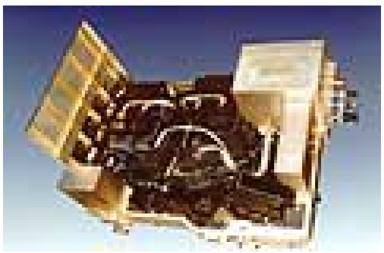

Figure 3.2: GOME-2

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) × 2.75° (along track)
Entrance slit	0.2 mm (across track) × 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 × 40 km (1920 km swath and integration time of 1.5 s)
	Band 1b - 4: 80 km × 40 km (1920 km swath and int. time of 0.1875 s)
	PMD: 10 km × 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, SCIAMACHY and OMI. This document may contain references and particular details from these instruments for legacy and comparison purposes.

Chapter 4

Algorithm background

4.1 Absorbing Aerosol Index

The Absorbing Aerosol Index (AAI) indicates the presence of elevated absorbing aerosols in the troposphere like desert dust and smoke. It separates the spectral contrast at two ultraviolet (UV) wavelengths caused by absorbing aerosols from that of other effects, including molecular Rayleigh scattering, surface reflection, gaseous absorption and aerosol and cloud scattering.

The AAI emerged as an error estimate in the Total Ozone Mapping Spectrometer (TOMS) ozone retrieval algorithm. As TOMS instruments have flown, on various platforms, from 1978 to 2006 providing nearly daily global coverage, the TOMS AAI record is the longest aerosol record available and it is used extensively to investigate aerosol impact on climate and study heavy dust, biomass burning and volcanic eruption events.

Traditionally, aerosol optical thickness measurements are being made using space-borne sensors operating in the visible and infrared (IR), where multiple scattering in the atmosphere is less important than in the ultraviolet (UV) and inversion calculations are relatively simple. In the visible and near-IR the large surface albedos of many land types make retrieval of aerosols difficult over these regions. With the ongoing development of numerical radiative transfer codes and increasing computational speeds accounting for multiple scattering is no longer a problem, allowing for new techniques of aerosol measurements in the UV. Because the surface albedos of both land and ocean are small in the UV, this wavelength range should be suitable for aerosol detection over land.

The AAI is derived directly from another quantity, the residue, which is defined in the following way [*Herman et al.*, 1997]:

$$r_\lambda = -100 \cdot \left\{ {}^{10}\log \left(\frac{I_\lambda}{I_{\lambda 0}} \right)^{\text{meas}} - {}^{10}\log \left(\frac{I_\lambda}{I_{\lambda 0}} \right)^{\text{Ray}} \right\} \tag{4.1}$$

In this equation, R_λ denotes the Earth's reflectance at wavelength λ. The superscript R^{meas} refers to TOA reflectances which are measured by GOME-2, while the superscript R^{Ray} refers to modelled TOA reflectances. These modelled reflectances are calculated for a cloud-free and aerosol-free atmosphere in which only Rayleigh scattering, absorption by molecules, Lambertian surface reflection as well as surface absorption can take place. As a result, the residue is a residual term caused by the presence of cloud and aerosols in the real scene as opposed to the modeled scene. More details about the calculation of the residue can be found in the ATBD

([RD1]).

The presence of clouds tends to make the residue negative. Scattering aerosols will generally do the same. Absorbing aerosols, on the other hand, increase the residue and will lead to a positive residue. For that reason, the AAI is defined as the positive part of the residue. The two wavelengths λ and λ_0 that constitute the AAI wavelength pair are set to 340 and 380 nm, respectively.

The name AAI is traditionally used for indicating absorbing aerosols, for which the residue has positive values. In the GOME-2 ARS product we will use the AAI as being synonymous to the residue, so the full range of residue values, positive as well as negative, will be reported in the AAI product.

4.2 Interpretation

The direct interpretation of the AAI in terms of aerosol properties is difficult. The residue (AAI/SCI) is a unitless quantity that depends on many aspects of the aerosol scene. In the paper by *de Graaf et al.* [2005] [RD3] a sensitivity study was performed.

In this sensitivity study it was shown that there are at least two possibilities to create a positive residue. Firstly, an absorbing aerosol layer can absorb Rayleigh scattered radiation from below the layer. Because the Rayleigh optical thickness is strongly wavelength dependent this creates a difference in the reflectance at two UV wavelengths relative to that of a Rayleigh atmosphere, even with gray absorbers (i.e. wavelength independent absorbing particles). When the absorbing ability of the layer increases more radiation is absorbed and the deviation increases, increasing the residue. The same is true when the amount of atmosphere under the absorbing layer increases.

Secondly, the aerosol absorption itself can be wavelength dependent, creating a spectral difference in the TOA reflected radiation. This will also create a positive residue if the absorption at the shorter wavelength is stronger, even when the aerosol layer is close to the surface. When the spectral absorption difference increases the residue will increase, meaning that different aerosol types produce different residues under the same circumstances. For an atmosphere which is dominated by scattering (either by particles, molecules, the surface or clouds) the reflectance will not deviate much from the reflectance of a Rayleigh atmosphere with an adjusted surface albedo, yielding zero or small negative residues.

The residue is sensitive to sun glint, which should be flagged. Sun glint is expected in GOME-2 data at the east side of the swath.

The residue is very sensitive to the absolute radiometric calibration of satellite radiances at 340 and 380 nm [RD1]. Deviations in the residue due to calibration errors may be presents in the level 1B data.

The residue (or AAI in case of GOME-2) ranges typically from about -1 for cloudy scenes to +2 and larger for desert dust or smoke plumes.

4.3 Level 1 Input

The basic level 1B data consists of a calibrated solar spectrum and spectra of calibrated geo-located 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 spectral level 1b data used in the calculation of the AAI are 1-nm averaged reflectances at 340 and 380 nm.

4.4 Level 2 output

Aerosol data are calculated and written as one or more HDF5 product files per orbit. The product contains the geolocation, angles and the retrieved AAI. At a later stage, the other aerosol parameters will be added to the product as they come available.

4.5 Delivery time to users / user access

The Aerosol Absorbing Index is classified as an NRT product, and can be obtained via EUMETCast or the EUMETSAT/AC SAF archive. Please see the AC SAF website at http://acsaf.org or contact the AC SAF helpdesk at helpdesk@acsaf.org for more information. The delivery time of the offline ARS product to the EUMETSAT/AC SAF archive will be within two weeks maximum, but usually within a day or two.

4.6 Geographical coverage and Granularity of the level 2 product

The geographical coverage of the aerosol product is practically all of the sun-lit side of the earth. 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 possibility that the same surface area is viewed more than once a day. Because the algorithm uses information from the wavelength region between 340 and 380 nm, the granularity of the default AAI output product is the same as the Band 2b measurements. This means that with nominal conditions the pixel size is 40 $\times$ 80km in flight-direction $\times$ cross track-direction.

Chapter 5

The ARS/AAI Product

5.1 Structure of the ARS Product File

The format of the offline Level 2 ARS profile product file is HDF5. 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 taken either from the level-1b or other input data files, copied from the configuration file, or calculated by the program.

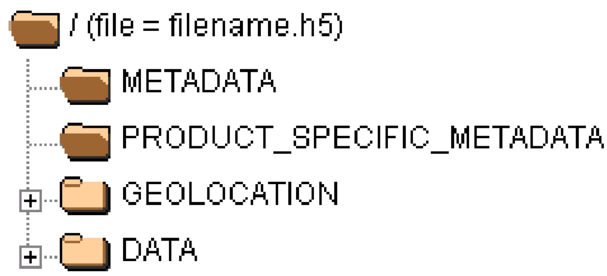

Figure 5.1: Structure of the HDF5 file.

The Metadata group contains parameters about the satellite instrument required by UMARF, such as metadata given in the AC SAF software requirements, 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, 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 Geolo-

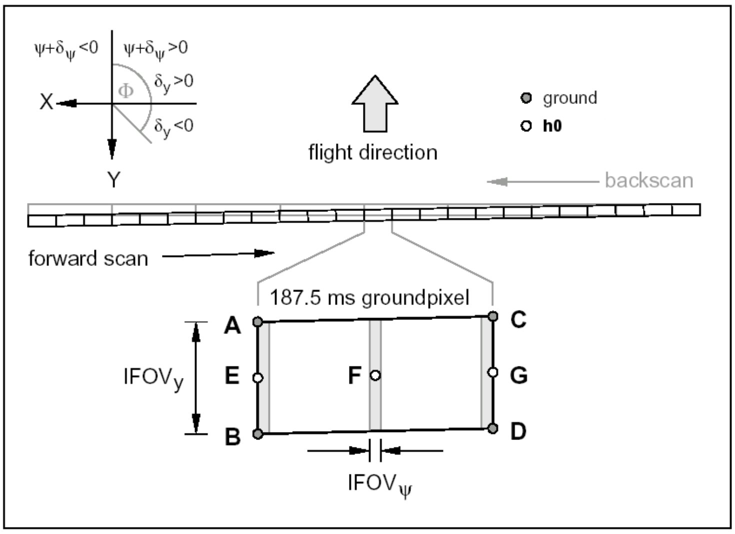

Figure 5.2: Ground pixel geometry (ref: [RD4])

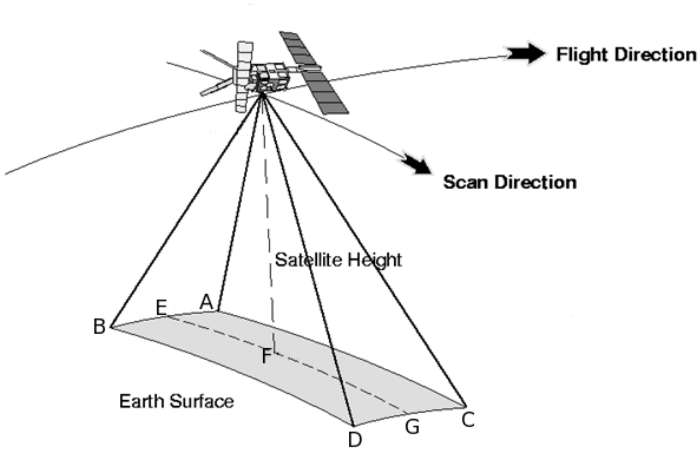

Figure 5.3: Ground pixel geometry (ref: [RD4])

cation group is organized in multi-dimensional arrays. The first dimension always corresponds to the total number of pixel sets which has been processed, hereafter referred to as NSets, the total number of retrievals per set is referred to as NElements.

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.

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 Table 5.1. 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

Continued on next page

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 ARS products 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	**Data Type**	**Description**
Wavelengths	float array, rank 1	Wavelengths used for calculating the AAI

FullWidthTriangle	float	FullWithHalfMaximum of the reflectance averaging function around the Wavelengths above.

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.

Table 5. Geolocation group contents.

Table 5.4: Geolocation group contents.

Dataset name	Data Type	Unit	Description
Time	string array rank 2	-	UTC time in CCSDS format
LongitudeCenter	float arr rank 2	degree	Longitude of the center of the ground pixel (F)
LatitudeCenter	float arr rank 2	degree	Latitude of the center of the ground pixel (F)
LongitudeCorner	float arr rank 3	degree	Longitude of corner A of the pixel
LatitudeCorner	float arr rank 3	degree	Latitude of corner A of the pixel
SolarZenithAngle	float arr rank 2	degree	Solar zenith angle center of the ground pixel
SolarAzimuthAngle	float arr rank 2	degree	Solar Azimuth angle w.r.t. north for center of ground pixel at H0
LineOfSightZenithAngle	float arr rank 2	degree	LineOfSight zenith angle for center of the ground pixel
LineOfSightAzimuthAngle	float arr rank 2	degree	Line of Sight Azimuth angle w.r.t. north of the ground pixel

Continued on next page

Table 5.4 – *Continued from previous page*

Dataset name	**Data Type**	**Unit**	**Description**
RelAzimuthAngle	float arr rank 2	degree	Relative Azimuth angle between sun and viewing angles
SubSatellitePointLongitude	float arr rank 2	degree	Geocentric longitude of subsatellite point
SubSatellitePointLatitude	float arr rank 2	degree	Geodetic latitude of subsatellite point
ScatteringAngle	float arr rank 2	degree	Total scattering angle the photon made from sun beam to satellite assuming single scattering
ScanDirection	float arr rank 2	N/A	Direction of the scan mirror (1 = forward, 2 = backward)
ScannerAngle	float arr rank 2	degree	Angle of the scan mirror.
NrOfPixelsInScan	int arr rank 2	N/A	Number of pixels within the scan line.
NElements	int arr rank 2	N/A	Number of pixels in each AAI set
IndexInScan	int arr rank 2	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)).

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 the same as for the Geolocation group.

Table 6. Data group contents.

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]

Continued on next page

Table 5.5 – *Continued from previous page*

Dataset name	Data Type	Unit	Description
			3. Groundpixel is in SAA; F_SSA in Level1b/PCD_BASIC [RD1] 4. Sunfile of date missing: older sunfile used 5. [not used] 6. [not used] 7. [not used] 8. Earthshine radiance data missing 9. Earthshine radiance data invalid 10. Solar irradiance data missing 11. Solar irradiance data invalid 12. [not used] 13. [not used] 14. Absorbing Aerosol Index data invalid (due to input errors ((ir-)radiance) or out of bound geometry conditions (Solar Zenith Angle, Solar Azimuth Angle, Viewing Zenith Angle, Viewing Azimuth Angle, Relative Azimuth Angle, ScatteringAngle) or external input valies like out of bound surface pressure or total ozone column). 15. Failure in setup of the Forward Model Input 16. [not used] 17. Sunglint flag 18. [not used] 19. Cloud Pressure Adjusted to Surface Pressure 20. Solar Eclipse Corrections applied 21. Other error 22 - 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 - 6: [not used] 7: No retrieval done! (due to any kind of input errors) 8 - 32: reserved for future use

Table 5.6: Data group contents, Output section.

Output Section **Dataset name**	**Data Type**	**Unit**	**Description**
NElements	int arr, rank 1	-	Number of AAI elements per set
AAI	float arr, rank 2	-	Absorbing Aerosol Index; Dimension = NElements x NSets
SunGlintFlag	float arr rank 2	-	Flag is sum of following subflags: 0=no sun glint; 1=land 4=Cloud fraction >0.3; 8=Cloud pressure <850 hPa (and Cf >0.1), 32=sun glint angle <18 degrees, 64=sun glint angle <11 degrees. Use only flag values 0, 1, 4, 8, 33-63, not 32 or >=64.
CorrectionFactor	float arr rank 2	-	Degradation Correction factor
UncorrectedResidue	float arr rank 2	-	Residue values that were not corrected for degradation.
DegradationCorrected-Residue	float arr rank 2	-	Residue, with degradation correction applied, before application of the End Of Orbit Corrections.
PMD_CloudFraction	float arr rank 2	-	Cloud fraction from AVHRR copied directly from L1b for PMD band AAI retrievals and averaged on B1b resolution in case of MSC based retrievals
PMD_SceneHomogeneity	float arr rank 2	-	Scene homogeneity from AVHRR copied directly from L1b for PMD band AAI retrievals and averaged on B1b resolution in case of MSC based retrievals
OrbitCorrectionValue (optional)	float arr rank 2	-	End of Orbit Correction values
OrbitCrossTrack-CorrectionValue (optional)	float arr rank 2	-	Cross track correction values

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_ARP_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 ARP indicates the PMD Absorbing Aerosol Index product. Note that these three letters are replaced by NAP for the Near Real Time products.

5.4 File size estimate

5.4.1 Estimated size of ARS output file

The size of the output file can vary. The size is affected by different string lengths, the maximum number of profiles per set, the actual number of AAI retrievals, the addition of optional data sets to the file, and possibly the compression factor in the HDF5 output file. On average, each PDU-sized data product of ARS data is about 113Kb.

5.5 Using the data

5.5.1 AAI

An example of the Absorbing Aerosol Index is given in Figure 5.4. In this figure, a large Saharan desert dust plume is transported over the Atlantic Ocean from Africa to South America.

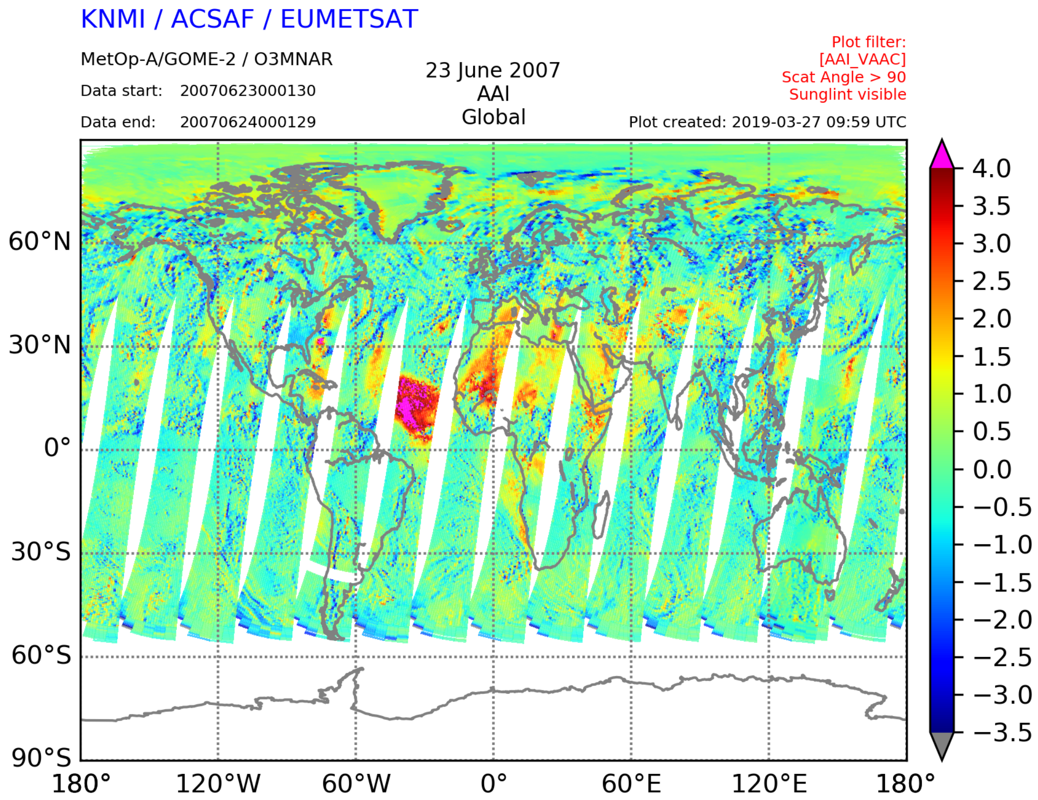

Figure 5.4: Absorbing Aerosol Index (AAI) from GOME-2 for June 23rd 2007.

5.5.2 Quality flags

Quality flags are very important as indicators for the correctness of both the input and the retrieved AAI. 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 sun glint. The sun glint causes a spurious AAI signal. This sun glint flag in the QualityInput comes directly from the Level-1b, and is on a scan level basis (i.e.: valid for the whole scan instead for the subpixel.

5.5.3 SunGlintFlag

There is a data record in the Data Group called SunGlintFlag. This indicates on a ground pixel basis whether there is a risk of sun glint. Flag is the sum of the following subflags:

- 0 no sun glint;
- 1 land;
- 4 Cloud fraction >0.3;
- 8 Cloud pressure <850 hPa (and Cf >0.1);
- 32 sun glint angle <18 degrees;

64 sun glint angle <11 degrees;

Users are advised to use pixels with flag values exactly 0, 1, 33-63.

Users are advised NOT to use flag values of exactly 32 or values larger or equal than 64.

5.5.4 ScatteringAngle

In the north and south eastern edges of the swath there are increased values of the AAI due to geometric effects. The light from the sun is scattered in a forward direction to the satellite and the algorithm does not handle this at the moment. Users are advised to use pixels with scattering angles larger than 90 degrees.

5.5.5 Scattering Aerosol Index (SCI)

Although most aerosol types have the ability to scatter as well as absorb radiation, we distinguish between scattering and absorbing aerosols. As explained in section 4.1, the presence of absorbing aerosols result in a positive value for the residue (AAI). Clouds and scattering aerosols on the other hand both scatter radiation and therefore tend to lower the residue. As a result, a positive value for the AAI may be considered as a clear and unambiguous sign of the presence of absorbing aerosols, whether the scene is cloud-free or not.

The detection of scattering aerosols is more complicated and challenging. As both scattering aerosols and clouds tend to lower the residue, it is not possible to distinguish between clouds and scattering aerosols in such circumstances, unless the scene is sufficiently cloud-free.

In order to use the residue product to detect scattering aerosols, the presence of potential clouds needs to be excluded first. For this purpose, an alternative cloud mask is available in the AAI output product to look for cloud-free scenes. The cloud parameters are "PMD_CloudFraction" and "PMD_SceneInhomogeneity", and these may be used to screen out potential clouds, depending on the user needs.

The cloud fraction and scene inhomogeneity parameters stored in the AAI output product were taken from the L1b product, where they are provided on PMD footprint resolution. However, the original data were measured by the imager AVHRR, with a much higher spatial resolution. For the PMD-AAI the cloud information is available for the individual PMD footprints. For the Main Science Channel AAI, the cloud information was made available for each of the MSC footprints by binning of PMD footprints.

Chapter 6

Product quality and characteristics

The product quality is determined mainly by the quality of the input parameters reflectances, ozone column, and surface height. The ozone column and surface height are both known with a (relatively) high accuracy. The impact of errors in the radiometric calibration can be strong, though. The most important example of this is the impact of instrument degradation on the AAI. Instrument degradation has a strong impact on the AAI. The GOME-2 AAI is suffering from scan-angle dependent instrument degradation. If it would be left uncorrected, there would be an east-west bias which amounts to $\sim$3 index points for data measured at the end of 2012 compared to the beginning of the mission. The instrument degradation and scan angle bias are corrected for.

As for the quality of the ARS/AAI products, it has been studied using a number of different verification techniques. An extended report of these studies and their results may be found in the AC SAF Validation Report.

Here we summarise the main conclusions:

1. Global maps of GOME-2 AAI compare well to global maps of OMI AAI.

2. From a pixel-to-pixel comparison with the AAI from SCIAMACHY it is found that the GOME-2 MSC AAI is of good quality. This we conclude from the good (one-to-one) correlation between GOME-2 and SCIAMACHY AAI. The offset between the GOME-2 MSC AAI and SCIAMACHY AAI is found to be close to zero. Additionally, the bias-corrected uncertainty in the GOME-2 MSC AAI was found to be $\sim$0.5 index point. This is only an upper limit, because this value is also determined by the quality of the SCIAMACHY AAI and the performance of our intercomparison approach. In any case, the (bias-corrected) value of 0.5 index points relates well to the target uncertainty of 0.5 index points mentioned in the PRD.

3. More quantitative results follow from the analyses of the global mean residue. The global mean MSC residue in particular revealed a similar seasonal variation for GOME-2 (on MetOp-A) as was found earlier for GOME-1. However, a modest offset of $\sim$0.4 index points w.r.t. the GOME-1 global mean value was found. When the calculation was repeated taking only those measurements that are located in the inner (GOME-1) part of the GOME-2 swath, the offset was reduced to $\sim$0.2 index points.

4. For GOME-2 on MetOp-B we found the MSC AAI to agree nicely with the MSC AAI from the MetOp-A platform. Only a small offset of $\sim$0.3 index points seems to be present. For GOME-2 on MetOp-C we found the MSC AAI to agree well with the MSC AAI from the MetOp-A and MetOp-B platforms. Only a small offset of 0.4–0.8 index points seems to be present, depending on the scanner mirror position.

5. The PMD AAI from MetOp-A, -B, and -C show behaviour similar to that of the MSC AAI products. For instance, statistical analyses show that the PMD AAI from MetOp-A is very close to the MSC AAI from MetOp-A. A small offset of 0.3 index points is found. An explanation for the differences between the MSC and PMD product is the (known) different radiometric calibration between MSC reflectances and PMD reflectances.

6. The GOME-2 AAI products have, like any other AAI product, a number of characteristic properties that need to be kept in mind. First of all, sun glint leads to anomalously high values for the AAI. Measurements affected by sun glint should therefore not be used. A sun glint flag is present in the product for filtering out sun glint situations. Secondly, solar eclipse events lead to very high and unphysical values for the AAI. These data should not be used. Thirdly, the uncorrected GOME-2 AAI would show a modest scan-angle dependence (not caused by instrument degradation).

7. At the east side of the swath at high latitudes (both North and South) there are areas showing too large values for the AAI. This is known behaviour of the AAI product but the physical background is yet unknown. These increased values are taken care of by the End-of-Orbit corrections.

8. The resulting AAI should be a relatively clean product, where instrument degradation, scan angle dependencies and systematic anomalies are taken care of.

Chapter 7

Further information

7.1 AC SAF website

Further up to date information and documentation on the ARS aerosol 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.

7.2 User Notification Service

EUMETSAT maintains a User Notification Service (UNS) that disseminates instantaneous messages relating to the various satellite platforms they operate, the (GOME-2) instruments 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.

7.3 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 Absorbing Aerosol Index are provided by KNMI in the framework of the EUMETSAT Satellite Application Facility on Atmospheric Composition (AC SAF)".

Chapter 8

Algorithm Change log

Algorithm Change log.

Alg/Sw/Conf/OPF	Changes
1.00/1.32/-/4.01	Inclusion of cloud parameters on PMD pixel resolution in the AAI product
1.00/1.33/-/4.10	The NRT/Offline Absorbing Aerosol Index products will start to use a GOME-2 instrument degradation correction factor. This will bring the global mean of the AAI signal back to the signal level at the beginning of the mission (both for GOME-2-A and GOME-2-B respectively). There will be two additional parameters in the Data group: CorrectionFactor and UncorrectedResidue.
1.00/1.34/-/4.10	Less stringent spectral quality control in order to allow retrieval of AAI of significantly more ground pixels. This leads to more pixels being retrieved at the northern and southern edges of the orbits, and a more stable degradation correction of the AAI.
1.01/1.35/-/4.10	Bugfix of the date index selection of the instrument degradation correction values for the PMD AAI (for reprocessed dates before 2013-07-16).
1.20/1.50/1.50/4.50	Use of AAI End of Orbit corrections
1.30/2.00/1.5x/4.60	General update to software version 2.0. Albedo / LER month selection; Adding Nprofiles to SPMG in O3P; Filling in AlbedoSource when using LER
1.30/2.01/1.5x/4.60	Bugfix: Albedo / LER interpolation of time was inverted
1.31/2.02/1.5x/4.60	Fix to handle the fill values in the irradiance error from the temporary Solar Model spectrum of GOME-2A.
1.32/2.03/1.5x/4.60	Fix to handle infinity and NaN values across compilers in a uniform way.
1.32/2.06/1.5x/4.60	Interpolation of the viewing zenith angle for the DLER calculation.
1.40/2.10/1.5x/4.70	Solar Eclipse Correction flag.

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