



O3MSAF
Algorithm Theoretical Basis
Document for ARS


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0.2	2007-06-06	Revisions after ORR-A2 comments.
0.3	2007-10-19	Revised after ORR-A2 review
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1. INTRODUCTION

1.1 Purpose

This document is the Algorithm Theoretical Baseline Document for ARS, the GOME-2 aerosol product, which is part of the O3MSAF. This document presents the scientific background of the algorithm, presents an outline of its implementation and assists the user of this product in its physical interpretation. The document also presents a sensitivity study.


1.2 Scope

This ATBD provides information on the AAI part of the ARS product. This algorithm was developed a KNMI in the PhD thesis work of Martin de Graaf and was implemented in the Opera software for ozone profile retrieval.

1.3 Glossary

1.3.1 Acronyms

AAI	Absorbing Aerosol Index
ARS	Aerosol Retrieval System
ATBD	Algorithm Theoretical Basis Document
B&P	Bass and Paur
CHEOPS	Climatology of Height-resolved Earth Ozone and Profiling Systems
DAK	Doubling-Adding KNMI
DFS	Degrees of Freedom for Signal
ECMWF	European Centre for Medium-range Weather Forecast
ERS	European Remote Sensing Satellite
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FRESCO	Fast Retrieval Scheme for Cloud Observables
FWHM	Full Width Half Maximum
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Instrument
KNMI	Royal Netherlands Meteorological Institute
LIDORT	LInearized Discrete Ordinate Radiative Transfer
LUT	Look Up Table
O3MSAF	Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring


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OE	Optimal Estimation
OMI	Ozone Monitoring Instrument
OPERA	Ozone Profile Retrieval Algorithm
PMD	Polarization Measurement Device
PSC	Polar Stratospheric Clouds
RMS	Root Mean Square
RTM	Radiative Transfer Model
SAF	Satellite Application Facility
SAGE	Stratospheric Aerosol and Gas Experiment
SBUV	Solar Backscatter Ultra-Violet radiometer
SZA	Solar Zenith Angle
TOMS	Total Ozone Mapping Spectrometer
UV	Ultra Violet
VIS	Visible

1.4 Reference documents

[RD1] 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


[RD2] De Graaf, M., Remote sensing of UV-absorbing aerosols using space-borne spectrometers, Ph.D. thesis, Free University, Amsterdam, 2006

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2. OVERVIEW

The AAI algorithm retrieves information on absorbing aerosols contained in the GOME UV/VIS Earthshine spectrum. In the next sections we will give a physical interpretation of the AAI and a theoretical sensitivity analysis.

The Absorbing Aerosol Index (AAI) indicates the presence of elevated absorbing aerosols in the Earth's atmosphere. Since the AAI distinguishes between scattering and absorbing effects, it does not suffer much from cloud contamination. The aerosol types that are mostly seen in the AAI are desert dust and biomass burning aerosols. The AAI in the O3MSAF ARS product is derived from the reflectances measured by GOME-2 at 340 and 380 nm.

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3. ALGORITHM BACKGROUND

3.1 GOME Absorbing Aerosol Index

The Absorbing Aerosol Index (AAI) indicates the presence of elevated absorbing aerosols in the troposphere. 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 (Torres et al., 1998).

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.

We will adopt here the name residue (r) for the result of equation (1) in section 3.2.1, which is a quantity derived from measured reflectances. 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 (see also section 3.4).

The residue emerged as an error estimate in the Total Ozone Mapping Spectrometer (TOMS) ozone retrieval algorithm (Torres et al., 1998, 1999). 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 (e.g.: Hsu et al., 1996, Herman et al., 1997, Seftor et al., 1997, Chiapello et al., 1999, Pandi et al., 2001, Alpert et al., 2001, Moulin et al., 2004).

In this document we will give a physical interpretation of the absorbing aerosol index, facilitated by presenting an analysis of the main sensitivities of the index. A theoretical basis for the AAI was given by Torres et al. (1998), using aerosol models with spectrally independent refractive indices. The radiance changes for different surface albedos, aerosol refractive indices, aerosol layer height and solar zenith angles were discussed, giving insight in the behaviour of an aerosol laden atmosphere and the resulting residue values therein. The main sensitivities were known qualitatively since 1997-1998: the residue is dependent on aerosol type (Torres et al., 1998) and on aerosol single scattering albedo and aerosol layer height (Herman et al., 1997). The quantitative sensitivities have been investigated fully in [RD1] and [RD2], and are presented here.

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Recently, new evidence showed the incorrectness of the assumption of a spectrally independent refractive index for mineral dust and the implications for the AAI (Sinyuk et al., 2003, Mahowald et al., 2004). The sensitivity of the residue for spectrally dependent refractive indices is compared to the residues found for spectrally independent refractive indices. The definition of the residue is given in section 3.2.1 and the calculation method used in this paper is presented in section 3.2.2. In section 3.3 the influence on the residue of aerosol micro- and macro-physical parameters, atmospheric optical, physical and chemical parameters and surface parameters are given separately, by means of a radiative transfer model study.

3.2 Residue Method

In this section, the definition and derivation of the residue is given and the method of calculation used for the GOME-2 data.

3.2.1 Definition of the Residue

The residue r is a wavelength-dependent variable defined as (Herman (1997))

$$r_{\lambda} = -100 \cdot \left\{ {}^{10}\log\left(\frac{I_{\lambda}}{I_{\lambda 0}}\right)^{meas} - {}^{10}\log\left(\frac{I_{\lambda}}{I_{\lambda 0}}\right)^{Ray} \right\} \quad (1)$$

where I_{λ} is the radiance at the top of the atmosphere (TOA) at a wavelength λ .

The superscript I^{meas} refers to a measured TOA radiance of a real atmosphere with aerosols, as opposed to a calculated TOA radiance for an aerosol-free atmosphere with only Rayleigh scattering and absorption by molecules and surface reflection and absorption. The latter is referred to as I^{Ray} .

The reflectance is defined as

$$R = \frac{\pi I}{\mu_0 E_0} \quad (2)$$

where E_0 is the solar irradiance at TOA perpendicular to the direction of the incident sunlight and μ_0 is the cosine of the solar zenith angle ϑ_0 . So $\mu_0 E_0$ is the solar irradiance at TOA incident on a horizontal surface unit. Using equation (2) we can replace all quotients of radiances in equation (1) with quotients of reflectances.

If the surface albedo A_s for the Rayleigh atmosphere calculation is chosen so that

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$$R_{\lambda_0}^{meas} = R_{\lambda_0}^{Ray}(A_s) \quad (3)$$

where λ_0 is a reference wavelength, equation (1) can be reduced to

$$r_\lambda = -100 \cdot 10 \log \left(\frac{R_\lambda^{meas}}{R_\lambda^{Ray}} \right) \quad (4)$$

where $R_{\lambda_0}^{Ray}$ is calculated for surface albedo $A_s(\lambda_0)$, so the surface albedo is assumed to be constant in the range $[\lambda, \lambda_0]$. We will use for GOME-2 the wavelength pair $\lambda/\lambda_0 : 340 \text{ nm}/380 \text{ nm}$.

3.2.2 Calculation of the Residue

Equation (3) involves finding a surface albedo for which the measured reflectance at the reference wavelength is equal to the reflectance of a pure Rayleigh atmosphere with all scattering and absorption effects accounted for in the surface albedo. This inversion process was performed with Lookup Tables (LUTs) of the reflectances, as described below.


On the assumption that the atmosphere is bounded from below by a Lambertian surface, which reflects incident radiation uniformly and unpolarised in all directions, the surface contribution to the reflectance at TOA can be separated from that of the atmosphere (Chandrasekhar, 1960):

$$R(\mu, \mu_0, \phi - \phi_0, A_s) = R_0 + \frac{A_s t(\mu) t(\mu_0)}{1 - A_s s^*} \quad (5)$$

The first term, R_0 , is the path radiance, which is the atmospheric contribution to the reflectance. The second term is the contribution of the surface with an albedo A_s . t is the total atmospheric transmission, s^* is the spherical albedo of the atmosphere for illumination from below, μ is the cosine of the viewing zenith angle ϑ and $\phi - \phi_0$ is the relative azimuth angle.

The path radiance can be expanded in a Fourier series. For a Rayleigh atmosphere, when $R_{\lambda_0}^{Ray}$, the expansion is exact with only three terms in $\phi - \phi_0$, because of the cosine-squared scattering angle dependence:

$$R_0(\mu, \mu_0, \phi - \phi_0) = a_0 + \sum_{i=1}^2 2a_i(\mu, \mu_0) \cos i(\phi - \phi_0) \quad (6)$$

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R_0 is calculated with LUTs of $a_i(\mu, \mu_0)$, $t(\mu)$ and s^* for all wavelengths used. Then the surface albedo A_s in Equation (3) can be found from

$$A_s = \frac{R - R_0}{t(\mu)t(\mu_0) + S^*(R - R_0)} \quad (7)$$

by replacing R by $R_{\lambda_0}^{meas}$ in equation (7). Note that this equation allows negative surface albedos, which occurs for highly absorbing (aerosol) layers.

Lookup tables of a_i , $t(\mu)$, and s^* were prepared as a function of μ and μ_0 , surface pressure P_s and ozone column density Ω with the radiative transfer model DAK. The coefficients were calculated for 42 Gaussian distributed μ and μ_0 points, ozone columns of 167 and 501 DU and surface pressures of 1013, 802, and 554 hPa, as the dependence of the residue on total ozone column was found to be linear, whereas the dependence on surface pressure was non-linear. The surface albedo and reflectance were found by interpolation between these points. Interpolation between ground pressure points was performed with a second order polynomial, all other interpolations were linear.

The residue is calculated from the GOME-2 reflectances by taking 1-nm wide windows around 340 and 380 nm, in order to reduce the impact of small spectral shifts, Fraunhofer lines, etc.. The Rayleigh calculations are performed for exactly 340 and 380 nm.

3.3 Residue Sensitivities

The effects of several aerosol parameters on the residue were studied, as well as the effect of polarisation, clouds and atmospheric constituents, using the radiative transfer model DAK. Thereto the measured reflectances R_λ/R_{λ_0} were replaced by simulated reflectances. The 340 nm/380 nm pair was chosen as the default pair.

3.3.1 Radiative Transfer Model DAK

The Rayleigh atmosphere reflectances and the LUT coefficients were calculated with the Doubling-Adding KNMI (DAK) radiative transfer model (Stammes, 2001). This model computes the monochromatic reflectance and transmittance in a plane-parallel atmosphere including polarisation, using the polarised doubling-adding method (De Haan et al., 1987). This method calculates the polarised internal radiation field of the atmosphere in an arbitrary number of layers, each of which can have Rayleigh scattering, gas absorption, and aerosol and cloud particle scattering and absorption.

3.3.2 Standard Atmosphere, Geometry and Definition of Aerosol Models

For the atmospheric gas and temperature profile the standard Mid-Latitude Summer (MLS) atmosphere (Anderson, et al., 1986) was adopted throughout all calculations. The standard ground pressure was 1013 hPa, the standard ozone column was 334 DU. Linear polarisation was taken into account. A surface albedo of 0.05 was used to simulate dark surfaces and 0.6 to simulate bright surfaces. An aerosol layer could be introduced to simulate aerosol effects. The default altitude of the bottom of this one kilometer thick layer was three kilometers.

Two different types of phase functions were used to simulate the aerosols: the Henyey-Greenstein (HG) function and Mie phase functions. The HG phase function is defined as (Henyey (1941)):

$$\Phi(\cos \Theta) = \frac{1 - g^2}{(1 + g^2 - 2g \cos \Theta)^{3/2}} \quad (8)$$

Here Θ is the scattering angle and $g = \langle \cos \Theta \rangle$ is the asymmetry parameter. The asymmetry parameter is a measure for the amount of forward scattered radiation by aerosols; the greater g , the greater the amount of radiation scattered in the forward direction. For Rayleigh scattering the amount of radiation in the forward direction is equal to the amount of backward scattering, so g is zero. The default value for the asymmetry parameter chosen for HG aerosol was $g = 0.7$, representing moderately forward scattering aerosols. The analytic HG function can be used to separate the effects of the single scattering albedo and the asymmetry parameter.

Table 1: Parameters for the aerosol models used in this study.

	λ	C2	D1a	D3	HG
r_g		0.14	0.12	0.50	-
v_g		1.45	2.20	2.20	-
Re(m)		1.55	1.55	1.55	-
Im(m)	340	0.04	0.0006	0.0006	-
Im(m)	380	0.04	0.0042	0.0042	-
ω_0	340	0.82	0.90	0.75	0.90
ω_0	380	0.83	0.93	0.81	0.90
g	340	0.73	0.70	0.83	0.70
g	380	0.73	0.69	0.80	0.70
τ	340	1.00	1.00	1.00	1.00
τ	380	1.04	1.01	1.01	1.00

Mie aerosol phase functions were used to model more realistic aerosols. In Mie calculations the complex refractive index m needs to be changed to vary the single scattering albedo, which also affects the asymmetry parameter. This

introduces spectral variations in these parameters, which affect the residue calculations. Three types of aerosols were used, a carbonaceous aerosol model (C2), a small mode dust aerosol model (D1a) and a large mode dust aerosol model (D3). C2 is a smoke model with wavelength independent refractive index defined in Torres (1998), D1a is the fine dust model introduced in Torres (2002), with the updated imaginary part of the refractive index of Sinyuk (2003). D3 is the large mode dust aerosol model as defined by Torres (1998), also with the updated imaginary part of the refractive index of Sinyuk (2003). In Table 1 the values of the parameters of the different aerosol models used in this study are summarised. The size distribution of the Mie aerosols was assumed to be log-normal.

3.3.3 Sensitivity of the Residue for Mie Aerosol

Data on aerosol properties suggest that the refractive index of dust aerosol is strongly wavelength dependent in the UV (Patterson (1977), Sinyuk (2003)). This has implications for the residue, as will be shown below with the Mie aerosol models, in which this wavelength dependence is taken into account.

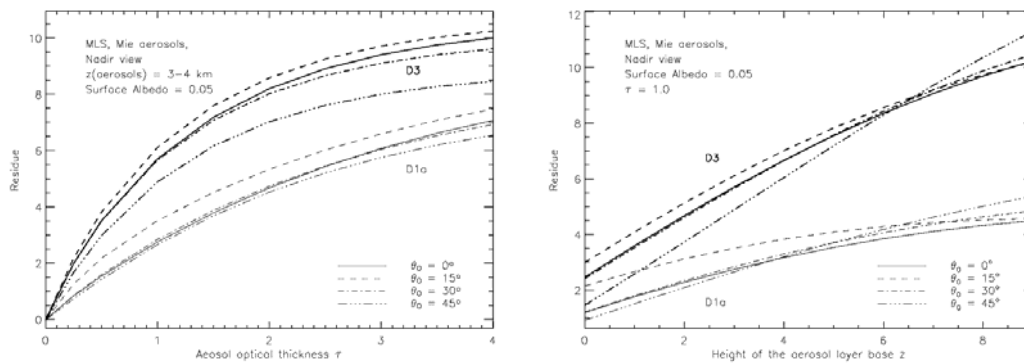



Figure 1: Mie aerosols: (a) Dependence of the residue on aerosol optical thickness. (b) Dependence of the residue on altitude of the aerosol layer z.

3.3.3.1 Aerosol optical thickness

Like with HG aerosol, the residue increases with aerosol optical thickness (Figure 1a). The increase is larger for larger aerosols, because the single scattering albedo is smaller (see Table 1). The residue is also much larger for aerosols with a wavelength dependent refractive index than for gray aerosols (cf. 1a); although the D1a aerosols have almost the same characteristics as the HG aerosols, they produce a much stronger residue increase for increasing aerosol optical thickness than the HG aerosols.

3.3.3.2 Aerosol layer altitude

The residue increases linearly with aerosol layer altitude, like it did for HG aerosol (cf. Figure 1b and 1b). The slope is proportional to the aerosol single scattering co-albedo, as was found in previous studies (Herman (1997), Torres

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(1998)). But there is an off-set for aerosols with a wavelength dependent refractive index: using gray aerosols the residue is positive only for aerosol higher than about one to two kilometers in altitude, whereas non-gray absorbing aerosols can be detected even very close to the surface.

This result is consistent with the study of (Mahowald (2004)), who found a stronger residue signal over mineral aerosol sources when gray dust aerosol models were replaced by aerosol models with wavelength dependent refractive indices. This implied the detection of non-gray aerosols closer to the surface, and thus closer to the source, than previously assumed.

3.3.4 Sensitivity of the Residue to Atmospheric, Surface and Geometric Parameters

3.3.4.1 Surface albedo

Increasing the surface albedo has two competing effects. Firstly, it will increase the role of absorption by the aerosol layer compared to that of the surface. The reason is that below the aerosol layer radiation is bounced back and forth between the surface and the aerosol layer before escaping to space. Absorption takes place each time both at the surface and in the aerosol layer.

When the surface albedo is raised, the relative importance of the absorption by aerosols is increased, amplifying the effect of the absorption characteristics of the aerosol layer. This can be spectrally flat, producing no effect on the residue with increasing surface reflection, or wavelength dependent, increasing the residue with increasing surface reflection.

Secondly, increasing the surface albedo increases the amount of directly reflected radiation emerging at the top of the atmosphere, which results in itself in a zero residue. This will reduce the effect of an aerosol layer and lower the residue for increasing surface reflection.

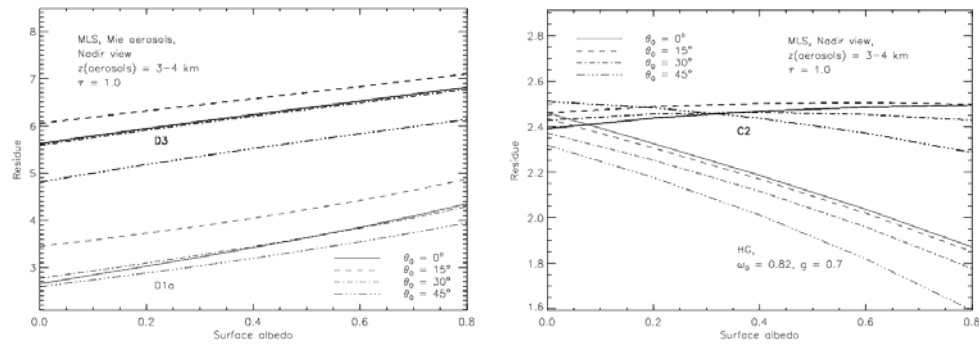


Figure 2: Dependence of the residue on surface albedo for nadir view and solar zenith angles between 0° and 45° . (a) Atmosphere with Mie aerosols type D1a (normal lines) and D3 (bold lines). (b) Atmosphere with Mie aerosols type C2 (bold lines) and HG aerosols with C2 characteristics: $\tau=1.0$, $\omega_0=0.82$, $g=0.7$. (normal lines).

For aerosols of type D1a and D3, with strongly wavelength dependent single scattering albedo, the first effect is most important. So the residue increases for increasing surface reflection (Figure 2a).

For HG aerosols, with wavelength independent single scattering albedo, the first effect results in a constant residue for increasing surface albedo, but the second effect reduces the residue (Figure 2b). This is also true for a thin aerosol (gray or non-gray) layer; the presence of such a layer will only be felt when the amount of directly reflected radiation by the surface is small. On the other hand, the residue of a very thick layer of gray aerosols is constant with increasing surface albedo (not shown).

For smoke aerosols, like the C2 model with a weakly wavelength dependent single scattering albedo, the two effects balance each other and the residue does not change much with increasing surface albedo (Figure 2b).

The above result for gray absorbers can also be found in Torres (1998), where the residue versus aerosol optical thickness was modeled using gray absorbing and scattering aerosols over a dark ($A_s=0.05$) and a bright surface ($A_s=0.6$). Using a bright surface instead of a dark surface hardly changed the residue for the absorbing aerosols (Figure 5 from Torres (1998)). The above result for the non-gray aerosols seems to be confirmed by observations. TOMS AAI values are larger over underlying clouds, which serve as a bright surface. Smoke aerosols have been observed over both dark surfaces (e.g.: biomass burning aerosols over tropical forests in South America, Gleason et al., 1998) and over bright surfaces (e.g. biomass burning aerosols over snow and ice in Greenland, Hsu et al., 1999).

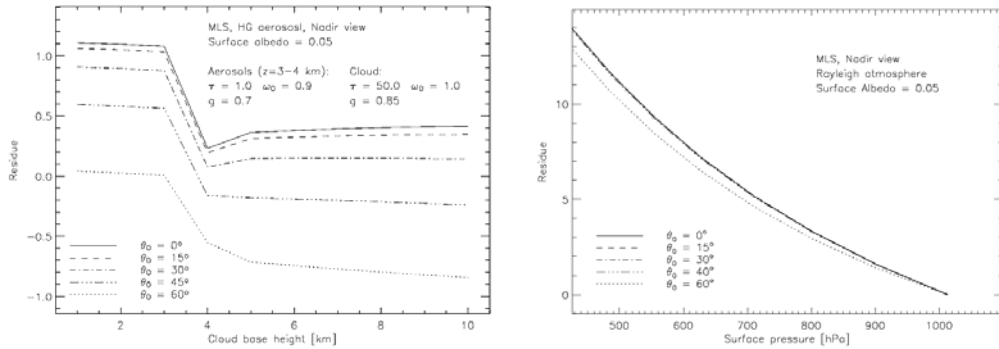



Figure 3: (a) Dependence of the residue on cloud base height, with an aerosol layer between 3 and 4 km altitude. The cloud has optical thickness $\tau = 50.0$ and scattering particles with $\omega_0 = 1.0$ and $g = 0.85$. The base of the 1 km thick cloud was varied between 0 and 10 km in steps of 1 km. (b) Dependence of the residue on surface pressure. Rayleigh atmosphere with MLS profile, nadir view, solar zenith angles vary between 0° and 60° .

3.3.4.2 Clouds

The effect of clouds on the residue is comparable to the effect of a high surface albedo when the aerosols overlie the cloud. But when the cloud overlies the aerosols the residue is completely determined by the cloud characteristics. This is illustrated in Figure 3a with HG aerosols (the effect for Mie aerosols can be inferred from Figure 2). In Figure 3a a cloud was present at different altitudes in an atmosphere with an absorbing HG aerosol layer at an altitude of 3 -- 4 km. The cloud is modeled as scattering HG aerosols characterised by a high optical thickness of $\tau = 50$, an asymmetry parameter $g = 0.85$ and a single scattering albedo $\omega_0 = 1.0$. The vertical extent of the cloud is 1 km.

When the cloud is present under the aerosol layer (left side of Figure 3a) the residue is the same as for an aerosol layer over a bright surface. The cloud reflects almost all light incident on it, so effectively it becomes the new surface. As the cloud base is raised from 0 to 3 km the residue is slightly reduced due to a decrease in the amount of intercepted radiation by the aerosol layer (the distance between the cloud and the aerosol layer is reduced). Then there is a transition to a new situation when the cloud base is between 3 and 4 km and coincides with the aerosol layer. The residue drops by about 0.9. When the cloud base is raised even further the residue stays almost constant. The cloud intercepts almost all incident radiation and acts as an opaque 'roof' over the aerosol layer; consequently the residue is almost entirely determined by the cloud characteristics. Cloud droplets are in fact scattering aerosols and produce zero or negative residues, depending on the solar zenith angle. This means that the residue method will not be affected very much by low clouds, but high clouds will certainly obscure absorbing aerosols layers.

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3.3.4.3 Ozone absorption

A linear relationship between residue and ozone was found by scaling the total ozone column Ω (not shown). The reduction of the TOA radiance due to ozone absorption is, to first order, equal to $\exp(-\tau_{O_3}M)$, where τ_{O_3} is the optical thickness of the ozone column and M is the geometrical air mass factor, $M = 1/\mu_0 + 1/\mu$. Since τ_{O_3} is about 0.01 at 340 nm, the exponential can be approximated by $1 - \tau_{O_3}$.

The dependence of the residue on Ω is limited: if Ω is increased from 100 to 500 DU, the 340nm/380nm residue increases linearly by 1. Therefore the ozone contribution in a Rayleigh atmosphere can be corrected for by linear interpolation. The LUTs include this dependence on Ω (see section 3.2.2).

Regarding the interaction of the absorption processes by ozone and aerosols, it has been shown that particle absorption effects introduce errors in the TOMS total ozone retrieval process, and a correction method making use of AAI has been developed (Torres (1999)).

3.3.4.4 Surface pressure / Surface Height


The residue is strongly dependent on surface pressure (Figure 3b). The surface pressure was lowered by removing the lower part of a Rayleigh atmosphere, which also simulates the effect of topography. In this way an apparent residue is introduced, as a result of the reduced multiple scattering due to the lower amount of Rayleigh scatterers in the atmosphere. This effect is wavelength dependent, with more multiple scattering at lower wavelengths, yielding a residue. The dependence is not linear (Figure 3b), therefore the surface pressure is accounted for by a second order polynomial interpolation in the residue calculations (see section 3.2.2). We assume that the surface height and the surface pressure are linked via the hydrostatic equation.

3.3.4.5 Geometrical dependence

Since the residue is a radiance quantity, it not only depends on atmospheric and surface parameters, but also on solar and viewing geometry. This dependence is shown in [RD1]. The dependence on geometry is however, much less than on aerosol parameters, and is most strong for large solar and viewing zenith angles, and for azimuths in the principal plane.

3.3.4.6 Scattering Angle

The geometrical dependence is especially visible in areas where the total scattering angle is less than 90 degrees. In these areas there is much more forward scattering/reflection and the algorithm does not handle this well at the moment.

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3.3.4.7 Sun Glint

The sea surface reflects sunlight like a mirror, and this increases the amount of light reaching up to the satellite. This mirror effect is not accounted for in the algorithm. Areas with risk of sun glint can be flagged, and some pixels can be permitted due to compensating or blocking effects of clouds. No sun glint is present over land. Two angles are used in the flagging procedure:

- Angle < 11 degrees; this is the 'core' angle and contains strongest reflectance.
- Angle < 18 degrees; this is the wider angle and sun glint in this area can be compensated / blocked by clouds with a cloud fraction larger than 0.3 or clouds with a cloud pressure lower than 850 hPa (cloud fraction must be larger than 0.1 in this case)


3.4 Defining the Absorbing Aerosol Index from the Residue

The above sensitivity study shows 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. 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.

Therefore the Absorbing Aerosol Index (AAI) is traditionally defined as the residue value only for cases where the residue is positive (Herman et al., 1997, Torres, 1998, De Graaf et al., 2005). Positive residue values exclude clouds and scattering aerosols. The calculation often involves using negative surface albedos and its absolute value has no unique interpretation, but high values of the AAI indicates the presence of absorbing aerosol layers, both over dark and bright surfaces. There have been some efforts of translating the AAI into physical meaningful parameters (Gleason (1998), Hsu (1999)), but we prefer to present the AAI itself rather than a derived product, because the interpretation of the AAI is still developing.


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[RD1] shows that the AAI from GOME-1 corresponds well to occurrences of biomass burning and dust events, which are major sources of absorbing aerosols.

The residue is also sensitive to sunglint, which scenes should be flagged. Sunglint is expected in GOME-2 data at the east side of pixels.

The residue is very sensitive to the absolute radiometric calibration of satellite radiances at 340 and 380 nm: 1 residue unit is equal to 2.3 % radiance change; a change of 0.1 residue units is well detectable by GOME-1, i.e. a change of 0.2 % in radiance ([RD1]). Recently, the residue has been found to provide also interesting information on calibration degradation of SCIAMACHY (L.G. Tilstra, 2007, private communication).

Since the negative values of the residue may contain interesting information on GOME-2 behaviour, we prefer to store both the positive and negative values of the residue in the GOME-2 ARS data product. Therefore, we will not limit the GOME-2 AAI to positive values of the residue. So in GOME-2 the AAI is synonymous to the residue. In plotting the AAI, one can set various minimum thresholds (AAI=0.0 or 1.0) to limit the result to only absorbing aerosol scenes.

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4. AAI RETRIEVAL IMPLEMENTATION

4.1 Framework

The AAI retrieval re-uses a lot of code from the general framework of the Opera Ozone Profile Retrieval Algorithm (see ATBD for the OOP product). The same Level-1B reading routines are used and a lot of the same internal structures. The implementation of the AAI retrieval algorithm is divided into steps detailed below.

4.2 Initialisation

In the initialisation step the software reads a configuration file, a workorder file and it reads the reference data. In the case of the AAI algorithm the reference data consists of the Rayleigh look-up-tables for the wavelengths selected by the user in the configuration file. Additionally, ozone columns from an Assimilated Total Ozone (ATO) file are used as input. If no ATO is available, the total ozone column is extracted from an ozone profile climatology selected via the configuration file. Next, some basic structures for reading the Level-1B data are set up, as well as structures for internal data records.


4.3 Ingestion and Data Selection

In the ingestion step, the software reads a number of MDR Earthshine records from the Level-1B file. From these MDR records the necessary information for the AAI retrieval is selected, and copied into an internal data structure: the 'AAI-Structure'. This AAI-Structure contains information on geolocation, date/time, solar and viewing angles, surface height, the ozone column (from ATO or climatology), and the reflectance around selected wavelengths, averaged with a triangular slit over a user defined width. The information is stored on a ground pixel granularity (size is following the Band-2b pixel size). Per ground pixel there is a flag indicating whether the information stored is valid.

4.4 Retrieval

The retrieval is done for pixels where the validity flag indicates valid spectral measurements and valid auxiliary data. The input for the retrieval are spectral measurements at two wavelengths, the surface height, the ozone column, and also the geometry (SZA, VZA and the Relative Azimuth Angle).

The lookup tables contain reflectances at the two chosen wavelengths, as well as the s^* , and t . The parameter t is the total atmospheric transmission for the given zenith angle, s^* is the spherical albedo of the atmosphere for illumination from below. The lookup tables were created using the radiative transfer code DAK (which stands for Doubling-Adding KNMI). This vector RTM takes polarisation into account, as well as ozone absorption and Lambertian surface

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reflection. Additionally, a pseudo-spherical description of the atmosphere was used and O₂-O₂ absorption was taken into account assuming a background level of oxygen. The dimensions of the lookup tables are: total ozone column, surface height, μ , and μ_0 .

The core of the retrieval computes the residue (AAI) by cubic spline interpolation in μ and μ_0 of path reflectance and analytically computed surface albedo. This is explained in the sections on algorithm description above.

At the end of the retrieval routine we perform a range check on the retrieved AAI value, setting it to an error value if it is out of range.

4.5 Storage

Data from the AAI-Structure has the dimensions of the width of the MDR and the number of MDRs that were read in at one time. This AAI structure does not contain the full PDU worth of data. The AAI-Structure is sent to the output module where, together with Product Specific MetaData such as the selected wavelengths and the width of the triangular slit used in the selection of the radiances, all relevant parameters are copied into an extensible data structure (geolocation, date/time, AAI).

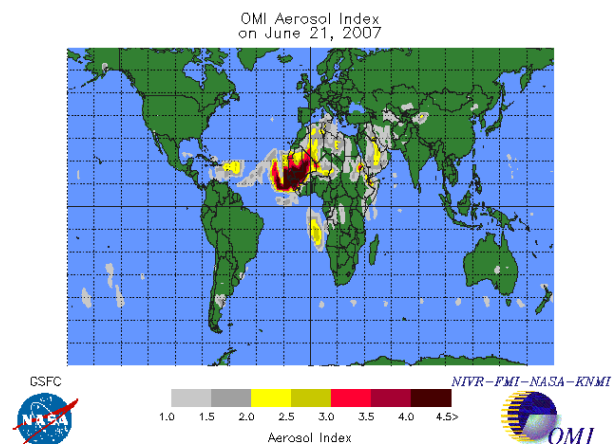
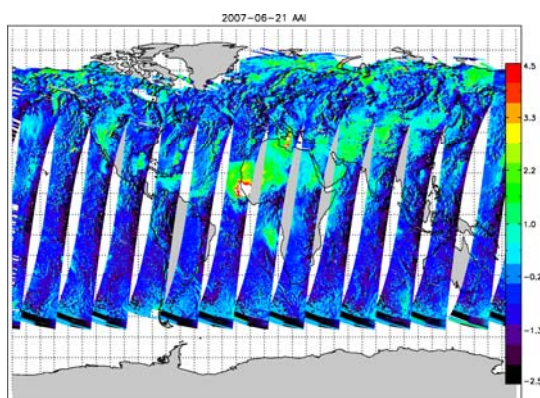
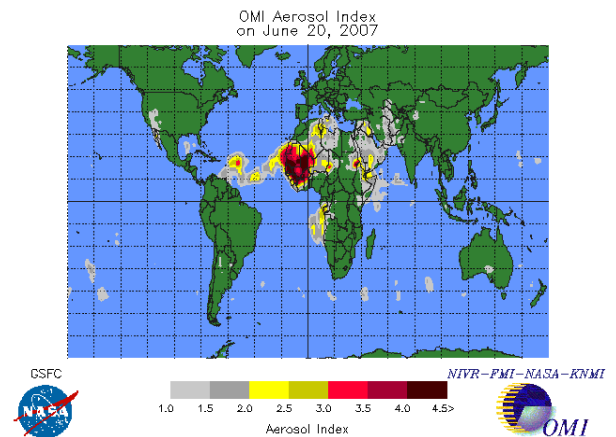
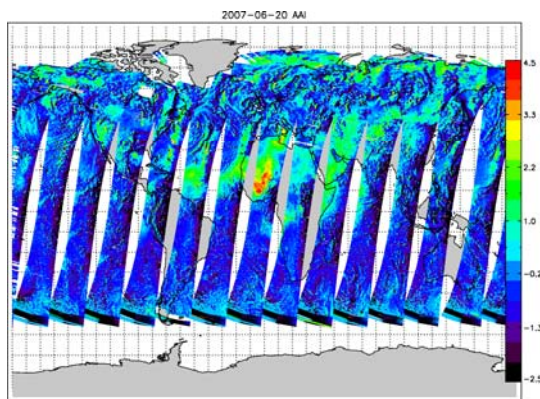
4.6 Output

When the main program has signaled that no more input data was found (e.g.: at the end of a Level-1B file), an output file is produced that conforms to the O3MSAF format: MetaData, Product Specific MetaData, a Geolocation Group and a Data Group. Please refer to the Product User Manual for detailed information on format and content.

5. VERIFICATION OF THE GOME-2 AAI PRODUCT

As a first verification of the GOME-2 AAI algorithm, we show in Fig. 4 a series of four days for which the GOME-2 AAI is compared globally to the OMI AAI, which has been taken from the OMI ozone product, processed according to the TOMS v8 algorithm (see <ftp://toms.gsfc.nasa.gov>).

The situation covers the period 20-23 June 2007, where a large Saharan desert dust cloud was transported westwards over the Atlantic Ocean (Fig. 4). Because the GOME-2 AAI map contains the entire range of the residue from -2.5 to 4.5, there are AAI values for the entire globe. The OMI AAI map only contains the residue values above 1.0, so it selects absorbing aerosol scenes. It is clearly visible that the Saharan dust storm is picked up nicely in the GOME-2 AAI data. A plume of biomass burning aerosol west of the coast of southern Africa is seen in both GOME-2 and OMI data.



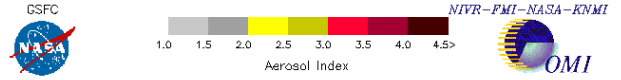
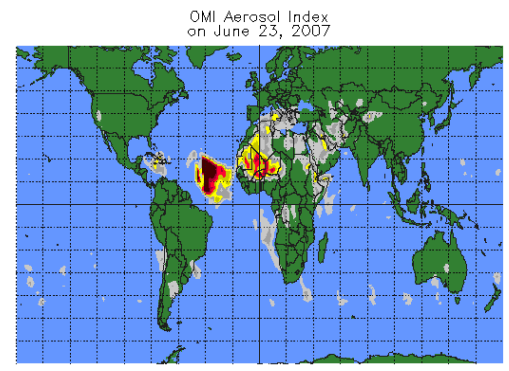
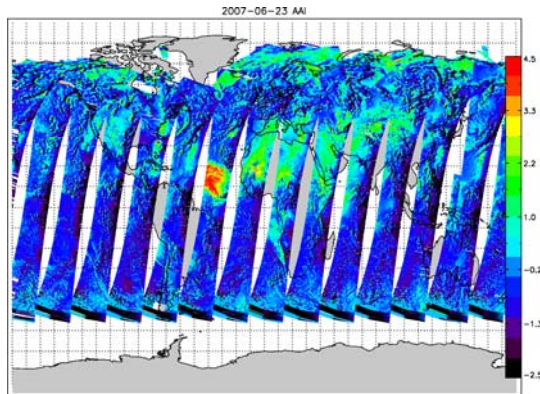
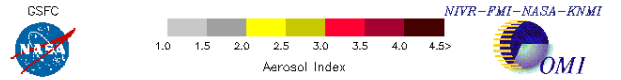
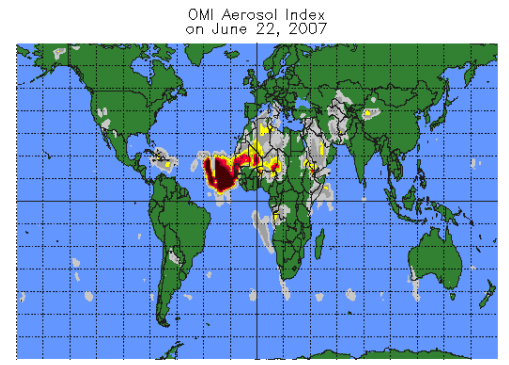
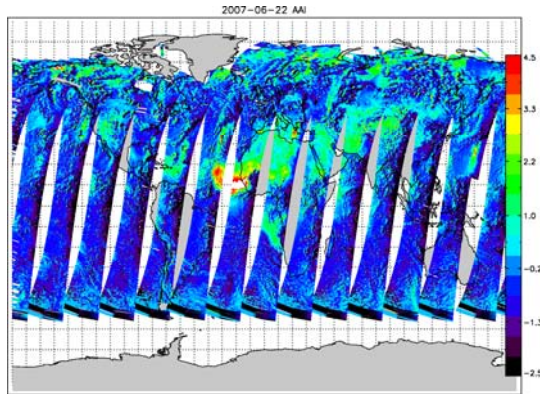




Figure 4: AAI from GOME-2 (left figures) and AAI from OMI (right figures) for the period June 20th-23rd 2007. Note the different AAI ranges and color scales for GOME-2 and OMI.

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