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aerosol_cci

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AATSR
Optimal Retrieval of Aerosol and Cloud (ORAC)

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Executive summary

This algorithm theoretical basis document provides an overview of the principles and structure of the Optimal Retrieval of Aerosol and Cloud (ORAC) algorithm, as used to produce the ORAC products for the ESA aerosol_cci prototype products (ORAC product version number 3.02 and 3.04).

Applied to Advanced Along Track Scanning Radiometer (AATSR) measurements in the aerosol_cci project, ORAC is a dual-view aerosol retrieval scheme for use over both land and ocean surfaces. ORAC retrieves both aerosol optical depth and effective radius, as well as the surface reflectance at each of the four AATSR short-wave channels, using a mixture of pre-defined aerosol components. The algorithm has also been shown to have limited skill at selecting aerosol type from a range of possibilities (represented by differing mixtures of aerosol components).

ORAC is built around the optimal-estimation retrieval formalism, and thus provides full uncertainty propagation (from estimates of measurement noise, forward model uncertainty and *a priori* constraint), the ability to apply *a priori* constraints in a mathematically rigorous and consistent way, and extensive retrieval statistics and diagnostics.

This ATBD is devided into 8 sections:

1. Introduction
2. Reference lists
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ISSUE	DATE	MODIFICATIONS / REASON FOR CHANGE
1.0	21/02/2011	First complete version
2.0	14/09/2012	Updated to reflect changes to algorithm after round-robin exercise.
2.1	4/11/2015	Addition of type selection for v3.04.

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1 Introduction

This document describes an optimal estimation retrieval scheme for the derivation of the properties of atmospheric aerosol from top-of-atmosphere (TOA) radiances measured by satellite borne visible-IR radiometers. The algorithm makes up part of the Optimal Retrieval of Aerosol and Cloud[1] (ORAC) retrieval scheme (the other part of the algorithm performs cloud retrievals and is described in detail elsewhere [RD 1, 2]).

Specific features of this algorithm include:

- A full implementation of the optimal estimation framework described by Rodgers [RD 3], enabling rigorous error propagation and inclusion of *a priori* knowledge.
- The ability to use multiple instrument viewing geometries in a single measurement, and in particular the dual-view system of the Along Track Scanning Radiometer (ATSR) series of instruments.
- Two forward modelling approaches which include bidirectional reflectance distribution function (BRDF) surface reflectance descriptions in different ways. The first of these (hence fourth referred to as *ORAC-classic*) is applicable to both single and multi-view instruments. The second (*ORAC-dev*) is specific to multi-angle instruments and is based on the surface reflectance treatment used in the SU-ATSR algorithm [RD 4] (which is also a partner algorithm in the aerosol_cci project).

Although both forward model versions of ORAC work over both land and ocean, it has been found that for the current versions of the algorithms ORAC-classic is the better of the two over water, while ORAC-dev performs better of land surfaces (particularly bright surfaces). For this reason, the ORAC product for aerosol_cci is a hybrid of the two schemes.

2 References

Applicable documents

[AD 1] Statement of Work “ESA Climate Change Initiative Stage 1, Scientific user Consultation and Detailed Specification”, ref EOP-SEP/SOW/0031-09/SP. Issue 1.4, revision 1, dated 9 November, 2009, together with its Annex C “Aerosols” (altogether the SoW).

[AD 2] The Prime Contractor’s Baseline proposal, ref. 3003432, Revision 1.0, dated 16 June 2010, and the minutes of the July 26, 2010 kick-off meeting.

[AD 3] Aerosol-cci project management plan (PMP), version 1.3.

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[1] ORAC has historically stood for Oxford-RAL Aerosol and Cloud, but this has been generalised to represent the wider pool of researchers currently involved in its development.

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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 2002, respectively. As the instruments were essentially the same in their operation, with the only major difference being the bandwidth available for data transfer, they can be described together. Although both ATSR-2 and AATSR are no longer operational, their measurement record will be continued with the forth instrument in the series, the Sea and Land Surface Temperature Radiometer (SLSTR), which is due to be launched in 2014 on the GMES Sentinel 3 platform.

The primary design goal of the ATSR series of 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 it's primary and secondary roles.

Both ATSR-2 and AATSR had seven spectral channels centred at 0.55, 0.67, 0.87, 1.6, 3.7, 10.7 and 12 μm. The instruments used 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 produced a scan centred on the nadir direction, while the other viewed the surface approximately 900 km ahead of the satellite (at a viewing angle of 55° from the nadir). This continuous scanning pattern produced a nadir resolution of approximately 1×1 km with a swath width of 512 pixels. The dual view system is one of the great strengths of the ATSR instruments, as it allows the atmospheric and surface contributions to the TOA radiance to be more effectively decoupled than is possible with a single view. This offers much improved accuracy in both derived surface and atmospheric parameters. In addition, the instruments are designed to be self calibrating, with two integrated, thermally controlled black-body targets for calibration of the thermal channels, as well as an opal visible calibration target (illuminated by sunlight) for the visible/near-IR channels.

Due to bandwidth limitations on the ERS-2 satellite, ATSR-2 was usually run in a “narrow swath” mode over the oceans, which produced a swath of only 256 pixels in some of the visible channels; or with some channels entirely missing (with the 0.55 μm channel being the most commonly affected, followed by 0.67 μm). Furthermore, usually one orbit per day had the digitisation resolution in the visible channels degraded from 12 to 8 bit, resulting in a only 256 reflectance levels being reported (rather than the usual 4096). In addition, although ATSR-2 continued to operate until 2009, the ERS-2 satellite developed a pointing problem in October 2001, which means that post 2001 data from the instrument has to have a geolocation correction applied before it can be used. Finally, in June 2003, the data tape recorder on ERS-2 failed, with the result that ATSR-2 data from this date was only available while the satellite is within range of a data downlink ground station. At the time of writing, level 1b data from ATSR-2 is available from mid 1995 through to June 2003, with a six month gap at the beginning of 1996 (due to an instrument problem at that time). AATSR provided nearly continuous data coverage from mid 2002 until the failure of ENVISAT in April 2012. There is thus a 12 month overlap between the data from the two instruments.

ERS-2 and ENVISAT were in similar polar orbits with periods of approximately 100 minutes. Both ATSR-2 and AATSR nominally provided global coverage every six days.

4 ORAC input and output data

When applied to (A)ATSR data, ORAC ingests standard ESA level1b data. Although the physical quantity measured by most satellite radiometers, including the (A)ATSR instruments, is radiance the data used by ORAC (and included in (A)ATSR level1b data) has been scaled by the cosine of the solar zenith angle and normalised, to produce a top of atmosphere reflectance. It is thus reflectance which is discussed in this document. In the configuration used for aerosol_cci, ORAC uses the first four (A)ATSR channels (i.e. 0.55, 0.67, 0.87, 1.6 μm) in both views.

The parameters retrieved by ORAC are:

- The $\log_{10}$ of aerosol optical depth at 0.55 μm.

- The $\log_{10}$ of aerosol effective radius (in units of $\log_{10}(\mu\text{m})$)
- Surface bi-hemispheric reflectance at each measurement wavelength.

In addition, the retrieval also provides $\log_{10}$ of aerosol optical depth at 0.87 μm, but this is not an independently retrieved value. One standard deviation uncertainty values are provided for all retrieved parameters.

Cloud cleared reflectance data is averaged onto a 10 km sinusoidal grid prior to retrieval (the grid is actually specified as having 4008 cells around the equator, which is the closest integer number to a 10 km spacing). For aerosol_cci, data is supplied in NetCDF files, following the CF-1.4 naming conventions. In these files the $\log_{10}$ values have been converted to a linear scale, i.e. the files contain aerosol optical depth and effective radius. The uncertainty on these values is expressed as $\log_e(10)\delta\log_{10}(x)x$, where x is the retrieved value transformed into linear space (optical depth or effective radius) and $\delta\log_{10}(x)$ is the uncertainty on the $\log_{10}$ value of x. Thus, the uncertainties provided on optical depth and effective radius do not directly correspond to the one standard deviation interval about the retrieved state, but are representative.

ORAC also makes use of a range of ancillary data, the use of which will be described in detail in later sections. In summary though, the following inputs are used:

- ECMWF reanalysis 10 m East-West and North-South (u and v) wind components. These are used by the sea-surface reflectance model to determine surface roughness and whitecap coverage.
- GlobCOLOUR monthly mean, 0.25° degree, chlorophyll-A and coloured dissolved organic matter (CDOM) products. These are also used by the sea-surface reflectance model to determine the volume scattering of the water.

In addition, if ORAC-classic were to be used over land the MODIS MCD43B BRDF model parameter product would be used to determine the *a priori* land surface reflectance and fix its directional dependence. In it's present form, the ORAC-dev forward model does not make use of any *a priori* surface reflectance information.

4.1 Cloud clearing

When retrieving aerosol properties from imaging satellite instruments, it is very important that data affected by the presence of clouds is excluded from the processing. The effect of cloud on visible and near-IR radiation is similar to that of aerosol, but many times stronger (due to the much larger size of cloud particles). Thus the presence of even a small amount of cloud within a scene can have a huge effect on the derived aerosol properties.

The primary cloud flag employed in ORAC is the operational flag provided in the standard level 1b products. Over oceans this consists of a series of threshold tests on both the thermal and shortwave channels, and a test on spatial inhomogeneity of a scene. Over land, the flag uses two normalised difference vegetation index (NDVI) type tests, which compare the TOA reflectance between the 0.55 and 0.67 μm channels and the 0.67 and 0.87 μm channels. These flags are described in detail by Birks [RD 5].

Generally the ocean flag is considerably more reliable than the one used over land and is, in most circumstances, very conservative (having been developed to minimise errors due to cloud contamination in sea surface temperature measurements, rather than providing an accurate map of cloud cover). However, we have discovered two significant problems with this cloud flag:

1. Due to its conservative nature, it has been found to flag optically thick aerosol, such as dense dust clouds or smoke/ash plumes, as cloud. A limited number of tests have been developed to

identifying specific thick aerosol plumes, which can be used to improve detection of such events. Details of these flags are given by Lean [RD 6].

2. The operational flag often misses low, warm stratiform clouds, particularly at northern mid-latitudes. These clouds are often quite thick and very obvious to the naked eye in the visible channels of ATSR. We have developed a simple NDVI type test, between the 0.55 and 0.67 micron channels. When applied over the ocean, a negative (or very small positive) value of this ratio, in both ATSR views, is indicative of such clouds. The test must be applied in both ATSR views, otherwise sun-glint is also flagged.

The operational land cloud flagging is also generally quite conservative, and visual inspection of the aerosol retrieval output suggests that regions which would be expected to show elevated aerosol loading are often flagged as 100% cloudy. Furthermore, this flag also suffers from a significant bug. If shortwave channels of (A)ATSR saturate, their reflectance value is set to zero in level 1b data; it appears that the operation cloud flag does not check for this and will therefore always return these pixels as cloud free. Unfortunately, this is not an uncommon occurrence for bright-thick clouds, so two additional tests have been developed to overcome this bug, and improve the detection of sub-pixel cloud:

1. Firstly, pixels over land which have a zero reflectance in either the 0.55 or 0.67 micron channels are marked as cloudy.
2. The so called “opening test” is used on the 12 micron brightness temperatures over land, with a 5 km radius kernel (whereby the erode and dilate image processing algorithms are sequentially applied to the scene). This test provides a powerful way of detecting regions of rapid change in the brightness of an image, which are indicative of cloud edges and sub-pixel clouds.

As a final pre-retrieval cloud flagging exercise, the opening test is again applied, but this time to all data (land and ocean) using the 1.6 micron channel.

ORAC also has the facility to read in an external cloud mask, such as the common cloud mask developed specifically for the aerosol_cci project. However, as the common cloud mask was not available in time for the initial delivery of the aerosol_cci prototype products, this has not been used[2].

5 The ORAC forward model

The core of the ORAC retrieval algorithm is the forward model, which uses radiative transfer code to predict the radiance observed at the satellite as a function of aerosol properties, using assumptions about the atmospheric state and the reflectance of the Earth’s surface. For the sake of numerical efficiency, ORAC makes use of two forward models: firstly a full radiative transfer model (referred to here simply as the forward model, FM), which attempts to accurately account for all relevant physical processes effecting the measurement, is run “off-line” to produce look-up tables of total atmospheric reflectance and transmission for the plausible range of viewing geometries and aerosol states. These look-up tables are then used to produce TOA radiances during a retrieval run using a simple arithmetic expression, known as the fast forward model (Fast-FM), which includes a BRDF surface characterisation.

The FM can itself be thought of as consisting of three separate elements:

1. A model of aerosol scattering and absorption.

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[2] Note: this point applies to all versions of the ORAC aerosol_cci product from 2.02.

2. A model of atmospheric gas absorption.

3. Radiative transfer code to produce TOA reflectance based on the output of the first two models, Rayleigh scattering and viewing geometry.

5.1 Aerosol scattering and absorption

In a given location, atmospheric aerosols are characterised by their morphology, 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 approximated by assuming the particles are spherical and applying Mie theory [RD 7], or by utilising various non-spherical scattering approximations, such as the T-matrix approach [RD 8], when the particles are known to be non-spherical.

The aerosol optical depth, τ, is the primary quantity obtained from ORAC. It is defined as:

$$\tau(\lambda) = \int_0^\infty \beta_\mathrm{e}(z,\lambda)\,dz = \int_0^\infty (\beta_\mathrm{s} + \beta_\mathrm{a})(z,\lambda)\,dz \tag{1}$$

The total extinction coefficient, β_e, is defined as the sum of the extinction due to absorption, β_a, and scattering, β_s. The vertical profile of β_a and β_s along with the scattering phase function, $P(\theta)$, (which determines the angular distribution of the scattered radiation) and the degree of polarisation as a function of scattering angle, fully describe the aerosol radiative characteristics. Other convenient ways of defining aerosol optical properties are the single scattering albedo, ω_o, which is the ratio of β_s to β_e, and the asymmetry parameter, g, which is the integral of $P(\theta)$ over all possible scattering angles ($0 \leq \theta \leq 180°$), weighted by $\cos\theta$ (i.e. it is the first moment of the phase function). For a given aerosol model (shape, size, and refractive index), β_e is proportional to the aerosol concentration while $P(\theta)$ is not.

Mie theory shows that the extinction coefficient is given by:

$$\beta(z,\lambda) = \int_0^\infty Q_\mathrm{e}(z,m,x)\,\pi r^2\,n(z,r)\,dr \tag{2}$$

where Q_e is the Mie extinction efficiency factor, and is dependent on the Mie size parameter $x = 2\pi r/\lambda$ (where r is the particle radius and λ the wavelength of light), and the refractive index of the particles ($m = m_\mathrm{r} + i m_\mathrm{i}$), and $n(z,r)$ is the number size distribution.

The log-normal distribution is the most suitable representation for characterising the size distribution of the atmospheric aerosols [RD 9]. The distribution, in terms of number density as a function of radius $n(r)$, is described by its median radius (r_m), standard deviation (σ) of $\ln r$, and total number density (N_0):

$$n(r) = \frac{N_0}{\sqrt{2\pi}}\frac{1}{\sigma r}\exp\left[-\frac{(\ln r - \ln r_\mathrm{m})^2}{2\sigma^2}\right] \tag{3}$$

For the production of the aerosol_cci prototype product, the aerosol components defined in the aerosol_cci Aerosol models technical note [RD 10] have been used. Using the climatology of aerosol component fractions provided in this document, a family of ten aerosol types have been defined, as described in table 1. These classes have been constructed using the optical and scattering properties provided by the aerosol_cci aerosol modelling working group.

The quantity used to define the size of the aerosol particles in ORAC is the effective radius, defined as the the ratio of the 3rd and 2nd moments of the size distribution:

Name	Mixing state			r_e (μm)
	Fine:Coarse	Coarse	Fine	
A70	99.0:1.0	100% dust	12.5% strongly-absorbing	1.218
A71	99.8:0.2	100% dust	50% strongly-absorbing	0.553
A72	99.8:0.2	75% dust	25% strongly-absorbing	0.553
A73	99.8:0.2	75% dust	12.5% strongly-absorbing	0.553
A74	99.8:0.2	50% dust	100% weakly-absorbing	0.553
A75	99.5:0.5	25% dust	100% weakly-absorbing	0.908
A76	99.0:1.0	100% sea-salt	100% weakly-absorbing	1.218
A77	99.5:0.5	50% dust	12.5% strongly-absorbing	0.908
A78	99.8:0.2	100% sea-salt	12.5% strongly-absorbing	0.553
A79	100.0:0.0	-	37.5% strongly-absorbing	0.142

Table 1: The ten aerosol ORAC classes produced from the four components defined by the aerosol_cci Aerosol models technical note. The Fine:Coarse ratio, and percentage mixtures of the coarse and fine modes are in terms of particle number. The fine:coarse ratio and effective radius figures are the a priori values.

$$r_e = \frac{\int_0^\infty r^3 n(r) dr}{\int_0^\infty r^2 n(r) dr} \tag{4}$$

In order to produce radiance look-up tables from the individual aerosol_cci components the scattering properties of each aerosol type are calculated for each AATSR channel across a range of effective radii from 0.01 to 10 μm. 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 effective radii other than those specified in 1, the relative concentration of the fine and coarse mode components are changed. For example, if the effective radius needs to be decreased, the relative concentration of the fine mode will be increased, while the coarse mode will be decreased.

  If the required effective radius is equal to that given by the fine or coarse mode of a given aerosol type, then the type effectively becomes a single mode aerosol[3]. If the size is outside of this range, then the mode radius of the smallest/largest components 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 composition 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 a vertical profile of aerosol extinction and phase function, based on vertical profiles of number density, N:

$$N(h) = N(0) \exp(-h/Z), \tag{5}$$

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[3] Note that is always the case for class A69.

Value	No. of points	Min. value	Max. value	Spacing
$\log_{10}(\tau)$	20	-2.0	0.75	logarithmic in τ
$\log_{10}(r_\mathrm{e})$	20	-2.0	1.00	logarithmic in r_e
θ_0	10	0°	90°	linear
θ_v	10	0°	81°	linear
ϕ	11	0°	180°	linear

Table 2: The dimensions of the ORAC LUTs used for aerosol_cci. Note that not all LUTs are functions of all variables (for instance, atmospheric transmission terms are functions of a single zenith angle only).

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 scattering albedo and the coefficients of a Legendre expansion of the scattering phase function are calculated for each instrument channel and over 20 logarithmically spaced effective radii between 0.01 and 10 μm.

Table 2 gives details of the tabulation of optical depth, effective radius and viewing geometry used in generating the ORAC look-up tables (LUTs).

5.2 Modelling atmospheric gas absorption

Once aerosol scattering properties have been calculated, gas absorption over the instrument band passes is calculated in terms of an optical depth, and convolved with the instrument filter transmission functions, using MODTRAN [RD 11]. MODTRAN provides tropical, mid-latitude summer and winter, subarctic summer and winter, and US Standard Atmosphere climatological atmospheres for the following gasses: H_2O, CO_2, O_3, N_2O, CO, CH_4, plus single profiles for: HNO_3, NO, NO_2, SO_2, O_2, N_2, NH_3 and the heavy molecules (CFCs). ORAC look-up 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 (A)ATSR channels are free from strong absorption features of gases which show large spatial and temporal variability (most notably, H_2O).

5.3 Modelling atmospheric transmission and reflectance

The final step in the FM is the prediction of atmospheric transmission and bidirectional reflectance, based on the aerosol phase functions and gas optical depth calculated in the previous two steps. The ORAC FM uses the DIscrete Ordinates Radiative Transfer (DISORT) software package [RD 12] to perform this step.

DISORT is a thoroughly documented and widely used general purpose algorithm for the calculation of time-independent radiative transfer calculations. The DISORT algorithm solves the equation for the transfer of monochromatic light at wavelength λ as described by the equation

$$\mu \frac{dL_\lambda(\tau_\lambda, \mu, \phi)}{d\tau} = L_\lambda(\tau_\lambda, \mu, \phi) - L^S_\lambda(\tau_\lambda, \mu, \phi), \tag{6}$$

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

It should be noted that DISORT still makes some important approximations, which can limit its accuracy in certain circumstances. The most important of these are:

- It assumes a plane parallel atmosphere, which makes it inapplicable at viewing or zenith angles above approximately 75°, where the curvature of the Earth has a significant influence on radiative transfer.
- It is a one dimensional model, so cannot reproduce the effects of horizontal gradients in the scattering medium. This is important where strong gradients exist, such as near cloud edges.
- It does not model polarisation effects and hence cannot be used to model measurements made by instruments which are sensitive to polarisation and does not take the polarisation introduced into the diffuse component of radiance by Rayleigh scattering.

DISORT is provided with the aerosol scattering properties defined by the scattering calculations and the gas absorptions defined by MODTRAN on 31 levels from 0–100 km and the vertexes shown in table 2. Although DISORT has the ability to include a surface of arbitrary reflectance below the modelled atmosphere, no surface reflectance is included at this step. Rather, the transmission and reflectance of the atmosphere alone is computed for both direct beam and diffuse radiation sources separately. These calculations produce five look-up tables for each aerosol type/channel combination:

- Bidirectional reflectance of the atmosphere, from the top of the atmosphere, $R_{\mathrm{bb}}(\theta_0, \theta_{\mathrm{v}}, \phi)$.
- Diffuse reflectance of the atmosphere to diffuse radiance, R_{dd}.
- Diffuse transmission of an incident beam, $T^{\downarrow}_{\mathrm{bd}}(\theta_0)$.
- Direct transmission of the beam, $T^{\downarrow}_{\mathrm{bb}}(\theta_0)$, or $T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}})$.
- Transmission of diffuse incident radiance, $T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}})$.

Here, a $\downarrow$ denotes transmission from the top to the bottom of the atmosphere, while $\uparrow$ indicates the reverse. Dependence on the solar zenith, viewing zenith and relative azimuth angles are denoted by θ_0, θ_{v} and ϕ respectively. The pairs of b and d subscripts denote the type of radiation each term operates on and produces; for example $T^{\downarrow}_{\mathrm{bd}}(\theta_0)$ operates on the direct beam (b) of solar radiation, and produces the diffuse radiation (d) that results at the bottom of the atmosphere. Each of these files contains tabulated transmission or reflectance (depending on the file) values for each of the twenty effective radii, nine 0.55 μm optical depths and sun/satellite geometry (specified by twenty equally spaced zenith angles and eleven equally spaced azimuth angles).

Effects of molecular absorption and Rayleigh scattering are included by adjustment of the layer's optical depth and the particle's single scattering albedo and phase function with the following:

$$\tau = \tau_{\mathrm{a}} + \tau_{\mathrm{R}} + \tau_{\mathrm{g}}, \tag{7}$$

$$\omega = \frac{\tau_{\mathrm{R}} + \omega_{\mathrm{a}}\,\tau_{\mathrm{a}}}{\tau_{\mathrm{g}} + \tau_{\mathrm{R}} + \tau_{\mathrm{a}}}, \tag{8}$$

$$P(\theta) = \frac{\tau_{\mathrm{a}}\omega_{\mathrm{a}}P_{\mathrm{a}}(\theta) + \tau_{\mathrm{R}}P_{\mathrm{R}}(\theta)}{\tau_{\mathrm{a}}\omega_{\mathrm{a}} + \tau_{\mathrm{R}}}, \tag{9}$$

where τ_{a}, τ_{R} and τ_{g} are the contributions to the total optical depth τ due to aerosol scattering, Rayleigh scattering and gaseous absorption within each layer respectively. The aerosol single scattering albedo is denoted ω_{a}.

For each layer bounded by lower and upper pressure levels p_{l} and p_{u}, respectively and ground level pressure p_0, τ_{R} is calculated from

$$\tau_{\mathrm{R}} = \frac{\tau_{\mathrm{RT}}[p_{\mathrm{l}} - p_{\mathrm{u}}]}{p_s}, \tag{10}$$

where τ_{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 [RD 13]:

$$\tau_{\mathrm{RT}}(\lambda) = \frac{1}{117.03\,\lambda^4 - 1.316\,\lambda^2}, \tag{11}$$

where p_{s} is the standard pressure ($p_{\mathrm{s}} = 1013.25$ hPa), p_0 is the ground pressure in hPa and λ is in μm.

Note that, at present, ORAC does not take the variation of surface pressure due to terrain height or meteorology into account. This, combined with the lack of polarisation in the radiative transfer calculations mean that ORAC is not currently suitable for use with instrument channels in the blue or ultraviolet (where the Rayleigh signal is much stronger and will vary significantly with terrain height).

6 Surface reflectance and fast forward model

Of crucial importance in the retrieval of aerosol properties from "near-nadir" visible/near-infrared satellite measurements (i.e. measurements in which the Earth's surface contributes to the measured radiances) is an accurate description of the surface reflectance. When applied to (A)ATSR dual view measurements, ORAC retrieves the surface reflectance in each measurement channel in addition to the aerosol optical depth and effective radius, however it is still necessary to provide a constraint on the angular dependence of the BRDF (i.e. the ratio of the various surface reflectance terms in the two instrument views). How this restraint is formulated is the essential difference between the ORAC-classic and ORAC-dev versions of the retrieval.

6.1 ORAC-classic implementation

In the ORAC-classic implementation, the BRDF is constrained using ancillary data which can be used to produce an *a priori* of the BRDF itself. The methodology used to produce this *a priori* surface reflectance differs between measurements made over sea or land. Over the sea a surface reflectance model, described by Sayer et al. [RD 14] is used. This model includes upwelling radiance from volume scattering within the water [RD 15], specular reflections from the wind-roughened surface (as modelled by Cox and Munk [RD 16 17]) and reflection from white-caps [RD 18, 19]. The model uses ECMWF reanalysis wind fields to determine wave statistics and white-cap coverage, as well as chlorophyll and CDOM concentrations provided by the GlobCOLOUR [RD 20] product.

Over land the MODIS[4] land surface bidirectional reflectance product, which carries the identifier MCD43B, [RD 21] is used to define the *a priori* surface reflectance. The product consists of a set of three parameters for the MODIS AMBRALS (Algorithm for Modelling Bidirectional Reflectance Anisotropies of the Land Surface) surface reflectance model [RD 22], which itself consists of three simple reflectance kernels for different surface types:

- Isotropic kernel. Lambertian reflectance, for which the kernel is $\equiv 1$.
- Ross-thick kernel, $K_{\mathrm{Rt}}(\theta_0, \theta_{\mathrm{v}}, \phi)$. Parametrises densely packed, randomly oriented reflectors, such as leaves.
- Li-sparse kernel, $K_{\mathrm{Li}}(\theta_0, \theta_{\mathrm{v}}, \phi)$. Parametrises the shadowing effects of isolated large objects, such as isolated trees.

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[4] MODerate resolution Imaging Spectrometer

The three coefficients, p_{iso}, p_{vol} and p_{geo} for the isotropic, Ross-thick and Li-sparse kernels respectively, provided by the BRDF product weight these models to reproduce the atmospherically corrected bi-directional surface reflectance observed by MODIS over a 8 day period.

The MODIS BRDF product has an uncertainty of ±10 %, with a minimum absolute uncertainty of 0.005 in the white sky albedo derived from the AMBRALS model coefficients[5].

Since the Ross-thick and Li-sparse kernels are both dependant only on the solar and viewing directions, the AMBRALS model can be written in the form:

$$\rho_{\mathrm{bb}} = p_{\mathrm{iso}} + K_{\mathrm{Rt}}(\theta_0, \theta_{\mathrm{v}}, \phi) p_{\mathrm{vol}} + K_{\mathrm{Li}}(\theta_0, \theta_{\mathrm{v}}, \phi) p_{\mathrm{geo}} \tag{12}$$

These coefficients can also be combined to form either a hemispheric reflectance:

$$\begin{aligned}\rho_{\mathrm{bd}} = p_{\mathrm{iso}} &+ \left(b_{\mathrm{bs1}} + b_{\mathrm{bs2}}\theta_0^2 + b_{\mathrm{bs3}}\theta_0^3\right) p_{\mathrm{vol}} \\ &+ \left(c_{\mathrm{bs1}} + c_{\mathrm{bs2}}\theta_0^2 + c_{\mathrm{bs3}}\theta_0^3\right) p_{\mathrm{geo}},\end{aligned} \tag{13}$$

or a bi-hemispheric reflectance:

$$\rho_{\mathrm{dd}} = p_{\mathrm{iso}} + b_{\mathrm{ws}} p_{\mathrm{vol}} + c_{\mathrm{ws}} p_{\mathrm{geo}}, \tag{14}$$

where the quantities b_{ws}, c_{ws}, b_{bs1}, etc. are constant coefficients published by the MODIS BRDF team [RD 23].

6.1.1 Mapping MODIS BRDF to AATSR channels

Although MODIS provides channels which closely match all of the (A)ATSR ones, the differences in the spectral response functions are great enough to produce a significant error when using the MCD43B product to predict the surface reflectance seen by AATSR [RD 24, 25] and it is necessary to correct the reflectances predicted by the MCD43B product. However, the required corrections depend on the particular spectral properties of the surface.

Thus the problem is to generate appropriate corrections, without needing to convolve a high spectral resolution model of the surface reflectance with the channel response function of each instrument, or knowledge of the spectral properties of the surface. This is achieved using a singular value decomposition (SVD) method to model the variability of the spectral albedo (bi-hemispherical reflectance) that would observed by MODIS and AATSR (or ATSR-2) over a wide range of surfaces, generated from the ASTER [RD 26] and USGS [RD 27] libraries of spectral reflectance.

A matrix of MODIS and AATSR measurements corresponding to the spectra of 147 representative surface types (i.e. a 8×147 element matrix) was decomposed using SVD, and it was found that the first four singular vectors captured 99.2 % of the variability observed in the spectra. Thus, a linear fit of these four vectors to the bi-hemispheric reflectance calculated from the MCD43B product provides an improved estimate of the corresponding AATSR reflectances. Error analysis of this technique by Sayer [RD 24] has shown that one standard deviation errors in the predicted AATSR reflectance due to the SVD correction from MODIS values are 8.6×10^{-4} at 0.55 μm, 1.5×10^{-3} at 0.67 μm, 6.6×10^{-4} at 0.87 μm and 3.4×10^{-3} at 1.6 μm.

6.1.2 Sun-glint

A major problem encountered in making nadir satellite measurements is the specular reflection of sunlight off the ocean surface, usually referred to as sun-glint. In sun-glint effected regions the TOA signal becomes dominated by the directly reflected radiance from the surface, which results in a much

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[5] C.B. Schaaf, private communication, 2010.

poorer signal-to-noise ratio for the atmospheric signal. For this reason, it is common for satellite aerosol products to mask out sun-glint regions. However, the geometry of the (A)ATSR dual-view system means that both views never effected by sun-glint at the same location, and ORAC-classic is still able to reliably retrieval aerosol properties. It should be noted that in sun-glint situations, ORAC is essentially working as a single view retrieval (as almost all information on the atmospheric aerosol is coming from the view not effected by sun-glint). Thus it is to be expected that retrieval error estimates will be correspondingly larger and there will be more noise in the results, as the retrieval is not as well constrained. However, barring forward model biases, the results should not show a decrease in overall accuracy.

6.1.3 The fast forward model

The ORAC-classic forward model works on the assumption that the surface BRDF can be parametrised by three reflectance terms:

1. The specular, or bidirectional reflectance, $\rho_{\mathrm{bb}}(\theta_0, \theta_{\mathrm{v}}, \phi)$. This is the reflectance of the surface to direct beam illumination, as viewed from a specific direction. It is the reflectance that would be observed by a satellite instrument in the absence of an atmosphere.
2. The hemispheric reflectance (black-sky albedo) $\rho_{\mathrm{bd}}(\theta_0)$ or $\rho_{\mathrm{db}}(\theta_{\mathrm{v}})$. This is the fraction of incoming, direct beam illumination that is reflected across all viewing angles (or, equivalently, the reflectance of the surface to purely diffuse illumination as viewed from a specific direction θ_{v}).
3. The bi-hemispheric reflectance (white-sky albedo), ρ_{dd}. This is the reflectance of the surface to purely diffuse illumination, across all viewing directions.

Using this surface reflectance description and writing down components of the TOA reflectance in terms of direct and diffuse transmission, we get:

$$R_{\mathrm{TOA}}(\theta_0,\theta_{\mathrm{v}},\phi) = \begin{array}{ll}
R_{\mathrm{bb}}(\theta_0,\theta_{\mathrm{v}},\phi) & \}\text{Reflection off the atmosphere} \\
\left.\begin{array}{l}
+T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bb}}(\theta_0,\theta_{\mathrm{v}},\phi)T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) \\
+T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bd}}(\theta_0)T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}}) \\
+T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{db}}(\theta_{\mathrm{v}})T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) \\
+T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{dd}}T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}})
\end{array}\right\} & \text{Single reflection off the surface} \\
\left.\begin{array}{l}
+T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bd}}(\theta_0)R_{\mathrm{dd}}\rho_{\mathrm{db}}T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) \\
+T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bd}}(\theta_0)R_{\mathrm{dd}}\rho_{\mathrm{dd}}T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}}) \\
+T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{dd}}R_{\mathrm{dd}}\rho_{\mathrm{db}}T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) \\
+T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{dd}}R_{\mathrm{dd}}\rho_{\mathrm{dd}}T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}})
\end{array}\right\} & \text{Double reflection off the surface} \\
\left.\begin{array}{l}
+T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bd}}(\theta_0)R_{\mathrm{dd}}\rho_{\mathrm{dd}}R_{\mathrm{dd}}\rho_{\mathrm{db}}T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) \\
+T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bd}}(\theta_0)R_{\mathrm{dd}}\rho_{\mathrm{dd}}R_{\mathrm{dd}}\rho_{\mathrm{dd}}T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}}) \\
+T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{dd}}R_{\mathrm{dd}}\rho_{\mathrm{dd}}R_{\mathrm{dd}}\rho_{\mathrm{db}}T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) \\
+T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{dd}}R_{\mathrm{dd}}\rho_{\mathrm{dd}}R_{\mathrm{dd}}\rho_{\mathrm{dd}}T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}})
\end{array}\right\} & \text{Triple reflection off the surface} \\
+\dots &
\end{array} \tag{15}$$

Here we have four terms resulting from a single surface reflection in Eq. 15, which can described as follows:

- $T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bb}}(\theta_0,\theta_{\mathrm{v}},\phi)T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}})$ is the direct transmission of the solar beam, reflected off the surface and transmitted directly to the satellite.

- In $T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bd}}(\theta_0)T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}})$ the diffusely reflected portion of the directly transmitted solar beam is diffusely transmitted (via multiple scattering in the atmosphere) into the viewing direction of the satellite.
- $T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{db}}(\theta_{\mathrm{v}})T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}})$ gives the portion of the diffusely transmitted solar beam, which is then reflected into the viewing direction of the satellite and directly transmitted back through the atmosphere.
- $T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{dd}}T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}})$ is the purely diffuse component, where solar radiation is diffusely transmitted to the surface, reflected off the surface and diffusely transmitted to the satellite.

The terms following on from these describe the rapidly diminishing series of multiple reflections between the surface and overlaying atmosphere. For these terms the assumption has been made that ground and atmosphere pair are essentially Lambertian reflectors; i.e. that only the bi-hemispherical reflectance of the atmosphere is needed. This is equivalent to saying, neglecting directly transmitted solar radiation, the sky is equally bright in all directions.

By assuming that the surface reflectance does not show any dependence on viewing angle when under diffuse illumination, terms involving $\rho_{\mathrm{db}}(\theta_{\mathrm{v}})$ can be combined with those involving ρ_{dd}

$$T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{db}}(\theta_{\mathrm{v}})T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) + T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{dd}}T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}}) \sim T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{dd}}\left(T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) + T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}})\right) \tag{16}$$

where the term $T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) + T^{\uparrow}_{\mathrm{db}}(\theta_{\mathrm{v}}) = T^{\uparrow}_{\mathrm{tb}}(\theta_{\mathrm{v}})$ is the total transmission of the atmosphere at the viewing zenith angle.

Applying this approximation and collecting terms leads to

$$\begin{aligned} R_{\mathrm{TOA}} = R_{\mathrm{bb}}(\theta_0, \theta_{\mathrm{v}}, \phi) &+ T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bb}}(\theta_0, \theta_{\mathrm{v}}, \phi)T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) \\ &- T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bd}}(\theta_0)T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}}) \\ &+ \left(T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bd}}(\theta_0) + T^{\downarrow}_{\mathrm{bd}}(\theta_0)\rho_{\mathrm{dd}}\right) T^{\uparrow}_{\mathrm{td}}(\theta_{\mathrm{v}}) \\ &+ \left(1 + R_{\mathrm{dd}}\rho_{\mathrm{dd}} + R^2_{\mathrm{dd}}\rho^2_{\mathrm{dd}} + \ldots\right). \end{aligned} \tag{17}$$

The term $T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bd}}(\theta_0)T^{\uparrow}_{\mathrm{bb}}(\theta_{\mathrm{v}})$ is taken away to account for the $T^{\uparrow}_{\mathrm{tb}}(\theta_{\mathrm{v}})$ term being applied to $T^{\downarrow}_{\mathrm{bb}}(\theta_0)\rho_{\mathrm{bd}}(\theta_0)$. Application of the appropriate series limit leads to the expression

$$\begin{aligned} R = R_{\mathrm{bb}}(\theta_0, \theta_{\mathrm{v}}, \phi) &+ T^{\downarrow}_{\mathrm{bb}}(\theta_0)\left(\rho_{\mathrm{bb}}(\theta_0, \theta_{\mathrm{v}}, \phi) - \rho_{\mathrm{dd}}\right)T_{\mathrm{db}}(\theta_{\mathrm{v}}) \\ &+ \frac{\left(T^{\downarrow}_{\mathrm{bb}}\rho_{\mathrm{bd}}(\theta_0) + T^{\uparrow}_{\mathrm{bd}}\rho_{\mathrm{dd}}\right)T_{\mathrm{db}}(\theta_{\mathrm{v}})}{1 - \rho_{\mathrm{dd}}R_{\mathrm{dd}}}. \end{aligned} \tag{18}$$

It is equation 18 that forms the basis of the ORAC-classic forward model. It should be noted that this expression does not obey the reciprocity principal (i.e. if the viewing and solar angles are swapped, the equation is not equivalent), due to the approximation made in equation 16. However, extensive testing of equation 18 against full radiative transfer calculations has shown it to be a very good approximation for realistic viewing geometries and surface BRDFs.

6.1.4 Retrieving the surface reflectance with the BRDF forward model

As mentioned above, when applied to dual-view measurements, ORAC-classic retrieves the surface reflectance in each measurement channel in addition to the aerosol optical depth and effective radius.

However, since the surface reflectance is described by three values (specular, hemispherical and bi-hemispherical) at each channel, a method of representing these as a single value is required.

As has been described already, the hemispherical reflectance describes the amount of radiation scattered into the entire hemisphere for a single incoming beam at a given zenith angle. Hence it can be derived from the BRDF:

$$\begin{aligned}\rho_{\mathrm{bd}}(\theta_0) &= \frac{\int_0^{2\pi}\int_0^{\pi/2}\rho_{\mathrm{bb}}(\theta_0,\theta_{\mathrm{v}},\phi)\cos\theta_{\mathrm{v}}\sin\theta_{\mathrm{v}}\mathrm{d}\theta_{\mathrm{v}}\mathrm{d}\phi}{\int_0^{2\pi}\int_0^{\pi/2}\cos\theta_{\mathrm{v}}\sin\theta_{\mathrm{v}}\mathrm{d}\theta_{\mathrm{v}}\mathrm{d}\phi} \\ &= \frac{1}{\pi}\int_0^{2\pi}\int_0^{\pi/2}\rho_{\mathrm{bb}}(\theta_0,\theta_{\mathrm{v}},\phi)\cos\theta_{\mathrm{v}}\sin\theta_{\mathrm{v}}\mathrm{d}\theta_{\mathrm{v}}\mathrm{d}\phi.\end{aligned} \tag{19}$$

Similarly the bi-hemispherical reflectance is the amount of light scattered over the entire hemisphere from isotropic diffuse down-welling radiance. It can be calculated by integrating ρ_{bd} across all solar zenith angles:

$$\begin{aligned}\rho_{\mathrm{dd}} &= \frac{\int_0^{\pi/2}\rho_{\mathrm{bd}}(\theta_0)\cos\theta_0\sin\theta_0\mathrm{d}\theta_0}{\int_0^{\pi/2}\cos\theta_0\sin\theta_0\mathrm{d}\theta_0} \\ &= 2\int_0^{\pi/2}\rho_{\mathrm{bd}}(\theta_0)\cos\theta_0\sin\theta_0\mathrm{d}\theta_0.\end{aligned} \tag{20}$$

It is clear from these two equations that a small change in any one of the three surface reflectance values will result in a proportional change in the other two, since a constant can simply be moved outside the integral.

Examining equations 12, 13 and 14 for the calculation of bi-directional, hemispherical and hemispherical reflectance from the MODIS BRDF product, it can be seen that, for a given pixel, we have three linear equations of the form

$$\rho = p_{\mathrm{iso}} + c_1 p_{\mathrm{vol}} + c_2 p_{\mathrm{geo}}. \tag{21}$$

Hence the reflectances calculated using these expressions also scale linearly. The proportionality constant between the three reflectance terms is set by the a priori surface reflectance (sea surface model over the ocean and MODIS BRDF over land), while the magnitude of the surface reflectance is retrieved.

ORAC-classic is set up to treat the white-sky albedo as the retrieved parameter, with the bi-directional and black-sky albedo values being derived from it, as the white-sky albedo is independent of the viewing geometry.

6.1.5 Derivatives of the forward model expression

The gradient of the forward model ($\partial y/\partial x$) where y is a radiance measurement in a single channel and x is one of the retrieved parameters 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.

The derivative of equation 18 with respect to optical depth can be shown to be

$$\begin{aligned}\frac{\partial R_{\mathrm{TOA}}}{\partial \tau} =& R'_{\mathrm{bb}} + (\rho_{\mathrm{bb}} - \rho_{\mathrm{bd}}) \left(T^{\downarrow}_{\mathrm{bb}} T'^{\uparrow}_{\mathrm{bb}} + T'^{\downarrow}_{\mathrm{bb}} T^{\uparrow}_{\mathrm{bb}} \right) \\ &+ \frac{\left(T^{\downarrow}_{\mathrm{bb}} \rho_{\mathrm{bd}} + T^{\downarrow}_{\mathrm{bd}} \rho_{\mathrm{dd}} \right) \rho_{\mathrm{dd}} T^{\uparrow}_{\mathrm{tb}} R'_{\mathrm{dd}}}{(1 - \rho_{\mathrm{dd}} R_{\mathrm{dd}})^2} \\ &+ \frac{\left(T^{\downarrow}_{\mathrm{bb}} \rho_{\mathrm{bd}} + T^{\downarrow}_{\mathrm{bd}} \rho_{\mathrm{dd}} \right) T'^{\uparrow}_{\mathrm{tb}} + T^{\uparrow}_{\mathrm{tb}} \left(\rho_{\mathrm{dd}} T'^{\downarrow}_{\mathrm{bd}} + \rho_{\mathrm{bd}} T'^{\downarrow}_{\mathrm{bb}} \right)}{1 - \rho_{\mathrm{dd}} R_{\mathrm{dd}}}\end{aligned} \tag{22}$$

where all $'$ indicate $\partial/\partial x$ and x is either τ or r_{e}.

The derivative with respect to surface reflectance requires that we express the derivatives of ρ_{bb} and ρ_{bd} in terms of a derivative of ρ_{dd}. Since ρ_{bb} and ρ_{bd} both depend linearly on ρ_{dd} for a given viewing geometry, we can write:

$$\frac{\partial R_{\mathrm{TOA}}}{\partial \rho_{\mathrm{bb}}} = \frac{\partial R_{\mathrm{TOA}}}{\partial \rho_{\mathrm{dd}}} \frac{\partial \rho_{\mathrm{dd}}}{\partial \rho_{\mathrm{bb}}} = \frac{1}{\alpha} \frac{\partial R_{\mathrm{TOA}}}{\partial \rho_{\mathrm{dd}}} \tag{23}$$

$$\frac{\partial R_{\mathrm{TOA}}}{\partial \rho_{\mathrm{bd}}} = \frac{\partial R_{\mathrm{TOA}}}{\partial \rho_{\mathrm{dd}}} \frac{\partial \rho_{\mathrm{dd}}}{\partial \rho_{\mathrm{bd}}} = \frac{1}{\beta} \frac{\partial R_{\mathrm{TOA}}}{\partial \rho_{\mathrm{dd}}}, \tag{24}$$

and the derivative can then be expressed as:

$$\begin{aligned}\frac{\partial R_{\mathrm{TOA}}}{\partial \rho_{\mathrm{dd}}} =& T^{\downarrow}_{\mathrm{bb}} (\alpha - \beta) T^{\uparrow}_{\mathrm{bb}} \\ &+ \frac{T^{\downarrow}_{\mathrm{bb}} \beta T^{\uparrow} + T^{\downarrow}_{\mathrm{bd}} T^{\uparrow}}{1 - \rho_{\mathrm{dd}} R_{\mathrm{dd}}} + \frac{\left(T^{\downarrow}_{\mathrm{bb}} \rho_{\mathrm{bd}} + T^{\downarrow}_{\mathrm{bd}} \rho_{\mathrm{dd}} \right) T^{\uparrow}_{\mathrm{tb}}}{(1 - \rho_{\mathrm{dd}} R_{\mathrm{dd}})^2}\end{aligned} \tag{25}$$

6.2 The ORAC-dev implementation

The ORAC-dev version of the retrieval is fundamentally more simple than the ORAC-classic formulation. The approach taken is to produce a single effective surface reflectance for each pixel, which can be viewed as a sum of the bidirectional and bi-hemispherical surface reflectances, weighted by the proportion of downwelling radiance at the surface which results from diffuse transmission. This effective surface reflectance is described by function of two parameters, one of which is only dependant on viewing geometry, $p(\omega)$ (where (ω) denotes dependence on the viewing geometry and is equivalent to $(\theta_0, \theta_{\mathrm{v}}, \phi)$ in the previous sections), while the other is dependant on wavelength, $s(\lambda)$ through the expression:

$$\rho_{\mathrm{tt}} = (1 - D(\lambda, \omega)) \left[p(\omega) s(\lambda) + \frac{g \gamma s(\lambda)}{1 - g} \right] + D(\lambda, \omega) \frac{\gamma s(\lambda)}{1 - g} \tag{26}$$

where ρ_{tt} is the surface reflectance to the total downwelling radiance (both diffusely and directly transmitted), $D(\lambda, \omega)$ is the fraction of downwelling radiance which has been diffusely transmitted, g is a factor defined by

$$g = (1 - \gamma) s(\lambda)$$

and the value $\gamma = 0.3$ has been determined experimentally. The first term in equation 26 is the reflectance of the surface to the directly transmitted portion of the solar illumination, while the second term is that for the purely diffusely transmitted solar illumination.

In the case of (A)ATSR, the above equation allows the surface reflectance in all four shortwave channels and both viewing directions to be described by 5 parameters; one $s(\lambda)$ per channel, plus a $p(\omega)$ parameter for one of the views[6].

The effective surface reflectance ρ_{tt} can then be applied in the widely used expression for calculating TOA reflectance under the assumption of a Lambertian surface reflectance:

$$R_{\mathrm{TOA}} = R_{\mathrm{bb}} + \frac{T_{\mathrm{bt}}^{\downarrow} \rho_{\mathrm{tt}} T_{\mathrm{tb}}^{\uparrow}}{1 - \rho_{\mathrm{tt}} R_{\mathrm{dd}}}, \tag{27}$$

where $T_{\mathrm{bt}}^{\downarrow}$ and $T_{\mathrm{tb}}^{\uparrow}$ refer to the total downwelling and upwelling transmissions. This forward model can be easily implemented using the same atmospheric transmission and reflectance terms used in the ORAC-classic forward model, and can thus be relatively easily switched in and out of the retrieval system.

A peculiar aspect of this formulation is that the surface reflectance as described by equation 26 is a function of the overlying atmosphere (including the aerosol) through the $D(\lambda, \omega)$ factor. However, if $D(\lambda, \omega)$ is set to unity, the expression is that for the bi-hemispherical reflectance (and the dependence on $p(\omega)$ is dropped). Conversely, setting $D(\lambda, \omega) = 0$ produces an expression of the hemispherical surface reflectance. The former of these two limits is used to produce the bi-hemispherical surface reflectance values in the aerosol_cci ORAC product over land from version 2.02.

This approach to parametrising the surface reflectance has one primary advantage over that used in the ORAC-classic implementation. As mentioned above, using the two views and four shortwave channels of (A)ATSR, the retrieval state vector has six elements, while the measurement vector has eight. Thus, provided the measurements are sensitive to both the aerosol and surface reflectance, the retrieval problem will be well constrained. This means the retrieval can be run without a priori constraints on the surface reflectance. Essentially equation 26 provides an implicit a priori constraint whereby the wavelength dependence of the ratio of the effect surface reflectance in each viewing angle is solely due to $D(\lambda, \omega)$.

Conversely, a method for efficiently introducing a priori knowledge of the true surface reflectance is still under development so that it is, as yet, impossible to apply a prior constraint to the surface in the ORAC-dev implementation. Thus, over very dark surfaces – in particular the ocean – where the measurements contain very little information on the surface, the retrieval becomes poorly constrained and the results are poor.

7 The retrieval algorithm

ORAC places the forward model described in the previous section into the optimal estimation framework described by Rodgers [RD 28 3]. If we define the vector made up of the retrieved parameters, the *state vector*, $\mathbf{x}$, then the probability density function of the state subject to the measurements, $\mathbf{y}$, is defined, by application of Bayes' theorem and Gaussian statistics, to be

$$-2 \ln P(\mathbf{x}|\mathbf{y}) = (\mathbf{y} - \mathbf{F}(\mathbf{x}))\, \mathbf{S}_{\epsilon}^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x})) + (\mathbf{x} - \mathbf{x}_{\mathrm{a}})\, \mathbf{S}_{\mathrm{a}}^{-1} (\mathbf{x} - \mathbf{x}_{\mathrm{a}}) \tag{28}$$

where $\mathbf{F}(\mathbf{x})$ is the forward function (i.e. the function which maps the state parameters to measurements, which we approximate with the forward model $\mathbf{f}(\mathbf{x})$ described in the previous section), $\mathbf{S}_{\epsilon}$ is the measurement error covariance matrix, $\mathbf{x}_{\mathrm{a}}$ is the *a priori* state vector and $\mathbf{S}_{\mathrm{a}}$ is the *a priori* error covariance matrix. Together $\mathbf{x}_{\mathrm{a}}$ and $\mathbf{S}_{\mathrm{a}}$ denote our best guess at the state before the measurement is

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[6] Strictly speaking there are two $p(\omega)$ parameters – one for each view – but one can be set to unity and the other allowed to vary.

made and the precision of this guess. The retrieval problem is, therefore, that of finding the minimum value of equation 28 (i.e. maximising the probability of $\mathbf{x}$ subject to $\mathbf{y}$), which is known as the cost function.

ORAC uses the Levenberg-Marquardt [RD 29, 30] numerical optimisation, with updates suggested by Press et al. [RD 31], to perform this minimisation. This is an iterative procedure, whereby, if the number of measurements in $\mathbf{y}$ is m, and there are n state parameters, $\mathbf{x}$ is incremented by

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \left(\mathbf{S}_\mathrm{a}^{-1} + \mathbf{K}_i^T \mathbf{S}_\epsilon^{-1} \mathbf{K}_i + \gamma \mathbf{D}_n\right)^{-1} \left[\mathbf{K}_i^T \mathbf{S}_\epsilon^{-1} \left(\mathbf{y} - \mathbf{F}(\mathbf{x})\right) - \mathbf{S}_\mathrm{a}^{-1} \left(\mathbf{x} - \mathbf{x}_\mathrm{a}\right)\right] \tag{29}$$

where $\mathbf{K}$ is the weighting function matrix, γ is variable parameter, $\mathbf{D}_n$ is a $n \times n$ diagonal scaling matrix and the i subscript denotes values for the current iteration. $\mathbf{K}$ is a $m \times n$ matrix, with each column containing the derivative of the forward model with respect to each state parameter, i.e.

$$k_{i,j} = \frac{\partial f_i(\mathbf{x})}{\partial x_j} \tag{30}$$

Thus, for a linear system, we could write $\mathbf{y} = \mathbf{K}(\mathbf{x} - \mathbf{x}_0)$, where $\mathbf{x}_0$ is some reference state.

The parameter γ is the key to the efficiency and robustness of the Levenberg-Marquardt algorithm. If $\gamma \to \infty$, equation 29 tends to the step given by the steepest descent algorithm, which will always lie in the direction of the local "downhill" gradient and is therefore very robust. If $\gamma \to 0$ however, the algorithm behaves like Gauss-Newton iteration, which, although less numerically robust than steepest descent, will provide an exact solution to a linear problem in one iteration. The procedure for determining the value of γ is to start with a fairly small value (so the initial iteration will resemble Gauss-Newton), then at each iteration:

- If, as a result of the step suggested by equation 29, the cost function increases, do not update the state vector and increase γ.
- If the cost function is decreased by a step, update the state vector and decrease γ for the next step.

ORAC uses a factor of 10 for increasing and reducing γ. The scaling matrix, $\mathbf{D}_n$, is used to ensure that the state parameters are of similar magnitude, in the interests of numerical stability.

This iterative procedure is continued until either a convergence criteria is satisfied, or a maximum number of iterations is exceeded (in the former case the retrieval is said to have converged, while the later case can generally be rejected as a failed retrieval). ORAC uses the change in the cost function between iterations to determine whether the algorithm has converged - a negligible change in cost between iterations indicates that the retrieval is no longer improving the fit between measurements and forward model.

The optimal estimation framework offers two main advantages over more ad-hock retrieval algorithms:

1. *A priori* information is explicitly included in the retrieval in a way which is consistent with the way measurement information is included.
2. Rigorous error propagation, including the incorporation of forward model and forward model parameter error, is built into the system, providing extra quality control and error estimates on the retrieved state.

Error estimates for the retrieved state can be calculated by applying

$$\hat{\mathbf{S}} = \left(\mathbf{S}_\mathrm{a}^{-1} + \mathbf{K}_i^T \mathbf{S}_\epsilon^{-1} \mathbf{K}_i\right)^{-1} \tag{31}$$

Wavelength (μm)	0.55	0.67	0.87	1.6
Relative reflectance error	2.4 %	3.2 %	2.0 %	3.3 %
Minimum absolute error	0.0005	0.0003	0.0003	0.0003
Interpolation error	0.81 %	0.67 %	0.66 %	0.68 %
Parameter error (land, nadir)	1.61 %	2.25 %	2.97 %	3.71 %
Parameter error (land, for.)	1.19 %	1.74 %	2.79 %	3.45 %
Parameter error (sea, nadir)	2.00 %	2.36 %	2.63 %	4.61 %
Parameter error (sea, for.)	1.32 %	1.50 %	1.61 %	2.94 %

Table 3: The uncertainties applied to the shortwave AATSR channels. Reflectance error was determined in pre-launch calibration, with the minimum absolute uncertainty set by the instrument digitisation resolution. LUT interpolation error and surface reflectance parameter errors determined by Sayer [RD 24]. Note that the parameter error terms are not in terms of TOA reflectance (as they must be scaled by $\mathbf{K}_p$).

after the final iteration, where $\hat{\mathbf{S}}$ is the covariance of the retrieved state. If there is a known limitation in the forward model, due to approximations or incomplete modelling of the relevant physics, this can be accounted for in the retrieval as forward model error described by a covariance matrix $\mathbf{S}_{\mathrm{fm}}$. Uncertainty in parameters on which the forward model depends, but which aren't retrieved (for instance, the height distribution of aerosol), can also be included in the retrieval as forward model parameter error. These extra error terms are combined within the measurement error:

$$\mathbf{S}_{\epsilon} = \mathbf{S}_{\mathrm{y}} + \mathbf{S}_{\mathrm{fm}} + \mathbf{K}_{\mathrm{p}}\mathbf{S}_{\mathrm{p}}\mathbf{K}_{\mathrm{p}}^{T} \tag{32}$$

where $\mathbf{S}_{\mathrm{y}}$ in the covariance matrix describing the uncertainty of the measurement itself, $\mathbf{S}_{\mathrm{p}}$ describes the uncertainty in the forward model parameters and $\mathbf{K}_{\mathrm{p}}$ is the weighting function which maps this error into measurement space (i.e. it is analogous to the $\mathbf{K}_i$ matrix used above).

7.1 Measurement and *a priori* error characterisation in ORAC

The validity of the optimal estimation approach, and particularly the uncertainty on retrieved parameters derived using it, is dependent on the accurate characterisation of measurement and *a priori* uncertainties.

The measurement covariance matrix is based on the pre-launch characterisation of the AATSR channel accuracy, with added terms to account for uncertainties in the parameters used in setting the ratios between the different surface reflectance terms (forward model parameter error), as well as error from the interpolation of the LUTs (forward model error). These various uncertainties are listed in table 3.

The reflectance uncertainties are first divided by the square root of the number of individual measurements included in each 10 km sinusoidal bin, to give the standard error. If this value is found to be below the noise threshold determined by the digitisation limit of AATSR, the threshold value is used instead. The interpolation and parameter errors are then added in quadrature, giving a diagonal $\mathbf{S}_{\mathrm{y}}$ to be used in the retrieval.

Setting of the *a priori* and its covariance matrix is done separately for the aerosol optical depth and effective radius and the surface reflectance. Each is set as summarised below:

- The *a priori* $\log_{10}$ aerosol optical depth is set to a fixed value of -1.0, but is only weakly constrained by the *a priori* variance, which is set to 1, regardless of aerosol type (i.e. this corresponds to one standard deviation bounds of 0.01 and 1). The *a priori* optical depth is assumed to be independent of the other state variables.

- The *a priori* $\log_{10}$ effective radius is set to the value given in table 1 and there is a tighter constraint applied, with an *a priori* variance of 0.15 on $\log_{10}(r_\mathrm{e})$. As with aerosol optical depth, the *a priori* effective radius is assumed to be independent of other state parameters; thus the aerosol optical depth and effective radius part of the *a priori* covariance matrix is diagonal.
- In the ORAC-classic algorithm the *a priori* surface reflectance is set by the sea surface reflectance model over the ocean and the MODIS MCD43B product over land. In this case the *a priori* covariance is set by the estimated uncertainties on the input products and correlation between the channels is explicitly included. The determination of the surface reflectance part of $\mathbf{S}_\mathrm{a}$ is described in more detail below.
- In the ORAC-dev algorithm the *a priori* surface reflectance parameters (see section 6.2) are very weakly constrained. p is given a value of 0.3 with a variance of 1.0, while s is set to 0.1 with a variance of 100.

The *a priori* covariance matrix for the ocean surface reflectance used in ORAC-classic was derived by Sayer et al. [RD 14] using an ensemble of runs of the sea surface reflectance model, with the input parameters perturbed by their estimated uncertainties. From this ensemble, a 20 % error on the bi-hemispherical reflectance was determined, which was found to be nearly independent of wavelength.

In calculating the ORAC-classic *a priori* covariance matrix over land [RD 25], the full spatial resolution of MODIS MCD43B product is used to provide the sample of surface reflectances within each grid cell, and a correlation matrix is calculated for each individually. This correlation is then scaled by the uncertainty on the MODIS surface albedo (10 %, with a minimum of 0.005), the SVD reconstruction errors (see section 6) and terms to account for temporal variability within the 8 day MODIS sampling period, to produce the surface reflectance part of $\mathbf{S}_\mathrm{a}$ over land.

8 Quality control and aerosol speciation

Although the ORAC algorithm does not directly retrieve any information on the composition of the aerosol, except the change in mixing state implied by the retrieval of effective radius (see section 5.1), it is still possible for the system to provide some indication of the aerosol type present in a given scene. This capability is achieved by running the retrieval repeatedly, using a different predefined aerosol type each time. The resulting set of aerosol retrievals can be merged into a single "speciated" product by comparing the retrieval cost function for each of the aerosol classes used, which can be weighted by *a priori* knowledge of the likely aerosol type at that particular location.

The version 3.02 product applies no prior weighting, simply selecting the aerosol type as that which converged to the lowest cost. The version 3.04 product uses an *ad hoc* weighting using the aerosol type climatology produced by Stephan Kinne for the AEROCOM model intercomparison project. The climatology provides up to three aerosol types for each $1^\circ \times 1^\circ$ area of the Earth. If a retrieval using any of these types converged to a cost less than 10, the type that produced the lowest cost of those three is selected. Otherwise, the retrieval with the lowest absolute cost is selected (as in v3.02). Version 3.02 is the intended aerosol_cci data set, while version 3.04 is an experimental data set intended to evaluate the performance of dust retrievals in ORAC.

All retrieval results from ORAC are passed through a series of quality checks before this merging is performed. The primary tests applied are:

- Retrieval convergence: If the retrieval algorithm has failed to converge in 25 iterations, it is deemed to have failed.
- Cost function: A high value of the retrieval cost function at the solution indicates the result does not provide a good fit to the measurements.
- AOD: To combat cloud contamination, a retrieved AOD of greater than 2.0 at 550 nm is deemed to be poor quality.
- Aerosol effective radius: For similar reasons, a retrieved effective radius of greater than 5.0 μm is also deemed to indicate a probable poor retrieval.
- Cloud fraction: A cloud fraction limit of 50% is applied to all 10 km retrieval pixels over land (i.e. at least half the level 1b pixels within a given 10 km cell must have been flagged cloud free), while over the ocean as 80% limit is applied.
- Cloud adjacency: Over land, if more than 50% of 10 km retrieval pixels adjacent to the current pixel have been masked as 100% cloudy, the current pixel is rejected.
- AOD variability: If the standard deviation of the retrieved AOD across a 3x3 array of adjacent retrieval pixels is greater than 0.1, the centre pixel is rejected. Again, this test is only applied over land.

The final two of these tests are a duplication of the post-retrieval cloud contamination removal implemented in the AATSR ADV aerosol_cci product produced by FMI.

ORAC results can be constrained by a aerosol-type climatology, such as that provided with the aerosol_cci common aerosol models [RD 10]. However, for version 2.02 this has not been done and the retrieval cost, as well as passing the quality control checks described above, have been the only selection criteria for the selection of the “best” aerosol type, as this has been found to product better agreement with AERONET AOD measurements.

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