An Optimal Estimation Aerosol Retrieval Scheme For (A)ATSR

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1 Introduction

This document describes the aerosol retrieval part of the Oxford/RAL Aerosol and Cloud (ORAC) retrieval scheme. It particularly relates to the aerosol-only version of the code developed as part of the ESA Data User Element GlobAEROSOL project, but is also applicable to the combined aerosol/cloud algorithm. The document gives a description of the retrieval methodology, including the forward model, generation of error estimates and required data inputs. The differences between the processor for ATSR-2 and AATSR instruments will also be covered.

2 Overview

This document is structured in the following way:

- A brief description of the ATSR-2 and AATSR instruments is given.
- The forward model used to generate radiance lookup tables is described.
- The description of surface reflectance within the retrieval is described.
- A description of the data preprocessing, including cloud clearing and spatial averaging is given.
- The retrieval method is described, including the production of error estimates.
- A listing of the various input data required by the retrieval scheme is given, including brief descriptions of why each data type is needed.

Firstly, the general structure of the retrieval is described in order to provide an overview of the entire processing scheme.

The retrieval scheme described in this document is an updated version of the aerosol component of the Oxford/RAL Aerosol and Cloud retrieval scheme described by Marsh et al. [1]. ORAC is itself a development of the Enhanced Cloud Processor [2], designed to retrieval cloud properties from ATSR measurements. The retrieval makes use of look up tables relating aerosol properties (i.e. aerosol optical depth at 550 and 865 nm) to top of atmosphere radiances, thus removing the need for computationally expensive radiative transfer calculations to be performed during the retrieval. In general, measured radiances will not correspond exactly to those given in the lookup tables and interpolation between lookup table values is required.

ORAC is an optimal estimation retrieval scheme which uses the Levenburg-Marquardt method to fit the forward model to the observed radiances. Optimal estimation produces the state for which the modelled radiances best match the observed radiances, weighted by the measurement errors, any a priori information of the state and the uncertainty in this a priori information. Because the formulation of optimal estimation is probabilistic, the retrieval not only produces a state estimate, but also information on the precision of that estimate.

As well as the retrieval scheme itself, ORAC includes extensive data preprocessing. The main tasks of the preprocessing are:

- To read in satellite and ancillary data and output it in the form required by the retrieval code.
- To provide cloud detection.
To flag the data as either over land or over ocean and produce first guesses of the surface reflectivity as appropriate.

To reduce the spatial resolution of the satellite radiances to the required product resolution.

3 The ATSR-2 and AATSR instruments

The second and third generation Along Track Scanning Radiometers (ATSR-2 and Advanced ATSR) were launched on the ESA polar orbit satellites ERS-2 and ENVISAT in 1995 and 2001, respectively. As the instruments are essentially the same in their operation, with the only major difference being the bandwidth available for data transfer, they can be described together.

The primary design goal of the ATSR instruments is the measurement of sea surface temperature, with a secondary objective of ATSR-2 and AATSR being the determination of land surface and vegetation properties. ORAC makes use of the atmospheric component of the ATSR signal, which is considered contamination in its primary and secondary roles.

Both ATSR-2 and AATSR have seven spectral channels centred at 0.55, 0.67, 0.87, 1.6, 3.7, 10.7 and 12 $\mu$m. The instruments use a dual view system, with a continuously rotating scan mirror directing radiation from two apertures and two on-board blackbody calibration targets onto the radiometer. One viewing aperture produces a scan centred on the nadir direction, while the other views the surface approximately 900 km ahead of the satellite (at a viewing angle of 55° from the nadir). This continuous scanning pattern produces a nadir resolution of approximately $1 \times 1$ km with a swath width of 512 pixels.

Due to bandwidth limitations on the ERS-2 satellite, ATSR-2 is usually run in a “narrow swath” mode over the oceans, which produces a swath of only 256 pixels. In addition, although ATSR-2 is still operational, the ERS-2 satellite developed a pointing problem in 2001, which means that post 2001 data from the instrument is currently unusable.

ERS-2 and ENVISAT are in similar polar orbits with periods of approximately 100 minutes. Both ATSR-2 and AATSR have repeat periods (i.e. the interval between successive measurements of the same location) of 3 days.
Figure 1: Schematic of the ATSR-2 instrument.
Figure 2: ATSR-2 showing the two viewing apertures and the blackbody targets.
4 Background

Remote sensing of aerosols from satellite is the most convenient tool for providing global information on aerosol spatial and temporal distributions. It is based on the concept that, when illuminated by the sun, aerosols absorb and backscatter a fraction of the radiation. This signal is detectable by the satellite instrument and allows the retrieval of aerosol properties, and it is this task the ORAC processor has been developed to undertake. The ORAC forward model is sensitive to aerosol size, chemical composition, shape and vertical distribution, as these characteristics determine aerosol radiative behaviour.

4.1 Description of aerosol microphysical and optical properties

In a given location, atmospheric aerosols are characterised by their concentration, size distribution, chemical composition (which determines their complex refractive index), and their vertical profile. With knowledge of these properties, the required radiative characteristics may be computed by assuming the particles are spherical and applying Mie theory [3].

The aerosol optical depth, $\tau$, is the primary quantity obtained from the satellite algorithm. It is defined in equation 1 as:

$$
\tau(\lambda) = \int_0^\infty \beta_e(z, \lambda) \, dz = \int_0^\infty (\beta_a + \beta_s)(z, \lambda) \, dz
$$

The total extinction coefficient, $\beta_e$, is defined as the sum of the extinction due to absorption, $\beta_a$, and scattering, $\beta_s$. The vertical profile of $\beta_a$ and $\beta_s$ along with the scattering phase function, $P(\theta)$, which determines the angular distribution of the scattered radiation, describe fully the aerosol radiative characteristics. Other convenient ways of defining aerosol optical properties are the single scattering albedo, $\omega_o$, which is the ratio of $\beta_s$ to $\beta_e$, and the asymmetry parameter, $g$, which is the weighted integration of $P(\theta)$ over all possible scattering angles ($\theta$) (from 0 to 180°). For a given aerosol model (shape, size, and refractive index), $\beta_e$ is proportional to the aerosol concentration while $P(\theta)$ is not.

Mie theory shows that the extinction coefficient is given by:

$$
\beta(z, \lambda) = \int_0^\infty Q_e(z, m, x) \pi r^2 n(z, r) \, dr
$$

$Q_e$ is the Mie extinction efficiency factor, and is dependent on the Mie size parameter $x = 2\pi r/\lambda$, and the refractive index of the particles ($m = m_r + im_i$), $n(r)$ is the number size distribution.

The log-normal distribution is the most suitable representation for characterising the size distribution of the atmospheric aerosols [4]. The distribution is then described by its mode radius ($r_i$), standard deviation ($\sigma$), and total number density ($N$).

5 Aerosol forward model

Aerosol optical depth at 0.55 $\mu$m and aerosol effective radius are retrieved from ATSR-2 and AATSR satellite data using four channels in the visible and near-infrared (0.55, 0.67, 0.87, and 1.6 $\mu$m). The retrieval algorithm uses lookup tables of atmospheric transmission and reflectance in these four
channels as a function of these two optical depths. These lookup tables are generated using assumed values for aerosol refractive index, size distribution, phase function, and vertical distribution, as well as assumptions of the absorption of atmospheric gases. The lookup tables are generated for a 32 layer plane parallel atmosphere stretching from 0 - 100 km in height, with a 1 km layer spacing up 25 km, stretching to 30 km for the top layer.

The primary source of aerosol properties used in the retrieval is the OPAC (Optical Properties of Aerosols and Clouds) database [5]. The database provides optical (most importantly the complex refractive index as a function of wavelength) and physical properties (such as the size distribution and vertical distribution) for a set aerosol components from which representative aerosol types can be built.

### 5.1 Modelling aerosol scattering and absorption

As has already been indicated, satellite radiometers are most sensitive to the total amount of aerosol along their line of sight. The next most important variable in determining the radiative effect of a given aerosol type is the size of the particles. One of the most robust measures of the average size of an aerosol distribution is the effective radius, defined as the ratio of the 3rd and 2nd moments of the size distribution:

\[
r_e = \frac{\int_0^{\infty} r^3 n(r) dr}{\int_0^{\infty} r^2 n(r) dr}
\]

where \( r \) is the radius, and \( n(r) \) is the number density as a function of radius. The vertical profile and other parameters also influence the radiance seen in the nadir direction to a lesser extent, but are neglected by the retrieval scheme due to a lack of information to parameterize them.

In order to produce radiance lookup tables from this data base the scattering phase function of each aerosol type are calculated using Mie scattering. Phase functions are calculated for the central wavelength of each channel across a range of effect radii from 0.02 to 20 \( \mu m \). Two assumptions are made during this step:

- That the radiative properties of the aerosol are constant across the width of each instrument channel. As the features of aerosol extinction spectra are very broad in comparison with gas features this is a reasonable approximation.

- Assumptions must be made in determining both the form of the aerosol size distribution and how its shape varies with changing aerosol effective radius. To model aerosol distributions with different effective radii to those prescribed by the OPAC database, the relative concentration of the different sized aerosol components which make up each aerosol class are changed. For example, if the effective radius needs to be decreased, the relative concentration of the smallest component of the aerosol (the accumulation mode) will be increased, while the larger components will be decreased.

If the required effective radius is equal to that given by the smallest or largest component of a given aerosol type, then the type effectively becomes a single component aerosol. If the size is outside of this range, then the mode radius of the smallest/largest comoponents is shifted (while keeping the width of the component’s distribution constant). Clearly, in such situations, the accuracy of the model can be called into question, so we are relying on the prescribed effective
radius being relatively close to that found in the real world. It should also be pointed out that in the case of very small aerosols, the optical properties of the particles become less important in determining their scattering effects, since they will act more like Rayleigh scatterers.

These scattering properties are then used to generate as vertical profile of aerosol scattering, based on vertical profiles of number density, \( N \): \[ N(h) = N(0) \exp(-h/Z) \] where \( h \) is the height and \( Z \) is a scale height, defined by the aerosol type. For each layer at which the aerosol distribution is defined, the extinction coefficient, single scatter albedo and the coefficients of a Legendre expansion of the scattering phase function are calculated for each instrument channel and over the 20 effective radii.

### 5.2 Modelling atmospheric gas absorption

Once aerosol scattering properties have been calculated, gas absorption over the instrument band passes is calculated, and convolved with the instrument filter transmission functions, using the MODTRAN database (version 3.5-v1.1)[6]. The MODTRAN database allows provides tropical, mid-latitude summer and winter, subarctic summer and winter, and US Standard Atmosphere climatological atmospheres for the following gasses: \( \text{H}_2\text{O}, \text{CO}_2, \text{O}_3, \text{N}_2\text{O}, \text{CO}, \text{CH}_4, \) plus single profiles for: \( \text{HNO}_3, \text{NO}, \text{NO}_2, \text{SO}_2, \text{O}_2, \text{N}_2, \text{NH}_3 \) and the heavy molecules (CFCs). ORAC lookup tables are generated using the mid-latitude summer atmosphere only. This simplification can be made as gas absorption is weak compared to aerosol extinction in the visible and the ATS-R-2 channels are free from strong absorption features of gases which show large spatial and temporal variability (most notably \( \text{H}_2\text{O} \)).

### 5.3 Modelling atmospheric transmission and reflectance

The final step in creating lookup tables is to predict atmospheric transmission and bidirectional reflectance values, based on the aerosol phase functions and gas absorption, using the Discrete Ordinates Radiative Transfer (DISORT) software package[7].

DISORT is a thoroughly documented and widely used general purpose algorithm for the calculation of time-independent multiple-scatter transfer calculations. The DISORT algorithm solves the equation for the transfer of monochromatic light at wavelength \( \lambda \) as described by the equation

\[
\frac{dL_\lambda(\tau_\lambda, \mu, \phi)}{d\tau} = L_\lambda(\tau_\lambda, \mu, \phi) - L_\lambda^S(\tau_\lambda, \mu, \phi),
\]

where \( L_\lambda(\tau_\lambda, \mu, \phi) \) is the intensity along direction \( \mu, \phi \) (where \( \mu \) is the cosine of the zenith angle and \( \phi \) is the azimuth angle) at optical depth \( \tau_\lambda \) measured perpendicular to the surface of the medium. \( L_\lambda^S(\tau_\lambda, \mu, \phi) \) is the source function.

DISORT is provided with the aerosol scattering properties defined by the Mie scattering calculations and the gas absorptions defined by MODTRAN, an underlying surface albedo (which is set as zero for the generation of the lookup tables), and a series of 9 logarithmically spaced aerosol optical depths (defined at a wavelength of 0.55 \( \mu \text{m} \)) between 0.008 and 2.0. From this four lookup tables (or Static Application Data files) for each aerosol type/channel combination are produced:
5.4 Surface reflectance

Bidirectional reflectance of the aerosol layer, $R_{BD}$: ATSR-2_A00_RBD_Ch1.sad
Reflectance of the aerosol layer to diffuse radiance, $R_{FD}$: ATSR-2_A00_RD_Ch1.sad
Diffuse transmission of the incident beam, $T_{BD}$: ATSR-2_A00_TBD_Ch1.sad
Directly transmission of the beam, $T_{DB}$: ATSR-2_A00_TB_Ch1.sad
Total transmission of diffuse incident radiance, $T_{D}$: ATSR-2_A00_TD_Ch1.sad
(In this instance the files are for the aerosol type A00, in channel 1 of ATSR-2.) Each of these files contains tabulated transmission or reflectance (depending on the file) values for optical depths at 0.55 and 0.865 $\mu$m corresponding each of the 20 effective radii, 9.55 $\mu$m optical depths and sun/satellite geometry (specified by 20 equally spaced zenith angles and 11 equally spaced azimuth angles).

5.3.1 Molecular absorption and Rayleigh scattering considerations

Within the aerosol layer the effects of molecular absorption and Rayleigh scattering are included in DISORT by a calculated adjustment of the layer’s optical depth and the particle’s single scattering albedo and phase function with the following:

\[
\begin{align*}
\tau &= \tau_a + \tau_R + \tau_g, \\
\omega &= \frac{\tau_R + \omega_a\tau_a}{\tau_g + \tau_R + \tau_a}, \\
P(\theta) &= \frac{\tau_a\omega_a P_a(\theta) + \tau_R P_R(\theta)}{\tau_a\omega_a + \tau_R},
\end{align*}
\]

where $\tau_a$, $\tau_R$ and $\tau_g$ are the contributions to the total optical depth $\tau$ due to aerosol scattering, Rayleigh scattering and gaseous absorption within each layer respectively. The aerosol single scattering albedo is denoted $\omega_a$.

For each layer bounded by lower and upper pressure levels $p_l$ and $p_u$ respectively and ground level pressure $p_0$, $\tau_R$ is calculated from

\[
\tau_R = \frac{\tau_{RT}[p_u - p_l]}{p_0},
\]

where $\tau_{RT}$, the wavelength dependent Rayleigh scattering optical depth for a column of atmosphere extending from the ground surface to the top of the atmosphere is obtained from[8]:

\[
\tau_{RT}(\lambda) = \frac{p_0}{p_s} \times \frac{1}{117.03 \lambda^4 - 1.316 \lambda^2},
\]

where $p_s$ is the standard pressure ($p_s = 1013.25$ mbar), $p_0$ is the ground pressure in mbar and $\lambda$ is in $\mu$m.

5.4 Surface reflectance

The third product retrieved by the ORAC processor is the surface reflectance. This is retrieved as a single value, with the spectral shape across the different channels being constrained. The method by which the spectral shape of the surface is prescribed differs for land and ocean pixels. In the case of ocean pixels the surface reflectance is modelled using the methods presented by Sidran [9] and [10], which includes upwelling radiance from volume scattering within the water itself and specular
reflections from the wind-roughened surface (as modelled by the Cox and Monk method [11]). Over land the MODIS\textsuperscript{1} land surface bidirectional reflectance product [13] is used. In both cases the an
effective Lambertian reflectance is calculated for compatability with the ORAC foward model.

5.4.1 Sun-glint

A major problem encountered in making nadir satellite measurements is the specular reflection of sunlight off the ocean surface, or sun-glint. In areas effected by sun-glint the surface contribution to the observed radiance becomes completely dominant and the determination of aerosol properties is unfeasible.

ORAC does not attempt aerosol retrievals in the sun-glint region and a reflectance thresold on ocean pixels is used to mask effected regions.

5.5 Computing top of atmosphere radiances

The forward model uses the transmission and reflectance lookup tables to predict a top of atmosphere radiance using a single layer radiative transfer model, which is shown diagrammatically in figure 3. The solar beam is incident on the aerosol layer \textsuperscript{2} and the first contribution to the TOA observed radiance is the direct bidirectional reflectance, $R_{BD}$, of the aerosol layer. Transmission through the layer is partly by direct transmission of the beam, $T_{DB}$, and partly by diffuse transmission of scattered radiance, $T_{BD}$. As an underlying Lambertian surface is assumed, any preferred directionality of the radiance is lost on reflection and these transmitted terms can be combined to give the total transmission downward through the aerosol layer, $T_B = T_{BD} + T_{DB}$. The reflected radiance is assumed to be diffuse and is partially transmitted, $T_D$, by the aerosol layer into the view direction, thereby giving the second term in the solar component. The aerosol layer also reflects downwards so there is a set of multiple reflections and transmissions giving rise to a series of rapidly decreasing contributions to the TOA reflectance. This process is represented in the following equation:

$$R = R_{BD}(\theta_0, \theta_v, \phi) + T_B(\theta_0)R_sT_D(\theta_v)R_{FD} + T_B(\theta_0)R_s^2T_D(\theta_v)R_{FD}^2 + \cdots$$

where $\theta_0$ is the solar zenith angle, $\theta_v$ is the satellite (view) zenith angle and $\phi$ is the relative (solar to satellite) azimuth angle. This expression can be simplified to give

$$R = R_{BD}(\theta_0, \theta_v, \phi) + T_B(\theta_0)T_D(\theta_v)R_s(1 + R_sR_{FD} + R_s^2R_{FD}^2 + \cdots)$$

which, in turn, can be simplified even further in terms of a geometric series limit,

$$R = R_{BD}(\theta_0, \theta_v, \phi) + \frac{T_B(\theta_0)T_D(\theta_v)R_s}{(1 - R_sR_{FD})}$$

It is this equation that is used to calculate the top of atmosphere radiances seen by the satellite.

\textsuperscript{1}MODerate resolution Imaging Spectrometer

\textsuperscript{2}A reminder that this layer is described by many layers in DISORT.
5.5.1 Forward model gradient

The gradient version of the forward model \( \frac{\partial y}{\partial x} \) where \( x \) is one of the state variables is required for the following two purposes:

1. The gradient with respect to parameters which are to be derived from the measurements (state parameters) is a vital quantity for the inversion of the non-linear reflectance model by the Levenberg–Marquardt algorithm.

2. The gradient with respect to parameters which might be considered known and not part of the inversion procedure (model parameters), e.g. surface reflectance spectral shape, is used to judge the sensitivity to these parameters and thus to estimate their contribution to the retrieval error.

If the equation 6 is rewritten as

\[ R = R_{BD} + S, \]

then without reproducing the algebra it can be simply stated that the gradient of the model w.r.t aerosol optical depth \( \tau \) is given by:

\[
\frac{\partial R}{\partial \tau} = R'_{BD} + S \left( \frac{T_B T'_B + T_D T_B}{T_B T_D} + \frac{R'_S R'_{FD}}{1 - R_S R_{FD}} \right)
\] (7)

where all \( ' \) indicate \( \frac{\partial}{\partial \tau} \).

The gradient of the model with respect to aerosol particle radius \( r_e \) is given by the same expression except that all \( ' \) indicate \( \frac{\partial}{\partial r_e} \).

6 Forward model error characterisation

It is not practical to accurately model the full range of variation in aerosol composition, size distribution, vertical distribution, atmospheric composition and surface properties which effect the radiance observed by ATSR-2. Even if all factors could be modelled, the measurements do not provide enough information to retrieve more than 2 or 3 independent pieces of information[1]. The resulting approximations and assumptions in the forward model will result in errors in the retrieved products and it is important that these errors be quantified.
6.1 Surface reflectance

Except in circumstances of high aerosol loading, or in the presence of cloud, the signal of a nadir viewing radiometer over land surfaces will be dominated by surface features, with the aerosol signature essentially adding a perturbation. Thus, the accuracy of the surface reflectance is of key importance in determining the overall accuracy of the retrieval. Although ORAC retrieves a surface reflectance, the spectral response of the surface is fixed for a given pixel. At present, work on quantifying the forward model error in surface reflectance is still ongoing, but some qualitative points can still be made:

- At present nothing is done to accurately model the surface reflectance of snow and ice surfaces, thus aerosol properties retrieved over such surfaces should be treated with great care. It should be noted that, due to the extremely high albedo of such surfaces, the retrieval of aerosol properties above them is inherently extremely difficult, as the relative contribution of aerosol extinction to the observed signal is very small. This fact also adversely effects the accuracy of the retrieval over other bright surfaces, such as desert regions.

- Over the land, the retrieval is limited by the accuracy of the MODIS surface reflectance product, which is in turn dependant on the atmospheric correction done in it’s own production, as well as the limitations of the surface reflectance model used. The MODIS surface reflectance product uses the Ambrals 3-kernel model [14], which is most effective at modelling vegetated or bare land – the accuracy of the product will be reduced built up or mixed use areas.

- The use of a fixed shape for ocean reflectance will introduce some error in regions where high surface roughness produces a large amount of foam, or where there are large plankton blooms (both of which will change the average spectral reflectance of the ocean).

6.2 Aerosol size distribution

Figure 6.2 gives an example of the difference between the scattering phase functions that correspond to two grossly different size distributions, which have the same effective radius. Even in this extreme case, however, the scattering phase function for the two distributions is remarkably similar and the single scatter albedo (which is the other aerosol parameter used by DISORT to calculate top of atmosphere radiances) for each distribution is almost identical. It is likely, therefore, that the method of setting the effective radius described in section 5.1 does not introduce significant errors in the modelled radiances.

6.3 Forward model: Sensitivity to vertical profiles of aerosol parameters

A simple five layer forward model from the ground to 2 km has been used to test whether the TOA radiance varies as a function of the aerosol number distribution, $\omega_0$ and $g^3$.

For aerosol number distribution the TOA radiance was investigated for a model with constant $\omega_0 = 0.8$ and $g = 0.61$ for all layers. The surface albedo was kept equal to 0.0.

The following four vertical profiles were tested:

$^*$Note that this analysis was done using a previous version of the lookup table generation that used the asymmetry parameter to describe the angular distribution of the aerosol scattering, rather than a Legendre expansion of the phase function.
6.3 Forward model: Sensitivity to vertical profile of aerosol parameters

**FORWARD MODEL ERROR CHARACTERISATION**

(a) (b)

![Graphs](image)

Figure 4: Comparison of the phase functions at 0.55 µm (panel a) of two size distributions (shown in panel b), both with an effective radius of 10.3 µm. The first distribution (solid line) consists of the accumulation mode and coarse mode sea salt components from the OPAC database[5] at 0% relative humidity, while the second distribution (dashed line) is the accumulation mode alone, with its mode radius increased by a factor of 14 to give it the same effective radius as the combined distribution.

- Exponentially increasing with height
- Exponentially decreasing with height
- Linearly increasing with height
- Linearly decreasing with height

The TOA radiances for the vertical profiles are shown in figure 5. From this figure it can be seen that the radiance values for all profiles are identical, i.e., if $\omega_0$ and $g$ were kept constant with height the forward model would not be sensitive to the aerosol profile.

Keeping all parameters constant and varying aerosol $\omega_0$ produces the set of graphs in figure 6. It can be seen that there is very little difference between the four plots when $\tau < 0.1$; however, for $\tau > 0.1$ the TOA radiance is dependent on whether $\omega_0$ increases or decreases with height. This is as one would expect and can be explained by more of the incoming radiation being absorbed high in the model atmosphere when $\omega_0$ decreases with height.

For the set of graphs in figure 7 the only parameter which is permitted to vary with height is the aerosol $g$. Again it can be seen that the TOA radiance varies with its vertical distribution.

From these tests it can be concluded that the forward model is sensitive to the vertical distribution of aerosol. Although the forward model is not directly sensitive to the vertical distribution of $N$ it is sensitive to the vertical profile of $\omega_0$ and $g$. From equation 5 it can be seen that values for $\tau$, $\omega_0$ and $g$ within the layers of the forward model are dependent on $\tau_a$ and hence on $N$.

Due to the lack of prior information about the vertical distribution of aerosol at a given location and time, this dependence cannot be accounted in some a priori, and the measurements do not provide enough information to allow the retrieval of the vertical distribution and the other retrieved parameters. Thus, this dependence simply adds a forward model error to the retrieval, since our model does not take it into account.
Forward model: Sensitivity to vertical profiles of aerosol parameters

Figure 5: TOA radiance values for each of the four vertical aerosol $N$ distributions at $\lambda = 0.67 \, \mu m$.

Figure 6: TOA radiance values for each of the four vertical aerosol $\omega_0$ distributions at $\lambda = 0.67 \, \mu m$. 

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7 Data preprocessing

The ORAC processor expects all input data to be presented in unformatted binary files. Since such files are an exact reproduction of a computer’s internal binary representation of data, the format of these files is architecture dependant and thus ORAC input files are not portable between different systems. The primary role of the preprocessing is to read in the required data in its own format (generally more portable standards), manipulate it and output it in unformatted form. The use of preprocessing code to in this way enables the FORTRAN retrieval code to be treated almost as a ‘black box’, while the preprocessing code can be written in a higher level language (in this case IDL) which is much better suited to the quick development of new routines for reading different data. This provides a stable, highly optimised retrieval scheme, while maintaining the flexibility needed to allow the easy application of the scheme to new input and ancillary data.

IDL has been selected as the language for the majority of the preprocessing code as there are readily available I/O routines for most scientific data formats and because of its inbuilt routines for data manipulation. The interactive nature of IDL is also a considerable advantage in the development and debugging of code, while, the freely available run-time only version of IDL (IDL Virtual Machine) makes it economical to implement the ORAC processing chain on multi-processor computational clusters.

In addition to file input and output, the preprocessing performs some important functions required by the retrieval:

7.0.1 Land flagging

The ORAC preprocessing produces its own land/sea flag, using the land flagging algorithm from the SADIST operational ATSR-1/ATSR-2 sea surface temperature processor [15].

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7 DATA PREPROCESSING

7.0.2 Setting surface reflectance

The \textit{a priori} land surface reflectance is set using the MODIS surface albedo product for the appropriate date. The MODIS surface product has been interpolated onto a regular longitude/latitude grid and then averaged to the resolution of the retrieval.

7.0.3 Determining sunglint region

As mentioned previously, the work of Cox and Monk [11] is used to model the surface roughness, based on ECMWF surface winds. From this the amount of sunglint within each pixel can be calculated and, if a given threshold is exceeded, the pixel is flagged so that no retrieval is attempted.

7.0.4 Cloud flagging

An important function performed by the preprocessing is the detection of clouds. Over the ocean, two options are available. The first to use the ESA cloud flag product, produced as part of the sea surface temperature retrieval, over the ocean. The ESA flag is included with the AATSR level 1b data, but is not present in the ATSR-2 UBT files used (see section 7.1). Thus the ATSR-2 processing uses the flag developed for the Global Retrieval of ATSR Cloud Parameters and Evaluation (GRAPE) project [12]. Both the ESA and GRAPE cloud flags are designed for use over the ocean only, over the land the Stevens Cloud Flag (a simple NDVI test developed by the Rutherford Appleton Laboratory) will be used for both instruments [16].

Note that cloud flagging is performed at the full instrumental resolution regardless of the spatial resolution required by the retrieval. This minimises the number of errors in cloud flagging due to sub-pixel clouds.

7.0.5 Viewing geometry interpolation

(A)ATSR level 1 files do not include sun/satellite geometries for every measurement pixel, but specify the geometry for 22 points at the start of each $512 \times 512$ pixel scene. The preprocessing therefore interpolates these values to fill in the rest of the scene.

7.0.6 Spatial averaging

In order to speed analysis and reduce the storage space required to store the products, ORAC can be run at a reduced spatial resolution. The preprocessing allows the $1 \times 1$ km resolution radiances to be averaged into “super-pixels” of any size. The mean and variance of all pixels which lie within a specified super-pixel are calculated and these values are then used as the radiance and associated variance for each retrieval pixel. The treatment of partially cloudy super-pixels is configurable - the super-pixel can either be flagged as partially cloudy (the ORAC cloud retrieval will then be run on the retrieval), or the cloud-free pixels can be averaged to produce a cloud-free radiance for the pixel (in which case the aerosol retrieval will be run).

7.0.7 Writing the driver file

The behaviour of the ORAC retrieval code is controlled by a driver. This is a text file which defines file paths, \textit{a priori} and first guess values, as well as other settings. This file is in turn generated by
the preprocessing code.

7.1 ATSR-2/AATSR differences

Due to the similarity between the ATSR-2 and AATSR instruments, there are very little differences between the preprocessing for each instrument. Indeed, aside from the absence of the ESA cloud flag in ATSR-2 data, the only difference in the preprocessing is the reading of the satellite data. AATSR top of atmosphere radiance data is currently only available in gridded brightness temperature (GBT) files, which are in a different format to the ATSR-2 GBT product. The ATSR-2 processing is currently based around ungridded brightness temperature (UBT) data.

The final difference between the ATSR-2 and AATSR processing chains is that they require different lookup tables, since the filter transmission functions are different for each instrument.

8 Retrieval algorithm

The ORAC retrieval scheme is an optimal estimation scheme using the Levenburg Marquardt algorithm. The basic principle of optimal estimation is to maximise the probability of the retrieved state conditional on the value of the measurements and any a priori. Formally, it is required to maximise the conditional probability $P = P(x|y, x_b, b)$ with respect to the values of the state vector $x$, where $x_b$ is the a priori value of the state vector and $b$ are all other parameters not modelled by the forward model. The full state vector $x$ is formally defined as

$$x = [\tau_{0.55}, \tau_{0.865}, a],$$

where $a$ is the factor by which the apriori surface reflectances, $R'_s$, are scaled:

$$R_s = aR'_s.$$ 

8.1 Definition of $J$

The assumption is made that errors in the measurements, a priori and model parameters are normally distributed with zero mean and variance given by $S_y$, $S_x$ and $S_b$ respectively. Then, the conditional probability takes on the quadratic form:

$$P(x) \propto \exp \left[-(y(x) - y_m)S_y^{-1}(y(x) - y_m)^T\right]$$
$$\times \exp \left[-(x - x_b)S_x^{-1}(x - x_b)^T\right]$$
$$\times \exp \left[-(b_t - b)S_b^{-1}(b_t - b)^T\right],$$

where the three terms represent weighted deviations from measurements, the a priori state and the model parameters respectively. $b_t$ has been written for the (unknown) true values of the model parameters. Maximising probability is equivalent to minimising the negative logarithm, so that $J$ is equivalently minimised where:

$$J(x) = (y(x) - y_m)S_y^{-1}(y(x) - y_m)^T$$
$$+ (x - x_b)S_x^{-1}(x - x_b)^T$$
$$+ (b_t - b)S_b^{-1}(b_t - b)^T.$$

$$16$$
Notice that the minimisation is done with respect to the state variable \( x \), so that the derivative of \( J \) is independent of the third term and \( b \) therefore cannot be part of the solution.

### 8.2 OE solution: minimisation of \( J \)

This section addresses the problem of the minimisation of \( J \), i.e. finding the solution. This is an area where many techniques and methods can be employed and where tuning of the adopted scheme can be as important as the scheme itself. Essentially any method of finding the minimum is acceptable in a sense, with the caveat that in an operational context it must be robust and fast. The particular characteristics of this problem are that:

1. First and second derivatives of \( J \) (with respect to \( x \)) are available and continuous,

2. Multiple minima are unlikely,

3. \( J \) is likely to be approximately quadratic in the region of the solution and far from quadratic elsewhere.

Characteristic 1) implies descent algorithms that make use of the local gradient are possible, and these are generally faster than methods that do not. 2) implies that extravagant domain searches to avoid minor minima are probably not required. 3) is a result of the reasonably strong non-linear nature of the forward (radiative transfer) problem. It means that quick convergence from a poor starting position is unlikely.

The cost function to be minimised is a reduced form of equation 8 since there is no explicit dependence on \( b \).

\[
J(x) = (y(x) - y_m)S_y^{-1}(y(x) - y_m)^T + (x - x_b)S_x^{-1}(x - x_b)^T.
\]

The first and second derivatives of \( J \) with respect to \( x \) are given by:

\[
J' = \frac{\partial J}{\partial x} = K_x^T S_y^{-1}(y(x) - y_m) + S_x^{-1}(x - x_b)
\]

\[
J'' = \frac{\partial^2 J}{\partial x^2} = K_x^T S_y^{-1} K_x + S_x^{-1}.
\]

The expression for \( J'' \) is a commonly-used approximation in that \( K_x \) is assumed to be independent of \( x \), i.e. the radiative transfer is linear in \( x \). This is only strictly true near the solution (in the region where \( J \) is quadratic) but (see next section) since \( J'' \) is only employed near the solution the approximation is acceptable.

#### 8.2.1 Levenburg-Marquardt algorithm

The minimum of \( J(x) \) is found by starting at some ‘first guess’ state \( x_0 \) (which in the absence of other information is usually set equal to the \textit{a priori} value) and then proceeding to make steps, \( \delta x_n \), based on some algorithmic theory. Assuming the value of \( J \) decreases at each step, the updated \( x \) vector is taking the process towards the cost function minimum. To be consistent with the three points made above, ORAC uses the Levenburg-Marquardt algorithm to define the value of \( \delta x_n \). The
8.2 OE solution: minimisation of \( J \)

The rationale of the Levenburg-Marquardt algorithm is to use a weighted combination of steepest descent and Newtonian descent according to the characteristic of the cost function. Thus, when the cost function is near quadratic (generally near the solution) the efficiency of the Newtonian scheme is employed, and when the cost function is far from the quadratic (generally when far from the solution) the robustness of the steepest descent algorithm is favoured.

The steepest descent algorithm is intuitively the simplest. The vector \(-J'\) defines the ‘downward’ direction of the local steepest gradient. A move \( \delta x = -\alpha J' \) where \( \alpha \) is a variable. If \( J \) is found to be decreasing \( \alpha \) can be increased to move faster; if \( J \) increases then \( \alpha \) is reduced until \( J \) decreases. \( J \) must eventually decrease with this method otherwise there is an error in the calculation of \( \partial J/\partial x \). The problem with steepest descent is that it can be very slow to converge, especially near the solution where the gradient necessarily becomes small. It is however very robust.

Newtonian descent on the other hand is very fast near the solution because it will find it in one iteration if \( J \) is quadratic. Newton’s method finds the root of an equation and is therefore applied here in the form to find the root of \( J' = 0 \). the Newton step is therefore defined as \( \delta x = -J'/J'' \).

The problem with Newtonian descent is that, away from the solution, \( J \) can be very non-quadratic; the \( J'' \) can easily be the ‘wrong’ sign and the step is taken away from the solution. No amount of scaling can cure this problem.

The combined use of steepest descent and Newtonian methods constitutes the method of Levenburg-Marquardt. The method tests before each step is taken to check whether the resulting cost is reduced. If so the step is taken and an adjustment is made to make the next step ‘more Newtonian’. If an increase in \( J \) is detected then the step is not taken and an adjustment is made towards more steepest descent. In this way, the Levenburg-Marquardt method adopts steepest descent away from the solution and makes use of Newtonian descent near the solution. Formally, the increment in the Levenburg-Marquardt method is:

\[
\delta x = - (J'' + \alpha I)^{-1} J',
\]

where \( I \) is the unit matrix (size \( x \times x \)) and \( \alpha \) is the control variable described. When \( \alpha \) is large (compared to the ‘average’ size \( J'' \)) the step tends to steepest descent; when small the step approximates Newtonian. To initialise the descent, \( \alpha \) is set proportional to the average of the diagonals of \( J'' \) to obtain a reasonable value.

\[
\alpha_0 = MQ_{start} \times \text{Trace}(J'')
\]

With a successful (decreasing \( J \)) step, the control parameter is decreased

\[
\alpha_{n+1} = \alpha_n \div MQ_{step},
\]

and with an unsuccessful step the control parameter is increased

\[
\alpha_{n+1} = \alpha_n \times MQ_{step}.
\]

In the ORAC the control parameters \( MQ_{start} \) and \( MQ_{step} \) have default values of 0.001 and 10 respectively but can be set otherwise if preferred.

8.2.2 Boundaries

The state space in which the solution is to be found is typically bounded by physical constraints and the retrieval needs to ensure that values are not retrieved outside of these boundaries.
8.2.3 Convergence criteria

The iteration process proceeds until the decrease in $J$ between consecutive iterations ($\delta J_n$) is so small as to be considered negligible. This is determined as being smaller than a preset value (the default is 0.05). This simple and robust technique prevents a parameter which is not well constrained from oscillating or becoming unstable (because the cost function is ‘flat’ in that direction). Such an instability makes it appear that the solution is not yet found whereas, in fact, the cost is minimal and cannot decrease further. The use of a convergence criterion on $\delta J_n$ avoids this problem.

8.3 Quality control information

This is a very important aspect of any retrieval as there needs to be an effective way of checking the validity of the result. Fortunately, optimal estimation provides diagnostics which allow a reasonably strict quality control to be applied.

There are three principal diagnostics directly available from the inversion method. The first is a check of the ‘goodness of fit’ of the solution to its constraints. This should identify situations where the scene is not modelled by the radiative transfer mixed aerosol layer. The second diagnostic is the error field for the retrieval. Scenes that are modelled successfully but have larger than expected errors can indicate problems with the scene, e.g. missing channels etc. The third diagnostic is the number of iterations taken to reach the solution. This is another indicator of problem scenes.

8.3.1 Model fit

The value of $J$ at the solution indicates via a single number whether the solution is good to within statistical accuracies assumed for the measurements and the a priori.

If, at the solution, none of the measurements deviate from the calculated values (i.e. $y(x) - y_m$) by significantly more than their expected noise values (given by $S_y$) and no state variables deviate from their a priori values (i.e. $x - x_b$) by significantly more than the a priori error (given by $S_x$) then $J$ will be of order $n_y + n_x$ (where $n_y$ is the number of measurements used and $n_x$ is the number of state variables retrieved). Because of the general lack of a priori and the bounded state variables there are actually fewer degrees of freedom than $n_y + n_x$. A bounded fraction ($0 - 1$) cannot contribute anywhere near its expected $S_x$ value ($\sim \infty$) to $J$. Therefore it can be stated that if there are $n_b$ state variables that are bounded but without significant a priori then an acceptable solution will have $J$ of order $n_y + n_x - n_b$. This is essentially a $\chi^2$ test on the solution.

In the present context, it is the measurement term which will mostly contribute to $J$ and indeed it is the final $y(x) - y_m$ that will most often indicate a problem with the solution. The aerosol retrieval keeps account separately of $J_y$ and $J_x$ where $J = J_x + J_y$. In examination of retrieval results there are various levels of checks depending on the level of post-mortem required: firstly check $J$ for a general retrieval success. Then check $J_x$ and $J_y$ for measurement or a priori misfit and finally either $y(x) - y_m$ or $x - x_b$ for the offending measurement or state variable.

Because the value of $J$ depends on the estimation of values for $S_y$ and $S_x$ it is likely that $J$ will not initially be of order $n_y + n_x - n_b$ as expected. Values too low imply an overestimation of (probably) measurement error; values too large imply either underestimation of noise levels or convergence criteria that are too loose.
8.4 Linear error analysis

One of the powerful features of OE is that a rigorous error analysis of the retrieved state vector is available. It is based on the assumption that, in the vicinity of the solution, the radiative transfer model is linear. In this case, it can be shown that the solution for the minimum of

\[ J(x) = (y(x) - y_m)^T S_y^{-1} (y(x) - y_m) + (x - x_b)^T S_x^{-1} (x - x_b) + (b_t - b)^T S_b^{-1} (b_t - b), \]

is found for

\[ \hat{x} = (S_x^{-1} + K_x^T S_y^{-1} K_x)^{-1} (S_x^{-1} x_b + K_x^T S_y^{-1} y_m), \]

and thus the so-called inversion operator \( D_y = \partial/\partial y_m \) at the solution is given by

\[ D_y = (S_x^{-1} + K_x^T S_y^{-1} K_x)^{-1} K_x^T S_y^{-1}. \]

Following [17], the following error sources can be identified: a) ‘null space’ or a priori smoothing error, b) measurement error and c) model parameter error. These are expressed as covariances \( S_N \), \( S_M \), and \( S_S \) respectively.

8.4.1 Null space error

This is given by

\[ S_N = (D_y K_x - I) S_x (D_y K_x - I)^T. \]

\( S_N \) expresses the error that arises from a basic lack of information in the measurement system, hence the term ‘null space’ error.

8.4.2 Measurement error

\( S_M \) expresses the mapping of the errors in the measurements onto the solution and is given by

\[ S_M = D_y S_y D_y^T. \]

8.4.3 Model parameter error

Given by

\[ S_S = (D_y K_b) S_b (D_y K_b)^T. \]

\( S_S \) expresses the mapping of the errors in the forward model parameters onto the solution. This term is frequently neglected from error analyses on the grounds perhaps that \( S_b \) is either small (all parameters are well known) or that all uncertain parameters are included in the state vector \( x \), and are therefore manifest through \( S_N \) and \( S_M \).

It should also be noted that the total of the null space and measurement errors gives the familiar total error:

\[ \hat{S}_T = (S_x^{-1} + K_x^T S_y^{-1} K_x)^{-1}. \]

All error terms are covariances and the correlations implied by the off-diagonal terms are important for interpreting the information content of the measurements. However, it is unrealistic to output
9 Calculation ofDerived Aerosol Parameters and Speciation

the full covariances for all three error sources in an operational code environment and these are only available as special breakpoint variables for diagnosis. The ORAC nominal output contains only the square root of the diagonals for the total error, $S_T$ (or optionally $S_T + S_S$).

It is important to note that this error estimate

1. Applies to each state parameter separately; a high expected error in one parameter does not necessarily imply a high error in another.

2. Is conditional upon the correct solution being found.

3. Is conditional upon the atmosphere and aerosol conditions corresponding to the model assumed.

Whether the retrieval satisfies the latter two points can be evaluated to some extent using the model fit analysis described in 8.3.

8.5 Defining the statistical constraints

The statistical constraints on the solution $\hat{x}$ are the error covariance matrices $S_x$ and $S_y$, i.e the quality of the measurements and a priori values of the state. The error covariance matrix $S_b$ defines the contribution of the model parameter error to the retrieval error and does not affect the behaviour of the retrieval (but see section 4.2 on inclusion of model parameter equivalent measurement errors).

9 Calculation of derived aerosol parameters and speciation

As described the ORAC retrieval scheme determines the optical depth at 0.55 $\mu$m, the effective radius and the surface reflectance, for a given aerosol type, which best reproduce the observed radiance. However, by making use of the spectral dependance of the extinction coefficient defined for each aerosol type, it is possible for ORAC to be configured to return optical depths at any wavelength, as well as associated parameters. This is done by making use of an extra aerosol lookup table, which tabulates the ratio of the extinction coefficient at the desired wavelength to that at 0.55 $\mu$m as a function of effective radius:

from these values, the optical depth at a second wavelength can be computed using,

$$\tau_\lambda = \tau_{0.55} \frac{\beta_{ext}(\lambda_2)}{\beta_{ext}(0.55)}.$$ (9)

It should be noted however that, since the optical depth at the second wavelength is being extrapolated from the directly retrieved value at 0.55 $\mu$m, using modelled optical properties, the accuracy of this quantity will depend strongly on the accuracy of the aerosol class used in the retrieval.

The $\beta_{ext}$ lookup table can also be used to derive other aerosol properties, such as the Ångström coefficient, defined as

$$\frac{d \log [\tau(\lambda)]}{d \log [\lambda]}.$$ (10)
By assuming that $\tau$ varies linearly with $\lambda$ in the visible, it can be directly calculated from the two retrieved optical depths:

$$A_{0.55,0.865} = \frac{\log [\tau_{0.865}/\tau_{0.55}]}{\log [0.865/0.55]}.$$  \hspace{1cm} (11)

Some degree of speciation of aerosol is also possible using ORAC retrievals. In principal this is done by repeating the retrieval using a series of different aerosol types and then selecting the one that best matches the measurements. However, due to the assumptions implicitly made in the modelling of the aerosol and the surface, as well as the small number of measurements available to characterise the spectral shape of the signal, this is only really feasible with grossly different aerosol classes and with strong apriori constraints. For example, it is feasible to distinguish background maritime aerosol from desert dust, but not from background continental aerosol (as both continental and maritime aerosol are predominantly scattering aerosol types, with fairly similar spectral signatures).
ORAC INPUT AND OUTPUT FILES

A ORAC input and output files

A.1 Preprocessing inputs

<table>
<thead>
<tr>
<th>Satellite data</th>
<th>The ORAC processing chain uses the Level 1 ATSR-2 ungridded brightness temperature/reflectance (UBT) product or the Level 1b AATSR gridded brightness temperature/reflectance product.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface winds</td>
<td>To produce the sun glint flag, surface winds are required for the Cox and Monk calculation. The standard $2.5^\circ \times 2.5^\circ$ ECMWF ERA-40 10 metre U and V wind component product can be used.</td>
</tr>
<tr>
<td>Surface albedo</td>
<td>The MODIS surface albedo product is required to set the land surface’s spectral shape as well as the a priori and first guess values. This is available from the NASA Earth Observing System Gateway web site (<a href="http://edcimswww.cr.usgs.gov/pub/imswelcome/">http://edcimswww.cr.usgs.gov/pub/imswelcome/</a>).</td>
</tr>
<tr>
<td>Landflag</td>
<td>The landflagging algorithm requires three land/sea database files, which are part of the SADIST landflagging package: sfa_world.landsea sfa_degrees.landsea sfa_tenths.landsea.</td>
</tr>
</tbody>
</table>

A.2 ORAC inputs

<table>
<thead>
<tr>
<th>Driver file</th>
<th>.dri</th>
<th>An text file containing setting which control the behaviour of the retrieval software.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radiances</td>
<td>.msi</td>
<td>Unformatted binary file of single precision floating point numbers representing the satellite radiances averaged over each super-pixel.</td>
</tr>
<tr>
<td>Variance of Radiances</td>
<td>.var</td>
<td>Unformatted binary file of single precision floating point numbers representing the variance of the radiances which made up the averaged radiance above.</td>
</tr>
<tr>
<td>Land/sea flag</td>
<td>.lsf</td>
<td>Unformatted binary file of bytes which flag each pixel as either land or sea.</td>
</tr>
<tr>
<td>Cloud flag</td>
<td>.clf</td>
<td>Unformatted binary file of single precision floating point numbers which flag each pixel as either clear or cloudy.</td>
</tr>
<tr>
<td>Geometry</td>
<td>.geo</td>
<td>Unformatted binary file of single precision floating point numbers denoting the solar zenith, satellite zenith and relative solar – satellite azimuth angles.</td>
</tr>
<tr>
<td>Location</td>
<td>.loc</td>
<td>Unformatted binary file of single precision floating point numbers denoting the latitude and longitude of each pixel at the surface.</td>
</tr>
<tr>
<td>Albedo</td>
<td>.alb</td>
<td>Unformatted binary file of unsigned long integers denoting the a priori surface reflectance for each pixel.</td>
</tr>
</tbody>
</table>
A.3 ORAC outputs

Retrieval output for the GlobAEROSOL project will be stored in NetCDF format. For each aerosol type an output file will written directly by the retrieval software using the NetCDF-3.6.0 FORTRAN library available from UCAR Unidata website (http://my.unidata.ucar.edu/). These data will then be read by an IDL post processing routine\(^5\) which will construct a single, speciated product, which will also be output in NetCDF format. This approach has the advantage that all retrieved aerosol properties, which may well prove to be useful to users of the final GAP, will be retained in the standard output format. The content of the output files is:

- Geolocation (longitude/latitude) of each pixel.
- Measurement time of each pixel.
- Cloud mask (including a cloud fraction).
- Aerosol type used for each pixel.
- Aerosol optical depth at 0.55 \(\mu\text{m}\).
- Aerosol effective radius.
- An aerosol optical depth at a second wavelength (usually 0.86 \(\mu\text{m}\)).
- Satellite radiances for channels 1, 2, 3 and 4.
- Variances for all retrieved values, as well as the radiances.
- Instrument and solar zenith angles for each pixel.
- Relative (instrument to solar) azimuth angle for each pixel.
- Number of iterations used for the retrieval to reach convergence.
- Retrieval cost at the solution for each pixel.
- Meta data, including a description and units for each data field, information on the processor used to create the data, etc.

References


\(^5\)IDL includes NetCDF manipulation routines.


