



# **ATBD 2.7**

# **ATMOSPHERIC CORRECTION OVER THE OCEAN**

# (CASE 1 WATERS)

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# Foreword

This Algorithm Theoretical Basis Document (MERIS ATBD 2.7) describes the present advancement of the algorithm for atmospheric correction of MERIS observations over oceanic Case 1 waters. The present document must be considered as a snapshot of the algorithm state; it may definitely not be seen as the description of a final, definitive, fully operational, algorithm. Several studies and tests remain to be carried out to reach such a level of maturity. Some of these studies are evoked in this ATBD, some others not. This ATBD has been peer-reviewed in spring 1997, and the suggested modifications or corrections have been incorporated in the present version.

In parallel to the generation of this ATBD, several papers have been published in the open literature. These publications describe in details (1) the theoretical work upon which the proposed algorithm is based (Antoine and Morel, 1998, "Relative importance of multiple scattering by air molecules and aerosols in forming the atmospheric path radiance in the visible and near infrared parts of the spectrum", *Applied Optics* 37, 2245-2259), (2) the algorithm itself and its implementation (Antoine and Morel, 1999, "A multiple scattering algorithm for atmospheric correction of remotely-sensed ocean color (MERIS instrument) : principle and implementation for atmospheres carrying various aerosols including absorbing ones", *International Journal of Remote Sensing*, in press), and (3) the test of the technique for detecting desert dust over the ocean (Antoine and Morel, 1998, "An algorithm for detection of desert dust from TOA ocean color spectra (MERIS instrument) : demonstration using SeaWiFS data, *Ocean Optics XIV conference*, Kailua Kona, Hawaii, 10-13 November 1998"). Two of these three publications are provided in Appendix, and the third one is available on request.





# **1. Introduction**

The feasibility of deriving the chlorophyll concentration from its influence on the spectral composition of the light backscattered by the upper oceanic layers (the "ocean color") was demonstrated by Clarke *et al.* (1970). Following this pioneer investigation, the Coastal Zone Color Scanner (CZCS) was developed and launched by NASA in November 1978, onboard the Nimbus-7 platform (Hovis *et al.*, 1980; Gordon *et al.*, 1980). This instrument has repeatedly observed the world ocean during 8 years (1979-1986), generating the first picture of the algal biomass distribution over the world ocean (Feldman *et al.*, 1989). Thanks to this experimental sensor, the capability of such a remote-sensing technique is now definitely proven. The success as well as the limitations and deficiencies of the CZCS, and the fact that it stopped its activity in 1986, led to the definition of a new generation of ocean color sensors, supported by the JGOFS (Joint Global Ocean Flux Study) community and designed to fill the need for a global, repetitive and operational coverage of the oceanic algal biomass.

The procedures used to extract the marine signal from the signals measured by the remote sensor in various spectral bands are collectively called the "atmospheric correction". The purposes of this document are (1) to propose a structure for the MERIS atmospheric correction algorithm over the open ocean (case 1 waters) and (2) to identify the studies that could be carried out in view of refining the algorithms. The theoretical work upon which the proposed algorithm is based is summarized in the present ATBD (section 3.1.1), and it is treated in details elsewhere (Antoine and Morel, 1998, *Applied Optics* 37, 2245-2259, given in Appendix 1). The algorithm itself and its implementation are fully devised in another paper (Antoine and Morel, 1999, *International Journal of Remote Sensing*, in press). A third paper was presented at the *Ocean Optics XIV conference*, Kailua Kona, Hawaii, 10-13 November 1998, and deals with some tests of the algorithm for detecting desert dust over the ocean.

## 2. Overview

## 2.1. What is the objective of the atmospheric correction algorithm ?

The atmospheric correction (its principles are recalled below) should allow the "water-leaving radiances" to be retrieved at each pixel of a MERIS scene, from the total radiance received by the instrument. At the top of atmosphere level, the "marine radiances" are those radiances originating from photons that have crossed the atmosphere down to the ocean and then have twice crossed the air-sea interface before reaching the sensor after a second atmospheric travel. These radiances carry information about the optical properties of the oceanic upper layers, and are related to the water-leaving radiances at the zero level, through a diffuse transmittance term.

The water-leaving radiances are combined into the "bio-optical algorithms", which allow the near-surface pigment (chlorophyll) concentration ( $Chl_{\langle sat \rangle}$ ) to be computed.  $Chl_{\langle sat \rangle}$  is, for instance, the parameter of interest for the bio-geo-chemical study of the carbon fluxes within the ocean interior (quantification and description of  $Chl_{\langle sat \rangle}$  distributions, primary production estimation, ecosystem modeling...), and is needed for other purposes (heating rate of the mixed layer, description of upper ocean dynamics, fisheries optimisation...).





## 2.2. The principle of "atmospheric corrections"

When an ocean-color sensor measures the radiance backscattered by the ocean-atmosphere system, it receives in the visible part of the spectrum a signal that is largely dominated by the "atmospheric path radiance". This radiance originates from photons scattered by air molecules and/or aerosols, which can also have been reflected at the sea surface, but have never penetrated the ocean. In the most favorable conditions of observation (clear atmosphere, small sun-zenith angle and favorable viewing angle), the water-leaving radiance represents only about 10% of the total radiance, and have then to be properly extracted (from the accuracy of this extraction depends the quality of the end-product of ocean-color data processing, *i.e.*, the near-surface chlorophyllous pigment concentration).

Under the assumption of separability of radiances, the determination of the radiances originating from molecular scattering (Rayleigh scattering) is easily handled, as only the illumination and observation conditions have to be known, even if a precise knowledge of atmospheric pressure (and wind speed) at the sea surface is also needed for accurate calculations. The central problem of atmospheric correction lies in the estimation of the radiances due to aerosol scattering. Indeed, the aerosol distribution (along the vertical as well as through the field of view), and the aerosol optical properties are not known when processing an ocean color scene.

Experience has been acquired in this domain since the launch of the CZCS, and even if the new ocean-color sensors have different, improved, characteristics, the work achieved with the CZCS provides guidelines to prepare the new atmospheric correction algorithm. Both the limited number of channels and the relatively poor radiometric sensitivity of the CZCS led to the development of specific correction schemes designed partly to remedy to these weaknesses. These schemes will be obsolete for processing data from MERIS, to the extent that increased radiometric sensitivity and additional channels in the near-IR spectral region considerably reduce the limitations encountered with the CZCS. The basic principle of the atmospheric corrections is to gain information about aerosol thanks to the radiances measured in near-IR bands (> 700 nm, where the water-leaving radiances are zero over case 1 waters), and to extrapolate this knowledge toward the visible domain.

## 2.3. Accuracy needed for atmospheric corrections.

Radiometric characteristics and calibration of MERIS are defined in terms of reflectances; radiances at the TOA level are accordingly converted into reflectances through (see Table of symbols and definitions)

$$\rho(\lambda, \theta_{\rm s}, \theta_{\rm v}, \Delta\phi) = \pi \, \mathcal{L}(\lambda, \theta_{\rm s}, \theta_{\rm v}, \Delta\phi) \,/ \,\mathcal{E}_{\rm s}(\lambda) \,\,\mu_{\rm s} \tag{1}$$

where  $E_s(\lambda)$  is the extraterrestrial irradiance for the wavelength in question,  $\mu_s$  is the cosine of the solar zenith angle  $\theta_s$ ,  $\theta_v$  is the satellite viewing angle, and  $\Delta \phi$  is the azimuth difference between the sun-pixel and pixel-sensor half vertical planes. Angular dependencies will be thereafter omitted for the sake of clarity.

Table 2.1 shows the radiometric characteristics of MERIS, compared with those of the CZCS and three future instruments, SeaWIFS, POLDER and MODIS (for these last 3 instruments, the central wavelength for some bands is slightly different from that of MERIS, at  $\pm 5$  nm). These values,





given in terms of reflectance, clearly show the increase in radiometric performance, from the CZCS to the new generation instruments.

Band	(λ),	ΝΕΔρ				$[\rho_W]_N$	
nm				-	-		
		CZCS <sup>‡</sup>	SeaWIFS <sup>‡</sup>	POLDER•	MERIS	MODIS <sup>‡</sup>	
412			0.00068		0.000427	0.00018	0.055
443		0.0011	0.00043	0.00036	0.000241	0.00016	0.035
560		0.00064	0.00027	0.00014	0.000201	0.00010	0.004
670		0.00051	0.00023	0.00020	0.000104	0.00004	0.0004
705					0.000143		0
775					0.000143	0.000085	0
865			0.00015	0.00016	0.000201	0.000076	0

‡ : taken from Gordon (1997)

•: taken from Deschamps et al. (1994)

**Table 2.1** : comparison of the radiometric characteristics of MERIS and other instruments. Approximate values of  $\rho_W$  are given for a chlorophyll concentration of 0.03 mg Chl m<sup>-3</sup> (see also Fig. 2.1 (a)).

Water-leaving reflectances,  $\rho_{\rm W}$ , are obtained after the measured total reflectances have been corrected for atmospheric effects. These water-leaving reflectances are related to the bio-optical state of the water body, through the ratio of the backscattering coefficient to the absorption coefficient,  $[b_{\rm h}/a]$  (see Morel and Gentili, 1991, 1993, 1996)

$$\rho_{\rm w}(\lambda,\theta_{\rm s},\theta',\Delta\phi) = \pi \ t_{\theta_{\rm s}}(\lambda) \ \Re(\theta') \ \frac{f(\lambda,\theta_{\rm s})}{Q(\lambda,\theta_{\rm s},\theta',\Delta\phi)} \left[\frac{b_{\rm b}(\lambda)}{a(\lambda)}\right]$$
(2)

The ratio  $[b_b/a]$  can be similarly related to the normalized water-leaving reflectance,  $[\rho_w]_N$ . This reflectance  $[\rho_w]_N$  is defined (Gordon and Clark, 1981) as the reflectance at nadir ( $\theta_v = 0$ ), for a sun at zenith ( $\theta_s = 0$ ), and without atmosphere ( $t_{\theta_s} = 1$ ). The relationships writes (see Morel and Gentili, 1996)

$$\left[\rho_{\rm w}\right]_{\rm N}(\lambda) = \pi \ \Re_0 \ \frac{f_0(\lambda)}{Q_0(\lambda)} \left[\frac{b_{\rm b}(\lambda)}{a(\lambda)}\right] \tag{3}$$







*Figure 2.1* : (a) Normalized water-leaving reflectances (Eq. (3)), plotted as a function of chlorophyll concentration (Chl), and for the wavelengths indicated.

The steps in the curves correspond to increments of 0.1 in log(Chl). (b) ratio of  $(b_b/a)$  at 443 or 490 nm to  $(b_b/a)$  at 560 nm  $(\Lambda_{443,560} \text{ and } \Lambda_{490,560})$ . (c) Allowable error in atmospheric correction at 443 nm,  $\Delta \rho(443)$  (*i.e.*, the maximum error above which a wrong chlorophyll concentration is retrieved, corresponding to the previous class). The error  $\Delta \rho(443)$  is calculated by assuming several ratios for  $[\Delta \rho(443) / \Delta \rho(560)]$ , as indicated (see text). The long-dashed curves are for errors of opposite signs at 443 and 560 nm. The shaded area is for errors within ±1 10<sup>-3</sup>. (d) as in (b), but for the wavelength couple 490-560.





where the subscripts 0 indicate that the corresponding quantities are for  $\theta_s = \theta_v = 0$ . In Eq. (3), the product  $(\pi \Re_0 (f_0/Q_0))$  is a constant (if the dependence of  $\Re_0$  upon wind speed is ignored), so that  $[\rho_w]_N$  can be considered as an inherent optical property of the medium.

#### **IMPORTANT NOTE:**

The MERIS Level 2 product is not the normalised water-leaving reflectance,  $[\rho_w]_N$ . as defined above, but a "semi-normalised" reflectance as follows:

$$\rho'_{w}(\lambda,\theta_{s},\theta_{v},\Delta\phi) = \pi.\,\Re(\theta') \frac{f(\lambda,\theta_{s})}{Q(\lambda,\theta_{s},\theta_{v},\Delta\phi)} \left[\frac{b_{b}(\lambda)}{a(\lambda)}\right]$$
(2a)

This is justified by the fact that the water-leaving reflectance product is also applicable above "Case 2" waters, where a normalisation procedure is not specified.

The MERIS instrument has been designed to allow, in principle, the detection of 10 classes of chlorophyll concentration, (Chl), within each of the 3 orders of magnitude between 0.03, 0.3, 3, and 30 mg Chl m<sup>-3</sup> (*i.e.*, a total of 30 classes). These classes are regularly distributed according to a constant logarithmic increment of 0.1. Shifting from one class to the next (previous) one corresponds to a change in (Chl) by a factor  $10^{\pm 0.1}$  (*i.e.*, +25% or -20%).

A first requirement for atmospheric correction is to allow 30 values of  $[\rho_w]_N$  to be discriminated at any wavelength where the pigment concentration influences the reflectance. The corresponding changes in  $[\rho_w]_N$ , as computed through Eq. (3), are displayed in Fig. 2.1(a) for several wavelengths, which are possibly used for retrieving (Chl). At 443 nm, the changes in  $[\rho_w]_N$  are of about 2.5 10<sup>-3</sup> when (Chl) < 0.1 mg m<sup>-3</sup>, of about 1 10<sup>-3</sup> when (Chl) ~ 1 mg m<sup>-3</sup>, and about 5 10<sup>-4</sup> for higher concentrations. At 490 nm, the changes are steadily of about 5-7 10<sup>-4</sup>, except when (Chl) < 0.1; they are of about 2 10<sup>-4</sup> for these low concentrations. At 560 nm, the changes in  $[\rho_w]_N$  are of about 2 10<sup>-4</sup> whatever (Chl). These values remain about the same when the constraints on  $\theta_s$ ,  $\theta_v$ , and  $t_{\theta_s}$  are relaxed, that is when  $\rho_w$  is examined for other geometries, instead of  $[\rho_w]_N$ , and they represent the desired discriminative skill of the atmospheric correction at these wavelengths. The change in  $[\rho_w]_N$  to be detected is smaller at 560 nm than it is at 443 nm or at 490 nm, and this more stringent condition was used to specify the noise equivalent reflectances for all wavelengths of the MERIS instrument (Ne $\Delta \rho$ , < 2 10<sup>-4</sup>; see Table 2.1). It should be reminded that this skill in discrimination, expressed in terms of reflectance changes, does not prejudge of the absolute accuracy of the instrument, and therefore of the correct retrieval of the true values of the reflectance.

It is now assumed that (Chl) is calculated, as usual, with a function  $\Phi$  of the ratio of  $[b_b/a]$  at two wavelengths, denoted  $\Lambda_{\lambda_1,\lambda_2}$ , which is used as an index of the bio-optical state.

$$\operatorname{Chl} = \operatorname{P}\left(\left[\frac{\mathbf{b}_{\mathbf{b}}}{\mathbf{a}}(\lambda_{1})\right] / \left[\frac{\mathbf{b}_{\mathbf{b}}}{\mathbf{a}}(\lambda_{2})\right]\right) = \operatorname{P}\left(\Lambda_{\lambda_{1},\lambda_{2}}\right)$$
(4)







*Figure 2.2.* The numbers which are contoured here represent 5 percent of the water-leaving reflectance at 443 nm, shown as a function of the solar zenith angle and viewing angle.

Left part : antisun and sun half-vertical planes. Right part : perpendicular plane. Upper and lower panels : chlorophyll concentration is 0.3 and 0.03 mg Chl m<sup>-3</sup>, respectively. The influence of the solar elevation on the diffuse reflectance of the ocean is taken into account (Morel *and* Gentili, 1991), as well as the anisotropy of the radiance field emerging from the ocean (Morel and Gentili, 1993).

A second requirement for atmospheric correction is that it must be accurate enough to allow 30 (Chl) values to be discriminated. In other words, 30 values of  $\Lambda_{\lambda_1,\lambda_2}$  must be discriminated between 0.03 and 30 mg (Chl) m<sup>-3</sup>. The  $\Lambda$  ratio is displayed in Fig. 2.1(b) as a function of (Chl), and for several couples of wavelengths. For a given geometry, it is related to  $([\rho_w]_N(\lambda_1) / [\rho_w]_N(\lambda_2))$  through the values of the  $(f_0/Q_0)$  ratio at the two wavelengths. The change in  $\Lambda_{443,560}$  between

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adjacent classes of chlorophyll, ( $\Delta A$ ), varies continuously from about 0.9 when (Chl) is 0.03 mg m<sup>-3</sup>, to 0.1 when (Chl) is 0.3 mg m<sup>-3</sup>, and to 0.03 when (Chl) is 30 mg m<sup>-3</sup>. For the wavelength couple 490-560 nm, and for the same values of (Chl), the changes in  $\Lambda_{490,560}$  are 0.2, 0.1, and 0.05.

After atmospheric correction, the allowable errors in  $[\rho_w]_N(\lambda_1)$  and  $[\rho_w]_N(\lambda_2)$  are those that would lead to an error in their ratio  $\Lambda_{\lambda_1,\lambda_2}$  equal, at the most, to  $\Delta \Lambda$ . These errors, denoted  $\Delta \rho(\lambda_1)$  and  $\Delta \rho(\lambda_2)$ , are accordingly computed as

$$\frac{([\rho_{w}]_{N}(\lambda_{1}) + \Delta\rho(\lambda_{1}))}{([\rho_{w}]_{N}(\lambda_{2}) + \Delta\rho(\lambda_{2}))} = \frac{[\rho_{w}]_{N}(\lambda_{1})}{[\rho_{w}]_{N}(\lambda_{2})} + \Delta\Lambda$$
(5)

For a given (Chl) class, Eq. (5) can be solved by fixing the relevant  $\Delta \Lambda$  value, by calculating the reflectances  $[\rho_w]_N(\lambda_1)$  and  $[\rho_w]_N(\lambda_2)$ , and by making an assumption about the error ratio  $(\Delta \rho(\lambda_1) / \Delta \rho(\lambda_2))$  (in such a way that the number of unknowns is reduced to 1). In the following,  $\lambda_1$ will be either 443 nm or 490 nm, and  $\lambda_2$  is 560 nm (*i.e.*, wavelengths possibly used for retrieving (Chl)). Errors at 443 nm and 490 nm are expected to be greater than those at 560 nm, because the accuracy of atmospheric correction may deteriorate when going away from the near infrared (*i.e.*, during the extrapolation toward the visible). The ratios  $(\Delta \rho(443) / \Delta \rho(560))$  and  $(\Delta \rho(490) / \Delta \rho(560))$ are thus fixed, somewhat arbitrarily, to 4, 2 or 1. It is as well conceivable that errors are of opposite signs at the two wavelengths, so that error ratios of -4, -2, and -1 have been also tested.

The acceptable errors  $\Delta \rho(443)$  resulting from these computations are displayed in Fig. 2.1(c) as a function of (Chl). They have been computed for each (Chl) class, and for the  $\Delta A$  values corresponding to an underestimation by one class of concentration. They are at first negative, and then positive after the  $\Lambda_{443,560}$  ratio becomes lower than the ratio ( $\Delta\rho(443)$  /  $\Delta\rho(560)$ ). A symmetrical pattern (*i.e.*,  $\Delta \rho$  at first positive and then negative) would have been obtained for errors corresponding to an overestimation by one class of concentration. The acceptable error  $\Delta \rho$ (443) is increasing as its ratio to  $\Delta \rho(560)$  increases. It is also increasing as the reflectances become closer at 443 and 560 nm (the error is undetermined when both reflectances are equal). The accuracy requirement for atmospheric correction is accordingly not too severe when ~  $0.3 < (Chl) < ~ 3 \text{ mg m}^-$ <sup>3</sup>; it is always greater than  $\pm 1 \ 10^{-3}$ , and most of the time greater than  $\pm 2 \ 10^{-3}$  when  $\Delta \rho(443)$  and  $\Delta \rho(560)$  have the same sign (*i.e.*, about 10% of  $[\rho_w]_N(443)$  when (Chl) = ~ 0.3 mg m<sup>-3</sup>). On the contrary, the accuracy requirement is increasingly demanding either for low or for high chlorophyll concentrations, and is between about  $\pm 1 \ 10^{-3}$  and  $\pm 5 \ 10^{-4}$ , depending on the ratio of errors at 443 and 560 nm. When the signs of the allowable errors  $\Delta\rho(443)$  and  $\Delta\rho(560)$  are opposite, they always must be below  $\pm 1 \ 10^{-3}$ , and often lower than  $\pm 5 \ 10^{-4}$  (see the two long-dashed curves in Fig. 2.1(c)). Therefore, an additional constraint on atmospheric correction would be identical signs for  $\Delta\rho(443)$ and  $\Delta \rho(560)$ . Fulfillment of this condition depends upon a correct retrieval of the spectral dependence of aerosol scattering.

When the wavelength couple 490-560 nm is used instead of the couple 443-560 nm (Fig. 2.1(d)), the conclusions about the allowable errors at 490 nm are roughly the same than those for  $\lambda =$ 





443 nm, except for concentrations below about 0.1 mg (Chl) m<sup>-3</sup>, where the  $\Lambda_{490,560}$  ratio is less sensitive to changes in (Chl) than is the ratio  $\Lambda_{443,560}$  (see Fig. 2.1(b)). The couple 490-560 could prove to be useful, however, for concentrations above about 3 mg (Chl) m<sup>-3</sup>, where the allowable errors are slightly greater at 490 nm than they are at 443 nm. In addition, when (Chl) is high, the water-leaving reflectance is a little larger at 490 nm than it is at 443 nm.

To sum up, the first requirement (retrieval of 30 reflectance values) requires that atmospheric correction errors be maintained within  $\pm 1-2 \ 10^{-3}$  at 443 nm, within  $\pm 5 \ 10^{-4}$  at 490 nm, and within  $\pm 2 \ 10^{-4}$  at 560 nm. If it is assumed that atmospheric correction errors in the 440-500 nm domain are about twice the errors at 560 nm, the second requirement (discrimination of 30 (Chl) values) requires errors within  $\pm 1 \ 10^{-3}$  at 443 nm (then  $\pm 5 \ 10^{-4}$  at 560 nm), or within  $\pm 5 \ 10^{-4}$  at 490 nm (then  $\pm 2 \ 10^{-4}$  at 560 nm). When expressed as relative errors, all the above requirements are greater than 1% of the normalized oceanic reflectances at 443 nm (and often 2-5%), except when (Chl) > 3 mg m<sup>-3</sup>. The situation is about the same for the wavelength couple 490-560 nm, except when Chl < 0.1 mg m<sup>-3</sup> and the  $\Lambda_{490,560}$  ratio is equal to 1.

Note, finally, that the accuracy requirement for the new generation ocean color sensors has been also defined as being a 5% accuracy on the reflectance in the 400 nm domain (*e.g.*, Gordon, 1997). The numerical values shown in Fig. 2.2, in the space defined by the solar zenith angle and the viewing geometry, represent five percents of water-leaving reflectances at 443 nm, computed for chlorophyll concentrations of 0.3 and 0.03 mg m<sup>-3</sup>. The requirement obtained by this way is consistent with the one derived here on the basis of the 30 (Chl) classes to be detected.

# 3. Algorithm description

## **3.1.** Theoretical description

## 3.1.1. Physics of the problem

## 3.1.1.1. Simulating the radiative transfer

The radiant field within the ocean-atmosphere system is described by the radiative transfer equation (RTE), which expresses the propagation of radiance within a medium of known inherent optical properties (Preisendorfer, 1961). For a passive medium (*i.e.*, with no internal source of radiation), this equation accounts for the loss of radiance due to scattering and absorption in the direction of propagation, and for the gain of radiance due to scattering from other directions. The two parameters of this integro-differential equation are the attenuation coefficient and the phase function. Even in the case of a homogeneous medium, there is no analytical solution for this equation (except for very peculiar, simplified, cases). A fortiori, there is no analytical solution for a complex system such as the atmosphere-ocean medium. Only numerical solutions are then possible.

The Monte Carlo technique has been used in the present study. With this method, any composition and vertical structure is possible for the various media, and no simplifying hypothesis is





needed. Furthermore, within the Monte Carlo code developed at LPCM, photons can be sorted out with respect to their history (number and type of scattering events), allowing any term to be studied (*i.e.*, radiances due to single or multiple scattering, radiances due to aerosol and/or molecules scattering, direct and diffuse part of the total radiances...).

With the purpose of defining an atmospheric correction scheme, some working conditions are necessary, and the ocean-atmosphere system is to be represented in a simplified manner. Indeed, even if realistic atmospheres can be simulated via the Monte Carlo technique, a simplified, more or less generic, vertical structure has to be defined in view of generalized calculations. Sensitivity studies will be accordingly needed in order to infer the differences caused when the actual conditions differ from those in the standard atmosphere adopted when defining the algorithm (see 3.1.1.6.1).

To generate TOA total radiances for molecular or compound (molecules plus aerosols) atmospheres, Monte Carlo simulations of the radiative transfer were carried out by using a code already described (Morel and Gentili, 1991, 1993), and validated against other radiative transfer codes (Mobley *et al.*, 1993). This code does not account for polarization, and the simplified geometry of a plane-parallel atmosphere is adopted. Photons are collected at the TOA level within 432 solid angles ("photon counters"), defined by a 5 degrees increment in zenith angle and a 7.5 degrees increment in azimuth; there is no counter aiming directly at nadir. The apparent diameter of the sun disk is set to  $0.5^{\circ}$ .

For Rayleigh scattering, a 50-layer profile is taken from Elterman (1968), in correspondence with  $\tau_{\rm r} = 0.0904$  at 550 nm, *i.e.*, a standard atmosphere with an atmospheric pressure of 1013.25 hPa. The anisotropy of the air molecules is ignored, the depolarization factor is zero, and the spectral dependency is expressed as  $\lambda^{-4.09}$ . Gas absorption is reduced to that of ozone, with a 50-layer vertical distribution also taken from Elterman (1968), and resulting in a total ozone content of 350 DU (1 DU = 2.69 10<sup>16</sup> molecules cm<sup>-2</sup>). The selection of various aerosol types and of their vertical distribution is dealt with later on (section 3.1.1.5).

This atmosphere is bounded by a flat, Fresnel-reflecting, interface with a perfectly absorbing ocean, so that multiple crossings of the interface by photons are not considered. This uncoupling of atmosphere and ocean is fully verified for Case 1 waters in the near infrared, and is an acceptable approximation for the visible wavelengths. The expression "TOA total reflectance" hereafter used means therefore the sum of the path reflectance simulated above a black ocean plus the water-leaving reflectance independently calculated through Eq. (2) and transmitted through the atmosphere. The algorithm uses at first the total radiance measured in near infrared bands, which is equal to the path radiance because there is no oceanic signal for Case 1 waters. The principle and implementation of the algorithm would remain the same over Case 2 waters, provided that the non-zero signal in the near infrared has been previously assessed or assumed in an independent way, and subtracted from the total reflectance.

Simulations were carried out to generate the  $\rho_{\text{path}}$  values for 6 wavelengths, several geometries ( $\theta_s$ ,  $\theta_v$ ,  $\Delta \phi$ ), and 4 aerosol optical thicknesses. The same geometries and wavelengths were considered to calculate  $\rho_{r,\tau a=0}$ , which the reflectance for a pure Rayleigh atmosphere. For each aerosol model and each ensemble made up of ( $\lambda$ ,  $\theta_s$ ,  $\theta_v$ ,  $\Delta \phi$ ), five couples ([ $\rho_{\text{path}} / \rho_{r,\tau a=0}$ ],  $\tau_a$ ), including the couple (1, 0) for an aerosol-free atmosphere, were fitted to a third order polynomial, to express the [ $\rho_{\text{path}} / \rho_{r,\tau a=0}$ ] versus  $\tau_a$  relationship, and the corresponding coefficients stored.





### 3.1.1.2. Signal decomposition

There are several ways to decompose the total signal received at the sensor level. The validity of any decomposition depends on a correct definition of the various terms involved. Coherence is also needed between the terms accounted for in the decomposition, the terms used in the correction algorithm, and the terms that we are able to calculate. A rapid insight is given below into the problem of signal decomposition; additional details can be found in Antoine and Morel, 1998, published in *Applied Optics* (given as Appendix 1 to this ATBD).

From this section and for the remaining of this document, the signals will be defined in terms of reflectance instead of radiance, according to the following transformation :

$$\rho(\lambda, \theta_{\rm s}, \theta_{\rm v}, \Delta\phi) = \pi \, \mathrm{L}(\lambda, \theta_{\rm s}, \theta_{\rm v}, \Delta\phi) \,/ \, \mathrm{E}_{\rm s}(\lambda) \,\,\mu_{\rm s} \tag{6}$$

where  $E_s(\lambda)$  is the extraterrestrial irradiance for the wavelength in question,  $\mu_s$  is the cosine of the solar zenith angle  $\theta_s$ ,  $\theta_v$  is the satellite viewing angle, and  $\Delta \phi$  is the azimuth difference between the sun-pixel and pixel-sensor half vertical planes. Angular dependencies will be thereafter omitted for the sake of clarity.

The total reflectance at the sensor level,  $\rho_t(\lambda)$ , can be split into the following components :  $\rho_{\text{path}}(\lambda)$ , the "path reflectance" generated by single and multiple scattering within the atmosphere and by reflection of diffuse radiation at the air-sea interface,  $T(\lambda)\rho_g(\lambda)$ , the reflectance due to direct specular reflection in the viewing direction (sun glint),  $t_d(\lambda)\rho_{wc}(\lambda)$ , the reflectance of whitecaps (if any), and  $t_d(\lambda)\rho_w(\lambda)$ , the water-leaving reflectance.  $T(\lambda)$  and  $t_d(\lambda)$  are the direct and diffuse atmospheric transmittances, respectively. The purpose of the atmospheric correction algorithm is thus to provide accurate estimates of  $\rho_{\text{path}}(\lambda)$ ,  $T(\lambda)\rho_g(\lambda)$ ,  $t_d(\lambda)\rho_{wc}(\lambda)$  and  $t_d(\lambda)$ .

$$\rho_{t}(\lambda) = \rho_{\text{path}}(\lambda) + T(\lambda)\rho_{g}(\lambda) + t(\lambda)\rho_{\text{wc}}(\lambda) + t_{d}(\lambda)\rho_{w}(\lambda)$$
(7)

For what follows  $T(\lambda)\rho_g(\lambda)$  and  $t_d(\lambda)\rho_{wc}(\lambda)$  are left out and the main term under examination is the path radiance. For that purpose  $\rho_{path}(\lambda)$  is decomposed into the following components, assuming that radiances due to aerosol or molecular scattering are separable :  $\rho_{r, \tau a=0}(\lambda)$ , the reflectance due to multiple scattering by air molecules (Rayleigh reflectance),  $\rho_a(\lambda)$ , the reflectance due to multiple scattering by aerosols, and  $\rho_{ra}(\lambda)$ , the reflectance due to combined, successive, scattering by air molecules and aerosols (coupling term)

$$\rho_{\text{path}}(\lambda) = \rho_{\text{r}}(\lambda) + \rho_{\text{a}}(\lambda) + \rho_{\text{ra}}(\lambda)$$
(8)

As said above, attention has to be paid to the definition of these various terms. Indeed, in the above expression,  $\rho_{\rm r}(\lambda)$  and  $\rho_{\rm a}(\lambda)$  are defined as the reflectances for a pure molecular atmosphere (*i.e.*, aerosol-free) and a hypothetical atmosphere with only aerosols (and no molecules) (*e.g.*, Deschamps *et al.*, 1983). The  $\rho_{\rm ra}(\lambda)$  term thus appears as a correction term, usually negative.





The reflectances  $\rho_r(\lambda)$  and  $\rho_a(\lambda)$  can also and more realistically be defined as the reflectances for a two component atmosphere (molecules and aerosols), and by abandoning the assumption that radiances are separable. In this situation, the  $\rho_{ra}(\lambda)$  term exactly represents the coupling of aerosol and Rayleigh scattering. These last terms are those that we can extract from a Monte Carlo simulation for a two component atmosphere, provided that the histories of the photons are kept. However, and from a practical viewpoint, it is necessary to compute the  $\rho_r(\lambda)$  term for aerosol-free atmospheres : this is the only term that we are able to calculate when processing ocean color observations, as aerosols are never a priori known (they are the term that we try to calculate).

In summary : from simulations, we shall retain the two following terms : the total reflectance at the sensor level, for a given ocean-atmosphere system and the Rayleigh reflectance for the same system when aerosols are removed. Such preliminary computations were carried out for several aerosol models, or aerosol model assemblages (see 3.1.1.5.2 for their definition), for optical thicknesses encompassing most of the plausible values over the ocean, and for which remote sensing is possible (from 0.03 to 0.5 at 550 nm), for six wavelengths among the 16 MERIS bands (3 in the visible : 443, 510 and 560 nm, 3 in the near IR : 705, 775 and 865 nm), 13 solar zenith angles (from 20 to  $60^{\circ}$ , each  $4^{\circ}$ ), and a flat air-sea interface (see 3.1.1.6 for sensitivity studies about the conditions at the air-sea interface). From the simulations, the radiances or reflectances can be expressed as a function of the above parameters and for any viewing geometry (for the Monte Carlo outputs, the sole limitation comes from the spatial discretisation).

No absorbing gases are considered, as it is assumed that their effect on the total radiances has been estimated before entering into the present atmospheric correction scheme.

The first step in the atmospheric correction for ocean color is to estimate  $\rho_{r, \tau a=0}(\lambda)$ . For that, the atmospheric pressure and the wind speed should be known. If they are unknown, standard, mean, values are adopted (the impact on the correction is treated as a sensitivity study, see 3.1.1.6.2). The path reflectance is now investigated in the realistic case of multiple scattering in a compound (molecules + aerosols) atmosphere.

#### 3.1.1.3. Accounting for multiple aerosol scattering.

Gordon (1997) has shown that for non-absorbing aerosols, and for moderate optical thicknesses (< 0.1), an algorithm based on the single scattering approximation could work well in most cases, with errors within  $\pm 0.002$  in reflectance at 443 nm. For higher optical thicknesses, or as soon as the actual aerosol absorbs radiation, multiple scattering has to be accounted for (but see 3.1.1.5.6).

It is known that multiple aerosol scattering enhances the signal with respect to that corresponding to single scattering (Deschamps *et al.*, 1983; Gordon *et al.*, 1988). This effect, which increases with increasing aerosol optical depth (in terms of signal magnitude), has to be accounted for in the present atmospheric correction for MERIS to meet the required accuracy (see Gordon and Wang, 1994; Gordon, 1997). In the same manner as for the single scattering, an indirect method is inevitable to cope with multiple aerosol scattering, which cannot be directly computed because the aerosols are unknown.





In our study about multiple scattering (see Appendix), we showed that the path reflectance is linearly (or nearly linearly) increasing with increasing aerosol load. For practical purposes, it has been decided to use the ratio of this path reflectance to the reflectance due to multiple Rayleigh scattering (for an aerosol-free atmosphere,  $\rho_{r, \tau a=0}(\lambda)$ ); this ratio also linearly increases when aerosol are progressively introduced in the atmosphere, and has a precise physical meaning.

Some examples of such relationships are displayed in Fig. 3.1, and for given geometric conditions and wavelengths. This figure shows that the relationship between both terms (the ratio and  $\tau_a$ ) is nearly linear. After some trials, we decided to fit the experimental points (obtained for 5 values of the aerosol optical thickness, including 0) by a quadratic function. The first step of the atmospheric correction lies on these relationships, so they have to closely match the data obtained from the simulated reflectances.

It is worth noting that the term used here  $(\rho_{r,\tau a=0}(\lambda))$  is not a realistic quantity, as far as it is compared with the "true" Rayleigh multiple scattering reflectance, resulting from a Monte Carlo simulation for a two-component atmosphere (aerosols + molecules). If this difference is of importance from the point of view of a systematic study of atmospheric reflectances, it is of no concern for our purpose. Indeed, our goal is to retrieve the global contribution of aerosol and Rayleigh reflectances in the MERIS channels, in view of retrieving the water-leaving reflectances. The above definition for  $\rho_{r,\tau a=0}(\lambda)$  is "operational", in that sense that it allows the correction to be done. The way this term is related to the "true" term is out of the scope of this ATBD (but see Appendix).

The principle for the algorithm and its implementation will be therefore to store in lookup tables the coefficients of relationships like those in Fig. 3.1, obtained for various aerosols. In parallel, a technique is necessary to navigate within this table, to identify the couple of aerosol that is the closest to the actual one.

#### 3.1.1.4. the algorithm

# 3.1.1.4.1. Computation of the ratio $[\rho_{path} / \rho_{r,\tau a=0}]$ and identification of the actual *aerosol*

A preliminary step consists in tabulating the  $[\rho_{\text{path}} / \rho_{\text{r},\tau a=0}]$  versus  $\tau_a$  relationships. Specific relationships are established for every aerosol model and wavelength, and for all illumination and observation conditions. One relationship is then necessary for each ensemble comprising aerosol (or fixed aerosol assemblage), wavelength, sun zenith angle, viewing angle, and azimuth difference. In parallel, the  $\rho_{\text{r},\tau a=0}(\lambda)$  values have also to be stored for the various illumination and observation conditions, to get the  $[\rho_{\text{path}}(\lambda) / \rho_{\text{r},\tau a=0}(\lambda)]$  ratio.

When starting the atmospheric correction, we dispose on one hand of  $\rho_{\text{path}}(\lambda)$  (measured) and  $\rho_{r,\tau a=0}(\lambda)$  (tabulated) for each wavelengths, and on the other hand of tabulated relationships linking the ratio of these 2 terms to  $\tau_a(\lambda)$ , for N aerosol models. The central problem to be addressed is therefore the selection, among the aerosol models used to generate the look-up tables, of the two models that most closely bracket the actual aerosol. The principle is to rely on the look-up tables, which should allow (numbering as in Fig. 3.1).





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way for identifying a couple of aerosol models enclosing the actual aerosol. The circled numbers identify the successive steps of this scheme, as discussed in the text (section 3.1.1.4.1).

(1-2) the values of  $\tau_a(865)$  to be calculated from the  $[\rho_{path}(865) / \rho_{r,\tau a=0}(865)]$  ratio, for several aerosol models,

(3) to extrapolate  $\tau_a$  from 865 to 775 nm, for each aerosol model,

2

2

(4-5) to obtain the  $[\rho_{path}(775) / \rho_{r, \tau a=0}(775)]$  ratios from  $\tau_a(775)$ , and therefore to select a couple of aerosol models, by comparing the actual  $[\rho_{path}(775) \, / \, \rho_{r, \, \tau a=0}(775)]$  ratio, and these various ratios. Finally, to estimate the  $[\rho_{path}(\lambda) / \rho_{r, \tau a=0}(\lambda)]$  ratio in the visible bands from the knowledge of the spectral behavior of this couple of aerosol models.

The principle is to firstly rely on a very simple set of candidate aerosol models, supposedly representing typical clear oceanic atmospheres (and described below). A "first-step" atmospheric correction is then carried out by using this first set of candidate aerosol models, and then the error that is made at 705 and 510 nm is examined. At 510 nm, the water-leaving reflectance for case 1 waters is almost constant for chlorophyll concentrations up to 1 mg Chl m<sup>-3</sup>, and thereafter smoothly decreases with increasing pigment concentration. The use of a mean value for this water-leaving reflectance, with its associated statistical error, is then possible (see later on; section 3.1.1.4.2). It is then feasible to obtain the error in the atmospheric correction at 510 nm, by subtracting from the total, measured, reflectance, the sum [path reflectance, estimated by the correction + supposed mean value of the water-leaving reflectance]. At 705 nm, the water-leaving radiance can be assumed zero for Case 1 waters, and the error in the atmospheric correction is therefore straightforwardly obtained.





If these errors are above predefined thresholds, we have an indication that the actual aerosols do not correspond to the simple cases first envisaged. We can then move to another (others) set(s) of aerosol models (see section 3.1.1.5, implementation).

The choice of the visible channel at 510 nm, in addition to the third near-IR channel of MERIS at 705 nm, actually comes out from the fact that the error at 705 nm, when a "non-standard" aerosol is present, is usually still very low, and does not allow to detect the failure.

The successive steps of such a correction scheme are as follows (see Fig. 3.2(a), (b), (c), and (d), and also section 3.1.2). For a given pixel, and thus for a given geometry  $(\theta_v, \theta_s, \Delta \phi)$ :

- (1) The ratio  $[\rho_{\text{path}}(\lambda) / \rho_{\text{r},\tau a=0}(\lambda)]$  is computed at 865 and 775 nm,  $\rho_{\text{r},\tau a=0}(\lambda)$  being taken in tabulated values (at these wavelengths, and for oceanic Case 1 waters,  $\rho_{\text{path}} = \rho_{\text{t}}$ ).
- (2) A first set of N aerosol models is selected, which, in principle, is representative of clear oceanic atmospheres (see 3.1.1.5 for details about the implementation). For these N aerosol models, N  $\tau_a(865)$  values are calculated from the  $[\rho_{path}(865) / \rho_{r, \tau a=0}(865)]$  ratio.
- (3) N values of  $\tau_a(775)$  are computed for the N aerosol models, from the knowledge of their spectral optical thicknesses (normalized by their values at 865 nm; tabulated values).
- (4) N values of  $[\rho_{\text{path}}(775) / \rho_{r, \tau a=0}(775)]$  are computed from the N values of  $\tau_a(775)$  for the N aerosol models, from the tabulated relationships between both quantities.
- (5) The actual  $[\rho_{\text{path}}(775) / \rho_{r, \tau a=0}(775)]$  is then compared to the N individual values obtained at step (4), and the 2 that most closely bracket the actual one indicate the two aerosol models that most likely are similar to the actual one.
- (6) 2 values of  $\tau_a(510)$  are calculated from the normalized spectral optical thicknesses of the 2 "bracketing" aerosol models. Step (2) is now inverted, to calculate two  $[\rho_{\text{path}}(510) / \rho_{\text{r.}\tau a=0}(510)]$  ratios from the two  $\tau_a(510)$ .
- (7) The following step lies on the assumption that, for a given wavelength  $\lambda$ , the actual  $[\rho_{\text{path}}(\lambda) / \rho_{\text{r},\tau a=0}(\lambda)]$  ratio falls between the two  $[\rho_{\text{path}}(\lambda) / \rho_{\text{r},\tau a=0}(\lambda)]$  ratios calculated at step (6), proportionately in the same manner as it does at 775 nm;  $\rho_{\text{path}}(510)$  is now known.
- (8) By making an assumption on the water-leaving reflectance at 510 nm (see below), the error in the atmospheric correction,  $\Delta \rho_{510}$ , can be assessed :

$$\Delta \rho(510) = [(\rho_{\rm t}(510)_{\rm measured} - \rho_{\rm path}(510)_{\rm estimated}) / t_{\rm d}(510)] - \rho_{\rm w}(510)_{\rm supposed}$$
(9)

The error at 705 nm is more straightforwardly obtained as





$$\Delta \rho_{705} = \rho_{\rm t}(705)_{\rm measured} - \rho_{\rm path}(705)_{\rm estimated} \tag{9'}$$

- (9) A test is then made on this  $\Delta \rho(510)$  value, and also on the value of  $\Delta \rho(705)$  (more straightforwardly obtained, because  $\rho_w(705)$  is zero). Following the answer, either the correction is continued at step (10), or it is carried out once more from step (2), by selecting however a different set of N' aerosol models. In the latter situation, the correction is actually carried out for several aerosol databases, so that steps 2-8 are carried out several times; several couples of aerosol models are then selected (one at each time steps 2-8 are done), and the couple kept at the end is the one leading to the lower  $\Delta \rho(510)$ . The practical way of navigating within the tables will be exposed later on (section 3.1.1.5.4).
- (10) For every wavelength  $\lambda$  of the visible domain, 2 values of  $\tau_a$  are calculated from the knowledge of the spectral scattering coefficients of the 2 "bracketing" aerosol models.
- (11) Step (2) is now inverted, to calculate two  $[\rho_{\text{path}}(\lambda) / \rho_{r,\tau a=0}(\lambda)]$  ratios from the two  $\tau_a(\lambda)$  for the visible bands, and then to obtain  $\rho_{\text{path}}(\lambda)$  (see step 7).
- (12) The water-leaving reflectance at the instrument level is then obtained as the difference between the total, measured, reflectance,  $\rho_{t}$ , and the estimated path reflectance,  $\rho_{path}$ .
- (13) the last step consists in calculating the diffuse transmittance, to derive the water-leaving reflectance.





## General sketch



Figure 3.2a : general sketch of the algorithm





### Aerosols correction



Figure 3.2b : detail of the aerosol correction (see also section 3.1.2.)





#### Aerosols selection



Figure 3.2c : detail of the aerosol selection (see also section 3.1.2.)





## **Detection of aerosol absorption**



Figure 3.2d : detail of the tests at 510 and 705 nm (see also section 3.1.2.)

3.1.1.4.2. The test at 510 nm





Experimental data suggested a nearly constant reflectance at 510 nm for oceanic Case 1 waters, whatever (Chl) (the "hinge point", Duntley et al., 1974; Gordon and Clark, 1981). Biooptical models (e.g., Gordon et al., 1988; Morel, 1988), mainly based on the interpretation of experimental data, accordingly predict a narrow range of values for R(0<sup>-</sup>)(510), over the whole domain of (Chl) (0.03 to 30 mg m<sup>-3</sup>). The curves displayed in Fig. 3.3 indeed show limited variations of  $R(0^{-})(510)$ . The data points in Fig. 3.3, extracted from measured reflectance spectra, as well confirm this constancy : however noisy may be these  $R(0^{-})(510)$  data, they at least do not show any significant trend. Therefore, it seems wise to assume a constant value for the diffuse reflectance at 510 nm, with a mean of ~ 2% if the data shown in Fig. 3.3 are considered. The corresponding mean value for the normalized water-leaving reflectance, hereafter noted  $[\overline{\rho_w(510)}]_N$ , is of about 1 10<sup>-2</sup> (with  $(\pi \Re_0 (f_0/Q_0)) \sim 0.47$ ) at least for the concentration range 0.03 to 3 mg(Chl) m<sup>-3</sup> (see Fig. 2.1(a)). This value for  $[\overline{\rho_w(510)}]_N$  is slightly larger than the value derivable at 520 nm from a normalized water-leaving radiance of 5 mW m<sup>-2</sup> nm<sup>-1</sup> sr<sup>-1</sup> (Gordon and Clark, 1981), and from an extraterrestrial irradiance of about 1900 mW m<sup>-2</sup> nm<sup>-1</sup> (Neckel and Labs, 1984). The natural noise in the reflectance at 510 nm, for a given chlorophyll concentration, is accounted for by attaching an uncertainty of  $\pm 3 \ 10^{-3}$  (at  $\pm 1\sigma$ ) to  $[\overline{\rho_w(510)}]_N$ .



*Figure 3.3* : Oceanic diffuse reflectance at 510 nm, for Case 1 waters with variable chlorophyll concentration.

The two curves have been obtained from the model of Morel (1988) (see also Morel and Gentili (1991) for the dependence of the reflectance on the sun zenith angle), either for a sun at zenith (bottom), or with a sun zenith angle of  $60^{\circ}$  (top). The various symbols correspond to values extracted from reflectance spectra measured at sea, as indicated.

To obtain the error in atmospheric correction at 510 nm, the  $[\rho_w(510)]_N$  value is "denormalized", in view of being compared with the apparent water-leaving reflectance (*i.e.*, the actual water-leaving reflectance plus the error in atmospheric correction). The transformation of  $[\rho_w(510)]_N$  into  $\rho_w(510)$  is performed through (see Morel and Gentili, 1996)





$$\rho_{\rm W}(510) = \left[\overline{\rho_{\rm W}(510)}\right]_{\rm N} \quad (\varepsilon_{\rm c} \ t_{\theta_{\rm s}}) \ \frac{\Re(\theta')}{\Re_0} \ \frac{f_1(\theta_{\rm s})}{Q(\theta_{\rm s},\theta_{\rm v},\Delta\phi)} \left[\frac{f_{1,0}(\lambda)}{Q_0(\lambda)}\right]^{-1} \tag{10}$$

with 
$$\Re(\theta') = \left[\frac{(1-\overline{\rho})}{(1-\overline{r}R)}\frac{(1-\rho_{\rm F}(\theta'))}{n^2}\right]$$
 (10')

The chlorophyll concentration has to be known to use the  $(f_1 / Q)$ , while actually it is not the case when the error in atmospheric correction is computed. The ratio of  $(f_1 / Q)$  for the actual geometry to  $(f_{1,0} / Q_0)$  (*i.e.*, f/Q for  $\theta_s = \theta_v = 0$ ) is, however, nearly insensitive to changes in the chlorophyll concentration (changes with Chl are within ±10%), at least in the concentration range 0.03-3. mg m<sup>-3</sup> and for geometries typical of ocean color remote sensing. Therefore, the knowledge of the chlorophyll concentration is not required to use the above equation, and the error in the atmospheric correction at 510 nm,  $\Delta \rho(510)$ , is obtained as

$$\Delta \rho(510) = \left[ \left( \rho_{\rm t}(510)_{\rm measured} - \rho_{\rm path}(510)_{\rm estimated} \right) / t_{\rm d}(510) \right] - \rho_{\rm w}(510)$$
(11)

If  $\Delta\rho(510)$  is greater than +0.0025, or lower than -0.0025, then the presence of continental and/or absorbing aerosols is indicated (positive answer). If the answer of the test is negative (clear maritime atmosphere), the atmospheric correction is extended to the whole spectrum (412 to 680 nm). If the answer is positive (*i.e.*, presence of peculiar, absorbing aerosols), then a confirmation is asked. Indeed, when  $\Delta\rho$  is above the selected thresholds, it could be due to a wrong estimate of  $\rho_{\rm W}(510)$ , rather than to an incorrect atmospheric correction. The verification is carried out as follows : if  $\Delta\rho$  is negative (positive) after the first test, a second test is carried out, using however the lower (upper) limit of [ $\rho_w(510)$ ]<sub>N</sub>, that is 0.013 (0.007). The situation is reset to that of a clear maritime atmosphere when the two tests do not lead to the same indication. Otherwise, the first test is confirmed and the correction performed again with additional aerosol models.

# 3.1.1.4.3 Computation of the diffuse transmittance, and getting the water-leaving radiance

This step of the atmospheric correction is of great importance, even if it has been usually considered as a routine operation. The diffuse transmittance term actually conceals several processes, each one either removing radiation from, or adding radiation to, the water-leaving radiance travelling along the pixel-to-sensor path. In addition, any error in  $t_d(\lambda, \theta)$  is directly transferred to as the same error in the water-leaving reflectance. The expression used to calculate the diffuse transmittance should account (1) for the loss of radiance due to absorption along the path from the pixel to the sensor, (2) for the loss of radiance due to the scattering of water-leaving radiances out of the viewing direction, and (3) for the gain of radiance due to the scattering of water-leaving radiance from the neighboring pixels into the viewing direction (this third contribution implies that  $t_d(\lambda, \theta)$  can be theoretically > 1).





In the following, point (3) (neighboring effect) is not considered, and  $t_d(\lambda, \theta)$ , where  $\theta$  is the viewing angle, is then

$$t_{d}(\lambda,\theta) = t_{oz}(\lambda,\theta)t_{w}(\lambda,\theta)t_{ag}(\lambda,\theta)t_{aa}(\lambda,\theta)t_{rs}(\lambda,\theta)t_{as}(\lambda,\theta)$$
(12)

where  $t_{oz}(\lambda,\theta)$  is the transmission factor related to absorption by ozone

- $t_{_W}(\lambda,\theta)$  is the transmission factor related to absorption by water vapor
- $t_{ag}(\lambda,\theta)$  is the transmission factor related to absorption by other absorbing gases
- $t_{aa}(\lambda,\theta)$  is the transmission factor related to absorption by aerosols
- $t_{\rm rs}(\lambda,\theta)$  is the transmission factor related to scattering by molecules
- $t_{as}(\lambda,\theta)$  is the transmission factor related to scattering by aerosols

In principle, the choice of the wavelengths for the MERIS channels ensures that  $t_w(\lambda,\theta)$  and  $t_{ag}(\lambda,\theta)$  are unity. The contributions of absorption by ozone and aerosols are simply expressed as :

$$t_{oz}(\lambda,\theta) = \exp\left(-\frac{\tau_{oz}}{\mu}\right)$$
 and  $t_{aa}(\lambda,\theta) = \exp\left(-\frac{(1-\omega_a)\tau_a}{\mu}\right)$  (13)

The individual contributions of scattering by aerosols and molecules are expressed as :

$$t_{as}(\lambda,\theta) = \exp\left(-\frac{\omega_a F_a \tau_a}{\mu}\right)$$
(14)

$$t_{rs}(\lambda,\theta) = \exp\left(-\frac{\omega_r F_r \tau_r}{\mu}\right)$$
(15)

where  $\mu$  is the cosine of  $\theta$ ,  $\tau_x$  is the optical thickness of the component x,  $\varpi_a$  and  $\varpi_r$  are the single scattering albedos of aerosols and molecules. the ratio  $\varpi_a$  can take different values depending on the aerosol model and  $\varpi_r$  is unity for the channels here considered.  $F_a$  and  $F_r$  are the backward scattering probabilities of aerosols and molecules, respectively (*i.e.*, the ratio of the backward scattering coefficient to the total scattering coefficient).  $F_a$  can take various values depending on the aerosol model, and  $F_r$  is 0.5. By assembling the expressions for  $t_{aa}(\lambda, \theta)$  and  $t_{as}(\lambda, \theta)$ , it follows that the contribution of aerosols to the diffuse transmittance is

$$t_{a}(\lambda,\theta) = \exp\left(-\frac{(1-\omega_{a}(1-F_{a}))\tau_{a}}{\mu}\right)$$
(16)

By reassembling the above expression with those for ozone and Rayleigh scattering, and by using the numerical values of  $\varpi_r$  and  $F_r$ , it follows that the diffuse transmittance is





$$t_{d}(\lambda,\theta) = \exp\left(-\frac{\tau_{oz} + (1 - \omega_{a} F_{a}) \tau_{a} + 0.5 \tau_{r}}{\mu}\right)$$
(17)

Note that F<sub>a</sub> stands now for the forward scattering probability of aerosols.

 $\tau_{\rm r}(\lambda)$  is set to a fixed value for standard atmospheric pressure (P<sub>0</sub>), and has to be multiplied by P/P<sub>0</sub> if P is the actual atmospheric pressure.  $\tau_{\rm oz}(\lambda)$  is computed from the knowledge of the ozone integrated content (mAtm cm), combined with the ozone absorption coefficients for the wavelength in question.  $\tau_{\rm a}(\lambda)$  is obtained at the end of the atmospheric correction (see below). The ratios  $\varpi_{\rm a}$  and F<sub>a</sub> are obtained in the same way, *i.e.*, by averaging the values for the 2 aerosols selected by the atmospheric correction.

Note that the aerosol contribution to  $t_d(\lambda, \theta)$  was ignored in the CZCS algorithms, because it is usually small, except for large optical thicknesses, *i.e.*, when the CZCS atmospheric correction was anyway unable to work properly. The aerosol term is included here in the calculation of the diffuse transmittance, to avoid introducing inaccuracies at the end of an a priori accurate atmospheric correction (see also 3.1.3.2).

#### 3.1.1.4.4 Retrieval of the aerosol optical thickness, $\tau_a$

Once a couple of aerosol models (the two "bracketing" aerosols) has been selected by the atmospheric correction algorithm, the two values of  $\tau_a(865)$  associated with these two aerosol models are simply averaged. The mean of these two values provides the best estimate of the actual aerosol optical thickness at 865 nm (rather than averaging the two estimates following the "mixing" ratio; see Gordon, 1997). From the tabulated spectral variations of the selected aerosol models (or aerosol model assemblages), the optical thickness can also be estimated at any wavelength in the visible, with however a lesser accuracy.

#### 3.1.1.4.5. Additional steps

The links with the other segments of the ground processing, as they are described in the ATBD(s) 2.5, 2.6, 2.8 and 2.9, are shown in Fig. 3.2a. The first link is with the "Case 2 bright waters flag", which should indicate if sediment-dominated waters are actually observed. Water-leaving reflectances in the near-IR are then passed on to the atmospheric correction algorithm. These reflectances are subtracted from the total reflectances, before entering the atmospheric correction. The other links are at the end of the atmospheric correction, which pass the water-leaving reflectances either at the Case 1 (ATBD 2.9) or Case 2 (ATBD 2.8) processing, depending on the value of the "Case 2 waters flag".

Another entry in the atmospheric correction (not discussed in this ATBD, and not implemented at present time) concerns the effect of stratospheric aerosols (in case of perturbed conditions; for instance after significant volcanic eruptions) or of thin cirrus clouds (see section 3.1.1.6.6). If such a correction is operated for MERIS, it should be at the top level of the algorithm, that is after radiances have been transformed into reflectances, and before entering the atmospheric correction. It can be anticipated that such a correction would be carried out *a priori*, by subtracting from the total reflectance known (precomputed) values of the reflectance due to the stratospheric





aerosols. Preliminary studies (Gordon et al., 1997) indicate that this kind of correction is not so straightforwardly carried out.

3.1.1.5. Implementation / test of the algorithm.

### 3.1.1.5.1. Aerosols over the ocean.

In principle, all kinds of aerosols are possibly encountered over the oceans. The presence of a peculiar aerosol type, and its relative proportion in the total aerosol load, are depending on the history of the air mass in question. When the region of interest is free from any continental influence, however, the situation can be described following a more or less general vertical structure and composition (WCRP, 1986) : The oceanic boundary layer (from the sea surface to an altitude of about 2 km) contains a "maritime" aerosol, mainly composed of the "sea-salt component" (liquid water and sea-salt particles), always containing however a small background of "water-soluble" particles (small particles, below about 0.05 µm, e.g., ammonium, calcium sulfate, organic compounds...). This boundary layer aerosol is non-absorbing ( $\omega_0$  about 0.97 0.98). Above the boundary layer, within the "free troposphere" (about 2-12 km), aerosols from continental origin are always present, even if their optical thickness is usually very low (e.g., WCRP, 1986). This aerosol of continental origin is usually moderately absorbing ( $\omega_0$  about 0.9-0.95). Finally, the stratosphere and the upper atmosphere (12-30-100 km) contain a background of non-absorbing aerosol, which can be represented by particles consisting of a 75% solution of sulfuric acid in water ( $H_2SO_4$ ). The optical thickness of this aerosol is extremely low (about 0.005 at 550 nm), except during the months (years) following large volcanic eruptions.

Within this ensemble of three aerosol types, the boundary layer aerosol usually contributes to about 75% of the total aerosol optical thickness at 550 nm.

Even in absence of volcanic eruptions, deviations from this "generic" vertical structure and composition are observed, and are usually due to air masses of continental origin. In this case, the layer that is frequently affected is the free troposphere, which can then contain significant concentrations of particles of continental origin (either desert dust or insoluble particles of other terrestrial origins, usually referred to as the "rural aerosol"). This kind of aerosols are moderately ("rural aerosol"), or strongly (desert dust), absorbing. In the case of desert dust outbreaks, the optical thickness can be very high. The other perturbation of continental origin is due to human activities. It is more confined to the coastal regions (and usually east of continents), and is characterized by the presence of "soot-like" absorbing particles, incorporated into the "rural" aerosol. This kind of perturbation usually concerns the boundary layer.

With such a sketch of aerosol climatology, it is obviously not intended to encompass all possible situations, either intermediate or clearly different from those exposed here. For example, the maritime aerosol can be slightly different from an ocean to another one (*e.g.*, between Pacific and Atlantic oceans, Villevalde *et al.*, 1994), desert dusts have different optical properties as a function of their origin (Sahara or Asian deserts); they are not only present in the free troposphere, as they ultimately sink into the ocean, etc...

3.1.1.5.2. conditions selected for simulating radiative transfer in the atmosphere.





#### Aerosol models and their optical properties.

The aerosol models used in the present work are constructed from the basic aerosol components defined in Shettle and Fenn (1979) (thereafter referred to as S&F79) and in WCRP (1986). These components consist of spherical particles (allowing the Mie theory to be applied), characterized by a peculiar particle mixing ratio, and size frequency distributions following lognormal laws or the modified gamma function (see Tables 3.1, 3.2 and 3.3). For some of these aerosols, the index of refraction of the particles depends on the relative humidity (RH); the real part of this index tends to that of water as RH increases, and its imaginary part (which determines absorption) decreases (Table 3.4). The aerosol models are the following :

• "Maritime model" (Shettle and Fenn, 1979) : this is a mixture of sea salt solution in water, plus a contribution of tiny continental particles. The index of refraction and the mean radius of particles is RH-dependent.

• "Urban model" (Shettle and Fenn, 1979) : this model is a mixture of water soluble and dustlike particles (with proportions 70% and 30%, both being 80% of the total), plus soot-like particles (20% of the total). The index of refraction and the mean radius of particles is RH-dependent. This model is the "small urban aerosol" as defined by Shettle and Fenn (1979) (they also defined a "large urban aerosol model"). It is selected because large particles are assumed to have sedimented when the urban aerosol is blown over the ocean.

• "Continental model" (WCRP, 1986) : this model is a mixture of water soluble (29%), dustlike (70%), and soot particles (1%). These 3 basic components are not necessarily the same than in Shettle and Fenn (1979).

• "Stratospheric model" (WCRP, 1986) : this model is represented by a 75% solution of sulfuric acid in water. It is non-absorbing, and the size distribution follows a modified gamma function (see below).

• "Desert Dust model" (Schütz, 1980) : the size distribution for this aerosol, which is assumed to be blown over the ocean (possibly over long distances), is characterized by the absence of large particles (the "long-range transport properties"). It is strongly absorbing.

The size distributions of the models defined by Shettle and fenn (1979) and by WCRP (1986) are represented by lognormal distributions, except for the  $H_2SO_4$  and volcanic ash models, which are represented by a modified gamma function :

$$n(\mathbf{r}) = \frac{d\mathbf{N}(\mathbf{r})}{d\mathbf{r}} = \sum_{i=1}^{2} \left[ \left( \frac{\mathbf{N}_{i}}{ln(10) \mathbf{r} \sigma_{i} \sqrt{2\pi}} \right) exp \left( -\frac{\left(log(\mathbf{r}) - log(\mathbf{r}_{i})\right)^{2}}{2 \sigma_{i}^{2}} \right) \right]$$
(18)

$$n(r) = \frac{dN(r)}{dr} = A\left(\frac{r}{r_0}\right)^{\alpha} \exp\left[-b\left(\frac{r}{r_0}\right)^{\gamma}\right], \text{ with } r_0 = 1 \ \mu m \tag{19}$$

Aerosol model	Particles	Volume	Particle
	(components)	percentage	percentage
Maritime	Rural aerosol mixtures <sup>‡</sup>		99 %
(S&F79)	Sea-salt solution in water ("oceanie	c")	1 %

<u> </u>	ļ



Urban	Rural aerosol mixtures		80 %	
(S&F79)	soot		20 %	
Continental	Water soluble	29	93.876 %	
(WCRP, 1986)	Dust-like	70	2.27 10 <sup>-6</sup> %	
	Soot	1	0.06123 %	
Dust	Desert dusts	100	100	
(Schütz, 1980)				
H <sub>2</sub> SO <sub>4</sub>	75% solution of	100	100	
(WCRP, 1986)	sulfuric acid in water			

*Table 3.1.* proportion of the aerosol components (‡ 70% of water-soluble particles, 30% of dust-like particles).

Aerosol component (S&F 79)		Parameters of	Parameters of the size distribution			
		r <sub>0</sub>	σ/ln(10)	$exp(\sigma)$		
Rural aerosol mixtures	RH 50%	0.02748	0.35	2.238724		
	RH 70%	0.02846				
	RH 80%	0.03274				
	RH 90%	0.03884				
	RH 99%	0.05215				
Sea-salt solution in water	RH 50%	0.1711	0.40	2.51188		
	RH 70%	0.2041				
	RH 80%	0.3180				
	RH 90%	0.3803				
	RH 99%	0.7505				
Urban (small particles)	RH 50%	0.02563	0.35	2.238724		
	RH 70%	0.02911				
	RH 80%	0.03514				
	RH 90%	0.04187				
	RH 99%	0.05996				
Desert Dust (Schütz, 1980)		0.5	0.35	2. 238724		

Table 3.2. parameters of the aerosol size distributions : models from Shettle and Fenn (1979)

(WCRP, 1986)	r <sub>0</sub>		σ/ln(10)	$exp(\sigma)$
Water soluble	0.00	)5	0.475	2.99
Dust-like	0.5		0.475	2.99
Soot	0.01	18	0.30	2.00
	А	α	γ	b
75% H <sub>2</sub> SO <sub>4</sub>	324	1	1	18
Volcanic ash	5461.33	1	0.5	16

<b>Table 3.3</b> .	parameters of	the aerosol	size distributions :	models from	WCRP (1986)
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	443 nm		510 nm		560 nm	
	n	n'	n	n'	n	n'
Sea salt (S&F79) <sup>‡</sup>	1.500	.251 10-7	1.500	.117 10 <sup>-7</sup>	1.499	.112 10-7



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Water-soluble (S&F79) <sup>‡</sup>	1.530	.500 10 <sup>-2</sup>	1.530	.500 10-2	1.530	.600 10 <sup>-2</sup>
Dust-like (S&F79) <sup>‡</sup>	1.530	.800 10 <sup>-2</sup>	1.530	.800 10-2	1.530	.800 10-2
Soot (S&F79) <sup>‡</sup>	1.750	.455	1.750	.450	1.750	.439
Oceanic, RH = 70%	1.416	.128 10-7	1.414	.622 10-8	1.412	.720 10-8
Oceanic, RH = 80%	1.358	.444 10 <sup>-8</sup>	1.355	.249 10 <sup>-8</sup>	1.354	.452 10-8
Oceanic, RH = 90%	1.349	.319 10 <sup>-8</sup>	1.348	.193 10 <sup>-8</sup>	1.345	.406 10 <sup>-8</sup>
Oceanic, RH = 99%	1.339	.165 10 <sup>-8</sup>	1.336	.124 10-8	1.335	.357 10-8
Urban S, $RH = 70\%$	1.487	.606 10-1	1.486	.600 10-1	1.486	.589 10-1
Urban S, RH = 80%	1.423	.345 10-1	1.420	.341 10-1	1.420	.335 10-1
Urban S, RH = 90%	1.389	.204 10-1	1.386	.202 10-1	1.384	.198 10-1
Urban S, RH = 99%	1.349	.466 10 <sup>-2</sup>	1.346	.461 10 <sup>-2</sup>	1.345	.453 10-2
Urban L, RH = 70%	1.476	.562 10-1	1.475	.556 10-1	1.474	.547 10-1
Urban L, RH = 80%	1.415	.313 10-1	1.413	.310 10-1	1.412	.304 10-1
Urban L, RH = 90%	1.380	.174 10-1	1.378	.172 10-1	1.377	.170 10-1
Urban L, RH = 99%	1.342	.187 10-2	1.339	.185 10 <sup>-2</sup>	1.338	.182 10-2
Water soluble (WCRP86)	1.530	.500 10-2	1.530	.500 10-2	1.530	.600 10-2
Dust-like (WCRP86) <sup>†</sup>	1.530	.800 10-2	1.530	.800 10-2	1.530	.800 10-2
Soot (WCRP86) <sup>†</sup>	1.750	.455	1.750	.450	1.750	.439
Volcanic ash (WCRP86)	1.500	.800 10-2	1.500	.800 10-2	1.500	.800 10-2
75 % $H_2SO_4$ solution	1.436	.100 10-7	1.431	.100 10-7	1.430	.106 10-7
Dust, (Schütz, 1980)	1.530	.550 10-2	1.530	.550 10-2	1.530	.550 10-2

Table 3.4. complex refractive indices, n - i n', for wavelengths 443, 510, and 560 nm.

‡ S&F79 stands for Shettle and Fenn (1979). These aerosol components are combined to generate the aerosol models listed in Tables 3.1 and 3.2.

Urban S means the urban model with small particles.

Urban L means the urban model with large particles.

 $\dagger$  WCRP86 stands for WCRP (1986). These aerosol components are combined to generate the aerosol models listed in Tables 3.1 and 3.3.





Table 3.4 continued, complex refractive indices, n - i n', for wavelengths 705, 775, and 865 nm.

	705 nm		775 nm		865 nm	
	n	n'	n	n'	n	n'
Sea salt (S&F79) <sup>‡</sup>	1.489	.287 10 <sup>-6</sup>	1.485	.151 10 <sup>-5</sup>	1.480	.793 10 <sup>-5</sup>
Watersoluble (S&F79) ‡	1.529	.732 10-2	1.525	.944 10 <sup>-2</sup>	1.520	.121 10-1
Dustlike (S&F79) <sup>‡</sup>	1.529	.800 10-2	1.525	.800 10-2	1.520	.800 10-2
Soot (S&F79) <sup>‡</sup>	1.750	.430	1.750	.430	1.750	.430
Oceanic, RH = 70%	1.408	.164 10-6	1.405	.822 10-6	1.402	.404 10-5
Oceanic, RH = 80%	1.351	.801 10-7	1.350	.346 10 <sup>-6</sup>	1.348	.138 10 <sup>-5</sup>
Oceanic, RH = 90%	1.343	.675 10-7	1.342	.275 10-6	1.340	.985 10 <sup>-6</sup>
Oceanic, RH = 99%	1.333	.521 10-7	1.332	.189 10 <sup>-6</sup>	1.330	.498 10-6
Urban S, RH = 70%	1.485	.582 10-1	1.482	.590 10-1	1.479	.600 10-1
Urban S, $RH = 80\%$	1.419	.332 10-1	1.417	.336 10-1	1.414	.341 10-1
Urban S, $RH = 90\%$	1.383	.196 10 <sup>-1</sup>	1.381	.198 10-1	1.379	.201 10-1
Urban S, RH = 99%	1.343	.448 10-2	1.342	.454 10-2	1.341	.462 10-2
Urban L, $RH = 70\%$	1.474	.540 10-1	1.471	.547 10-1	1.468	.557 10-1
Urban L, RH = 80%	1.411	.301 10-1	1.409	.305 10-1	1.407	.310 10-1
Urban L, $RH = 90\%$	1.375	.167 10-1	1.374	.169 10 <sup>-1</sup>	1.372	.172 10-1
Urban L, RH = 99%	1.336	.179 10 <sup>-2</sup>	1.335	.182 10-2	1.334	.185 10-2
Water soluble (WCRP86)	1.529	.733 10-2	1.525	.944 10 <sup>-2</sup>	1.520	.121 10-1
Dustlike (WCRP86) <sup>†</sup>	1.529	.800 10-2	1.525	.800 10-2	1.520	.800 10-2
Soot (WCRP86) <sup>†</sup>	1.750	.430	1.750	.430	1.750	.430
Volcanic ash (WCRP86)	1.500	.800 10-2	1.500	.800 10-2	1.500	.800 10-2
75 % $H_2SO_4$ solution	1.428	.304 10-7	1.427	.975 10-7	1.425	.212 10-6
Dust, (Schütz, 1980)	1.530	.550 10-2	1.530	.550 10-2	1.530	.550 10-2

‡ S&F79 stands for Shettle and Fenn (1979). These aerosol components are combined to generate the aerosol models

listed in Tables 3.1 and 3.2.

Urban S means the urban model with small particles.

Urban L means the urban model with large particles.

<sup>†</sup> WCRP86 stands for WCRP (1986). These aerosol components are combined to generate the aerosol models listed in

Tables 3.1 and 3.3.



Figure 3.4 : Examples of aerosol phase functions, for the aerosols as indicated. Wavelength is 550 nm.

The aerosol phase functions have been computed by using Mie theory, and for the six MERIS bands selected for the present study (443, 510, 560, 705, 775, and 865 nm). Examples are shown in Fig. 3.4. It has been previously checked that the use of the central wavelength (rather than averaging over the bandwidth) does not produce significant differences in the resulting phase function (*cf* JRC contract, 1995).

The extinction coefficients computed from these phase functions are shown on Fig. 3.5, for given conditions, as the ratio of  $c(\lambda)$  to c(865). This ratio characterizes the spectral dependency of the aerosol extinction


**Figure 3.5** : the ratio  $c(\lambda)/c(865)$  as a function of wavelength (linear-log scale), and for several aerosol models selected for the present study ("mar" is the maritime model for various relative humidities, "urb" is the urban model, etc..).

The "standard" atmospheric vertical structure.

The standard atmosphere vertical structure adopted here is based on the profile recommended by WCRP (1986) for open oceanic areas. It is typical of clear oceanic atmospheres, and is as follows :

- Boundary layer (0-2 km) :
  - Maritime aerosol model (Shettle and Fenn, 1979), for RH = 70, 80, 95, 99%Optical thickness is made varying from 0.03 to 0.50 at 550 nm.
  - (non-absorbing aerosols,  $\omega$  about 0.98-0.99)
- Free troposphere (2-12 km) :
  - Continental aerosol (WCRP, 1986)
    - Optical thickness is constant, and equal to 0.025 at 550 nm.
  - (slightly absorbing aerosol :  $0.95 < \omega < 0.98$ )
- Stratosphere (12-50 km) :
  - A 75% solution of sulfuric acid in water (WCRP, 1986)
  - Optical thickness is constant, and equal to 0.005 at 550 nm.
  - (non-absorbing aerosol,  $\omega$  about 0.99)

The constant contribution of the continental +  $H_2SO_4$  aerosols is not so important if we consider the aerosol optical thickness of the atmosphere; its influence on the spectral variation of this optical thickness, however, is significant and results in a spectral change close to that observed over remote ocean areas. The total optical thickness resulting from this aerosol assemblage is spectrally



varying according to Ångström exponents between about 0 and 0.5, when the wavelengths 443 and 865 nm are considered.



*Figure 3.6.* Aerosol extinction normalized at 865 nm, as a function of wavelength. From top to bottom : "standard assemblage" with the maritime model for RH = 70, 80, and 99%.

## Peculiar aerosol vertical repartitions.

The other sets of aerosol models are constructed as follows and their use dictated by the tests at 510 and 705 nm. As it is impossible to encompass all possible situations, the following assumptions have been made :

The "perturbing" aerosols are from three possible types :

- Desert dust.
- Continental aerosol.
- Urban-like aerosol.

When present, they are mainly located :

- In the free troposphere (desert dust, and continental aerosol)

- In the boundary layer (urban-like aerosol).

(deviations from these "vertical structures" will be examined as sensitivity studies, see 3.1.1.6.1).

So, additional sets of aerosol models (and the associated lookup tables for the relationship  $[\rho_{\text{path}} / \rho_{r, \tau a=0}]$  versus  $\tau_a$ ) have been constructed as follows

(i) In all situations, the stratosphere remains unchanged, as compared to the standard set of models.

(ii) When desert dust or a continental aerosol is present in the free troposphere, the problem is now to define how optical thickness is shared by this aerosol and the boundary layer aerosol.





Indeed, the relationships  $[\rho_{\text{path}} / \rho_{\text{r}, \tau a=0}]$  versus  $\tau_a$  are established for ONE aerosol and a given geometry (for the "standard" set of models, the presence of constant backgrounds in the troposphere and stratosphere allow to consider the assemblage as a unique, mean, aerosol). When the optical thickness of the tropospheric aerosol is not constant, it has been decided to define the aerosol assemblage by the relative contributions of the boundary layer aerosol (0-2 km) and of the tropospheric aerosol (2-12 km), to the optical thickness of the troposphere (0-12 km) at 550 nm.

For instance, for an aerosol optical thickness of 0.50, the contributions of the boundary-layer and tropospheric aerosols could be 0.25 and 0.25, or 0.1 and 0.4, etc... This proportion will be referred to as the "mixing ratio".

(iii) For the case of "urban-like" aerosols, the model containing soot particles replaces the «standard» maritime aerosol in the boundary layer. The free troposphere and the stratosphere remain as in the standard cases.

The complete set therefore contains 32 aerosol assemblages :

• Maritime model (standard cases)

4 RH (70, 80, 95, and 99%) for the maritime model (Shettle and Fenn, 1979), plus constant backgrounds in the free troposphere and the stratosphere => 4 assemblages

• Troposphere with continental aerosol :

3 "mixing ratios", *i.e.*, 25%, 50%, and 75% of the optical thickness due to the tropospheric aerosol, 4 values of the relative humidity for the boundary layer maritime aerosol (70, 80, 95, 99%), plus a constant background in the stratosphere.

	=> 12 assemblages.
• Troposphere with desert dust	
As for the continental model	=> 12 assemblages.

• Urban like aerosol

4 RH (70, 80, 95, and 99%) for the urban model (Shettle and Fenn, 1979), plus constant backgrounds in the free troposphere and stratosphere => 4 assemblages

The sign of the error  $\Delta \rho$  obtained either at 510 or at 705 nm actually depends on the spectral dependence of the aerosol extinction, as compared to that of the "standard aerosols". For the desert dust aerosol,  $\Delta \rho$  is systematically negative (at least when the error is significant), while it is always positive for the continental aerosol. This difference in the sign of  $\Delta \rho$  allows choosing unambiguously between these two aerosol types. The situation at 510 nm is not so clear for the urban model, which can lead either to positive or negative errors.

Therefore, we go through this database in the following way : if the tests at 510 and 705 nm indicate the presence of dust (negative error), then the 12 corresponding assemblages are not examined all together. They are examined by groups of 4, corresponding to the 3 selected values of the mixing ratio. For instance :

- Maritime model with mixing ratio = 25, for relative humidities of 70, 80, 95, and 99%
- Maritime model with mixing ratio = 50, for relative humidities of 70, 80, 95, and 99%
- Maritime model with mixing ratio = 75, for relative humidities of 70, 80, 95, and 99%





The set that leads to the lower error at 510 nm is selected at the end. The principle is the same when the flag indicates a positive error at 510 nm, for the presence of continental aerosols. A difficulty arises with the urban-like aerosols, which can lead either to positive or negative errors at 510 nm. As a consequence, they are always considered when the flag at 510 nm "rings". From the first tests carried out, it appears that the correct aerosol assemblages are selected in most cases.

## Generating the lookup tables (LUTs)

Lookup tables have been generated, containing (1) the 3 coefficients of the quadratic relationship between  $[\rho_{\text{path}} / \rho_{\text{r},\tau a=0}]$  and  $\tau_a$ , (2) the Rayleigh reflectances for an aerosol free atmosphere  $\rho_{\text{r},\tau a=0}$ , and (3) the aerosol extinction coefficients for the 32 aerosol assemblages, normalized by their value at 865 nm. The "data" needed to made up these tables have been generated by Mie computations (phase functions and extinction coefficients), and by radiative transfer computations, with the following conditions :

Aerosols	: the 32 aerosol assemblages, as described above.
$\tau_{a}(550)$	: 0.03, 0.1, 0.3, 0.5 (and 2, see section 3.1.1.6.5) for the "standard cases"
	0.05, 0.2, 0.5, 0.8 (and 2, see section 3.1.1.6.5) for the "non standard cases"
λ	: 443, 510, 560, 705, 775, 865 nm
$\theta_{\rm s}$	: From 20 to 68°, each 4° (13 values)
	1 1010 051 0

Atmospheric pressure is 1013.25 hPa.

The sea surface is flat, and the ocean is totally absorbing (no water-leaving radiances)

The values obtained for the ratio  $[\rho_{\text{path}} / \rho_{r, \tau a=0}]$  at 4 different aerosol optical thicknesses, and the ratio 1 for an aerosol-free atmosphere (so : 5 points) are fitted to a second order polynomial and the 3 coefficients are stored in the LUT. To test the algorithm, additional simulations are carried out, while their results are not incorporated in the lookup tables. The aerosols selected for testing the algorithm are :

- Maritime model with RH = 85% (clear maritime atmospheres).
- Assemblages with dust, and the boundary layer maritime aerosol for RH = 85%, and mixing ratios of 25, 50, and 75%.
- Assemblages with the continental aerosol, and the maritime aerosol for RH = 85%, and mixing ratios of 25, 50, and 75%.
- Urban model with RH = 85%

3.1.1.5.3. Test in "standard" conditions (the "standard" set of aerosol assemblages)



**Figure 3.7**. Error in the retrieved top of atmosphere water leaving reflectance at 443 nm, for the maritime aerosol with RH = 85%, and for the geometrical conditions indicated. Dotted line is for  $\tau_a(550)$  about 0.3, dashed line for  $\tau_a(550)$  about 0.1 (i.e., about the mean over remote oceanic areas).



**Figure 3.8**. Histogram of the error in the retrieved top of atmosphere water leaving reflectance at 443 and 560 nm (frequency of each class relative to the most represented class), for the maritime aerosol, RH = 85% The results for the 4 aerosol optical thicknesses and various geometries are here pooled together (4004 cases). The percentage of errors within +/ 0.002 is indicated.

#### Estimation of the path reflectance

The lookup tables described in the previous section have been used to test the proposed algorithm, by introducing into the algorithm total reflectances at the TOA level, as simulated with the maritime aerosol for RH = 85%. Results are presented either for specific geometries (Fig. 3.7; configurations typical of a MERIS scan), or in a more general form in Fig. 3.8; these results show that, for the clear maritime atmospheres, the required accuracy ( $\pm 0.002$  in reflectance at 443 nm) is reached by the algorithm. The error at 560 nm is usually  $\frac{1}{2}$  or  $\frac{1}{4}$  of the error at 443 nm, even if larger errors at 560 nm are sometimes encountered. Errors above the  $\frac{+}{-}$  0.002 limit are actually obtained either for geometrical configurations where sun glint should actually avoid any correction, or for high optical thicknesses. It is noticeable that better results are obtained when the Monte Carlo technique (with its unavoidable stochastic noise) is abandoned for the generation of the pseudo data and the lookup tables, and replaced by an exact technique. This has been tested for instance with the Matrix Operator Method.

### Retrieval of the aerosol optical thickness

Fig. 3.9 shows the relative error in the aerosol optical thickness, as retrieved for 865 nm. Most of these errors are within  $\pm 15\%$ , and often considerably less.



*Figure 3.9. Histogram of the relative error in the aerosol optical thickness retrieved at 865 nm (same 4004 cases as in Fig. 3.8).* 



*Figure 3.10.* Histograms of the error in the pigment index due to the error Δρ in the atmospheric correction, for 3 nominal values of Chl, as indicated (the same 4004 cases as in Fig. 3.8, for each panel). The percentage of "exact retrievals" is indicated, as well as the total number of cases for which a chlorophyll concentration has been computed.





## Impact on the pigment index retrieval

The impact of the errors in the atmospheric correction on the pigment index (Chl) retrieval can now be assessed. The bio-optical algorithms defined for MERIS (see ATBD 2.9 and Morel and Gentili, 1996) are used here, under the form of a polynomial expression

$$\ln(\text{Chl}) = 0.9791 - 2.3962\ln(r_{13}) + 0.8602\ln^2(r_{13}) - 0.6615\ln^3(r_{13}) + 0.2793\ln^4(r_{13}) + 0.0509\ln^5(r_{13})$$
(20)

where  $r_{13}$  is the ratio of  $(b_b/a)$  at 443 nm to  $(b_b/a)$  at 560 nm. Parameters  $b_b$  and a are the backscattering and absorption coefficients of algae, respectively.

The error  $\Delta \rho(\lambda)$  obtained at the end of the atmospheric correction is equal to  $t_d(\theta_v, \lambda) \Delta \rho_w(\lambda)$ so that the error in the water-leaving radiance,  $\Delta L_w(\lambda)$ , is equal to  $\Delta \rho(\lambda) E_s(\lambda) \mu_s / \pi t_d(\theta_v, \lambda)$ . To infer the impact of the error in atmospheric correction on the pigment concentration retrieval, coefficients  $b_b$  and a are retrieved from the "apparent" value of the marine reflectance (*i.e.*, its true value plus the error in atmospheric correction), through (see list of symbols)

$$\left[t_{d} \cdot \rho_{w}(\lambda, \theta_{s}, \theta', \Delta\phi)\right] = \pi t_{d}(\lambda, \theta_{v}) t_{\theta_{s}}(\lambda) \Re(\theta') \frac{f_{1}(\lambda, \theta_{s})}{Q(\lambda, \theta_{s}, \theta', \Delta\phi)} \frac{b_{b}(\lambda)}{a(\lambda)}$$
(21)

$$\Re(\theta') = \left[\frac{(1-\overline{\rho})}{(1-\overline{r}R)} \frac{(1-\rho_{\rm F}(\theta'))}{n^2}\right]$$
(22)

These coefficients  $b_b$  and a are used to calculate a new pigment concentration, Chl', which is then compared to the initial concentration, Chl. An iterative procedure is necessary, because the value of the f/Q ratio is dependent upon the chlorophyll concentration, which is the unknown of the problem (see Morel and Gentili, 1996; MERIS ATBD 2.9). The comparison has been made for pigment concentrations of 0.03, 0.3 and 3 mg m<sup>-3</sup>. The histograms of the errors in Chl are shown in Fig. 3.10.

Each of the three histograms in Fig. 3.10 merges the errors in the retrieved chlorophyll concentration for  $\tau_a = 0.03$ , 0.1, 0.3 and 0.5 at 550 nm, and for several geometries. These errors are expressed in terms of a number of (Chl) classes : values between x and x+1 (x being an integer between 0 and 4) mean that the retrieved (Chl) concentration is overestimated by x (Chl) class. Along the same line, values between x-1 and x mean that the retrieved (Chl) concentration is underestimated by x (Chl) class. Therefore, all values between -1 and +1 correspond to an "exact retrieval" in terms of (Chl) classes. Less than 40% of the retrieved fulfill this condition when Chl = 0.03 mg m<sup>-3</sup> (Fig. 3.10), and a slight positive bias affect the retrieved concentrations. The results for Chl = 0.3 mg m<sup>-3</sup> are in better shape, with no bias and 65% of exact retrievals. A bias of about minus one class (*i.e.*, - 20%) occurs for Chl = 3 mg m<sup>-3</sup>, and 46% of the errors are within the limit of ±1 class.

When  $Chl = 0.03 \text{ mg m}^{-3}$ , the low percentage of exact retrievals is actually consistent with the severe accuracy requirement for the domain of low (Chl) (see Fig. 3.1(c); remind that a shift of only





one class of concentration represents a -20% or +25% change in (Chl)). The discrimination of 10 (Chl) classes between 0.03 and 0.3 mg m<sup>-3</sup>, as initially aimed at, seems limited by the accuracy of the atmospheric correction. Lowering the number of (Chl) classes to be detected to 5 between 0.03 and 0.3 mg m<sup>-3</sup>, for instance, would increase the acceptable errors in  $\rho_w$ (443).

The bias observed when Chl = 3 mg m<sup>-3</sup> was not expected to the extent that the errors in atmospheric correction are the same for the three panels of Fig. 3.10. Errors that do not bias the pigment retrieval for low and moderate chlorophyll concentrations (*i.e.*, high  $\rho_w(443)$ ), have an impact for higher concentrations because the actual blue-to-green ratio is close to 1. This bias is a consequence of the nature of the algorithm, which performs extrapolation of the atmospheric contribution from the near infrared toward the visible, with, in general, increasing errors with decreasing wavelength. As far as we know, this problem, occurring for chlorophyll concentrations around 3 mg m<sup>-3</sup>, seems not to have been acknowledged.

### 3.1.1.5.4 Test with absorbing aerosols

### Correction of aerosol reflectance

The procedure used to test the algorithm for the clear maritime atmospheres is used now for "non standard" atmospheres, characterized by the presence of continental aerosols or desert dust (with the 3 "mixing ratios"), or of urban aerosols, always with RH = 85% within the marine boundary layer. These aerosols are of the same "family" than those used to generate the lookup tables (sensitivity studies are carried out in section 3.1.1.6.1).



*Figure 3.11.* Histogram of the error in the retrieved top of atmosphere water leaving reflectance at 443 nm, and for the three "nonstandard" aerosol assemblages, as indicated (and for RH = 85% in the marine boundary layer).

The results for the four aerosol optical thicknesses (i.e., 0.03, 0.1, 0.3, and 0.5 at 550 nm), the three "mixing ratios" (the proportion of aerosols within the boundary layer and the free troposphere), and various geometries, are here pooled together (see text). The percentage of errors within  $\pm$ .002 is indicated. The percentage between parentheses is the one obtained without detection of aerosol absorption.



*Figure 3.12.* Fraction of pixels that were well identified by the tests at 510 and 705 nm (i.e., recognized as "containing" absorbing aerosols), as a function of the aerosol optical thickness, and for the three "nonstandard" aerosol assemblages.

The test at 510 actually functions for situations with the continental aerosol or desert dust, while it is the test at 705 nm that identifies most of the urban aerosols. The 3 curves are for Chl = 0.03, 0.3, and 3 mg m<sup>-3</sup> (solid, dotted and dashed lines, respectively). Long dashed curves (black triangles) represent the percentages of pixels well identified as containing absorbing aerosols, while the aerosol models were wrongly selected.

Results are shown in Fig. 3.11, where the errors obtained for 4 optical thicknesses, and for various geometrical configurations are pooled together (*i.e.*, 12012 cases for atmospheres with either the continental aerosol or desert dust, and 4004 for the urban aerosol). The accuracy of the algorithm is obviously not so good as for the clear maritime atmospheres, even if a significant percentage of the errors remain within  $\pm 0.002$ . The errors outside of this range are obtained (1) when the test at 510 nm has failed in identifying the absorbing character of the actual aerosol, or









The results for the three "nonstandard" aerosol assemblages are shown. For the two upper panels, the results for the three "mixing ratios" (the proportion of aerosols within the boundary layer and the free troposphere) are pooled together (3003 cases for each panel). The percentage of errors within +/ 30% is indicated, as well as the total number of cases for which the optical thickness has been computed.





**Desert dust** 



*Figure 3.14. Histograms of the error in pigment concentration due to the error*  $\Delta \rho$  *in the atmospheric correction, for 3 nominal values of Chl, as indicated (same cases as in Fig. 3.11).* 

The percentage of "exact retrievals" is indicated, as well as the total number of cases for which the chlorophyll concentration has been computed.





(2) when the test at 510 nm was successful, while the choice of the couple of aerosol models was not the best possible. The global accuracy of the algorithm remains satisfying, however, and, in addition, errors outside  $\pm 0.002$  at 443 nm sometimes lead to negative water-leaving radiances, allowing the failure of the algorithm to be identified *a posteriori*.

Fig. 3.12 shows the percentage of success of the tests at 510 and 705 nm, as a function of the aerosol optical thickness. When the optical thickness of the "perturbing" aerosol is low, the flag usually remains silent; this is nevertheless without consequence because the slight additional aerosol load (with respect to the clear maritime atmosphere) allows the correction to be successfully carried out with the standard set of aerosols. When the optical thickness of the "perturbing" aerosol is higher, the test identifies about 60 to 80% of the "non standard" conditions.

## Retrieval of the aerosol optical thickness

Fig. 3.13 shows the relative error in aerosol optical thickness, as retrieved at 865 nm. The situation is degraded, as compared to Fig. 3.9. Most of the errors remain however within  $\pm 15\%$ .

## Impact on the pigment index retrieval

Fig. 3.14 synthesizes the results concerning the errors in the pigment index, for three nominal values (0.03, 0.3, 3 mg Chl m<sup>-3</sup>). The percentage of "exact retrievals" is less than for clear atmospheres, especially for the case of urban aerosols, and for the lower Chl concentration. It should be reminded however that the atmospheric correction would have totally failed without the use of the test at 510 and 705 nm. Therefore, the results shown here definitely represent an improvement with respect to what could be obtained with a "standard" algorithm, without the possibility of identifying at least part of the situations where absorbing aerosols are present.

### 3.1.1.5.5 Cancellation of the test at 510 nm

A significant number of reflectance spectra (as measured at sea) have been examined to infer the natural variability of the diffuse reflectance of oceanic Case 1 waters at 510 nm,  $R(0)_{510}$ . From these data, and also from the values obtained from a reflectance model (Morel, 1988), a mean value of  $R(0)_{510}$  and its associated uncertainty have been selected to implement the test at 510 nm, which aim at identifying the presence of absorbing aerosols. The results presented in the two previous sections have shown that the test is successful. It is nevertheless impossible to ensure that this test will function so well during the actual operation of the algorithm. The reason could be a greater than expected variability in  $R(0)_{510}$ .

The possibility of canceling the test at 510 nm should therefore be incorporated into the final, operational, algorithm. In this situation, only a subset of the 32 aerosol assemblages would be kept. It is probably useless (and even misleading) to carry out the atmospheric correction with the complete database; ambiguities will necessarily appear if the 32 assemblages are examined all together at once. The "restricted" database would be similar to that used by Gordon and Wang (1994a), with, for instance, only clear maritime atmospheres, and a few "special aerosols" to incorporate extreme values of the spectral selectivity of aerosol scattering.

This possibility has been tested here by using the entire database (32 aerosol assemblages). The errors of the atmospheric correction are shown in Fig. 3.15. The relative errors in the aerosol



optical thickness retrieved at 865 nm, and the error in the pigment index, are shown in Figs. 3.16 and 3.17, respectively. The results, in terms of errors at 443 nm, are degraded as compared to those obtained when the test at 510 nm and 705 nm are activated (Figs. 3.8 and 3.11); in addition, the aerosol type is wrongly retrieved in many cases (and especially for clear maritime atmospheres), because of ambiguities arising during the selection of the aerosol.



*Figure 3.15.* As in Figs. 3.8 and 3.11, but when the tests at 510 and 705 nm are removed and all aerosol models considered together when selecting the aerosol type.

### 3.1.1.5.6 Single scattering algorithm

In the previous section, the possibility of canceling the tests at 510 and 705 nm has been examined, because the use of the test at 510 nm could be problematic in some instances. A second source of misfunctioning of the algorithm could exist, if the aerosol models used to generate the lookup tables are not enough representative of reality (even if these models have been partly validated, *e.g.*, Schwindling, 1995). If these aerosol models reveal to be misadapted, then the only "life buoy" is a "CZCS-like", single-scattering algorithm, which allow to estimate the aerosol reflectance for any wavelength in the visible, without the use of any aerosol model (see *e.g.*, Gordon, 1997). In this situation, the path reflectance is assumed to be the sum of the Rayleigh reflectance (multiple scattering), and of the reflectance due to aerosol single scattering :

$$\rho_{\text{path}} = \rho_{\text{r}, \tau a=0} + \rho_{\text{as}} \tag{23}$$

So that, in the near-infrared (*i.e.*, 775 and 865 nm), where  $\rho_{\text{path}} = \rho_{\text{t}}$ :

$$\rho_{\rm as} = \rho_{\rm t} - \rho_{\rm r, \, \tau a=0} \tag{24}$$

For any visible wavelength,  $\lambda_i$  (e.g., Gordon, 1997)

$$\rho_{\rm as}(\lambda_{\rm i}) = \rho_{\rm as}(865) \exp\left[\frac{865 - \lambda_{\rm i}}{865 - 775} \log_{\rm e}\left(\frac{\rho_{\rm as}(775)}{\rho_{\rm as}(865)}\right)\right]$$
(25)







*Figure 3.16.* As in Figs. 3.9 and 3.13, but when the test at 510 and 705 nm is removed and all aerosol models considered together when selecting the aerosol type.



*Figure 3.17.* As in Fig. 3.14, but when the tests at 510 and 705 nm are removed and all aerosol models considered together when selecting the aerosol type.

The percentage of errors within +/30% is indicated, as well as the total number of cases for which the chlorophyll concentration has been computed (Chl = 0.3 mg m<sup>-3</sup>)

So that

$$t.\rho_{\rm w} = \rho_{\rm t} - \rho_{\rm r, \tau a=0} - \rho_{\rm as} \tag{26}$$

The errors in the pigment index, resulting from the errors of the single scattering atmospheric correction are shown in Fig. 3.18. There is about 30% of "exact retrievals" whatever the aerosol model. It has to be noticed, however, that the number of cases for which a chlorophyll concentration has been computed is reduced, as compared to the same number in Fig. 3.14 or 3.10. This difference is actually due to the calculation of negative, or unrealistically large, water-leaving radiances.



*Figure 3.18.* As in Fig. 3.14, when using the "CZCS-like" single scattering algorithm, however, and for a nominal value of the pigment index of 0.3 mgChl m<sup>-3</sup>.

The percentage of "exact retrievals" is indicated, as well as the total number of cases for which the chlorophyll concentration has been computed.





# 3.1.1.6. Sensitivity studies

In this section, the impact of various parameters on the atmospheric correction is examined through sensitivity studies. The principle is to operate the correction by using the database generated for the prescribed standard conditions (*i.e.*, a flat sea surface, and specified constant values for atmospheric pressure and ozone content), to process data issued from simulations where the conditions are different, regarding one parameter of interest. The amplitude of the error in the retrieved water leaving reflectances should then provide information to decide if the natural variability in the parameter in question has to be accounted for (by increasing the dimension of the lookup tables) or, on the contrary, if this parameter can be kept to a constant and mean value.

# 3.1.1.6.1 Vertical distribution of aerosols / "special" aerosols

Even if the standard vertical structure of aerosols adopted to implement the algorithm has been derived from observations and from the recommendations of aerosol specialists, it is clear that different vertical structures are possible over the ocean. Different aerosol types (*i.e.*, composed of other components than the standard aerosols used before) are also possibly encountered. The following have been tested here :

- (1) In the free troposphere, the desert dust model of Schütz (1980) is replaced by the dust-like aerosol component described in WCRP (1986). The dust and the boundary-layer aerosol (the maritime model, with RH = 80%) are each responsible for 50% of the optical thickness,  $\tau_a$ , which is set to 0.05 and 0.50 at 550 nm. This profile illustrates a situation where the aerosol in the lookup tables and the actual aerosol have a similar spectral behavior in the near infrared, whereas their absorption characteristics diverge in the visible.
- (2) The continental aerosol within the free troposphere is replaced by an aerosol whose particle size distribution follows a Junge law, with v = 3, with refractive indices of 1.33 (water) and 1.50 (continental particles), and with  $\tau_a = 0.1$  at 550 nm. The boundary layer is as above, with an optical thickness of 0.03 or 0.3. This situation corresponds to blowing over the ocean of continental, non-absorbing, particles.
- (3) The urban model with small particles is replaced by a model with a larger mode (Shettle and Fenn, 1979). The constant background in the free troposphere remains as in the standard cases (clear atmospheres). This situation could be encountered above near coastal waters, overlaid by air masses close to their source of soot particles.
- (4) A moderately absorbing mixture of oceanic particles and desert dust (dust particles being either 10 or 50% of the total particle number) replaces the pure maritime aerosol in the boundary layer. The constant background in the free troposphere remains as in the standard cases (clear atmospheres). This profile corresponds to the sinking of desert dust into the sea.
- (5) A convective atmosphere is simulated by annihilating the vertical structure in the boundary layer and the free troposphere, and by replacing the standard maritime and continental aerosols by the same mixtures as above, with a scale height of 3 kilometers within the whole troposphere. The total aerosol optical thickness is set to 0.05 and 0.3.
- (6) Idem as (5) but for the urban aerosol (with RH = 80 or 99%).





(7) The extension of the desert dust layer is reduced to 4 km (between the altitudes 2 and 6 km), instead of 10 km (2 to 12 km) in the previous profiles, with an optical thickness of 0.1. The boundary layer aerosol is the maritime model with RH = 80%. This structure aims at representing a dust layer after a long transport over the ocean (it is likely that this kind of layer tends to narrow during its transport; Powell, 1995).

The 7 aerosol distributions were used to simulate TOA total radiances for  $\theta_s = 20$ , 40, and 60°. The error of atmospheric correction at 443 nm obtained for these aerosols are pooled together for several geometries, and they are presented in Fig. 3.19 and discussed below in reference to the numbering used above. The corresponding errors in the retrieved pigment index are presented ni Fig. 3.20.

- (1) Absorption is systematically detected for  $\tau_a = 0.5$ , and less frequently for  $\tau_a = 0.05$ . The increasing departure of the  $[c(\lambda) / c(865)]$  ratios with decreasing wavelength, between the two desert dust models (WCRP (1986), used for the test, and Schütz (1980), in the lookup tables) leads however to an over-correction of about 0.004 at 443 nm. These rather bad results emphasize the need for a correct representation of the absorption properties of the aerosols in the visible domain.
- (2) The situation is approximately converse of that in (1), *i.e.*, an under-correction, with however a greater percentage of errors within  $\pm 0.002$ . Introducing aerosols with a strong scattering selectivity within the lookup tables (they are not represented now) would probably brought the bias observed here close to 0.
- (3) The reasonably good results for the correction of the large urban aerosols indicate that some uncertainty in the representation of the coarse mode of the aerosol size distribution is probably acceptable.
- (4) Atmospheric correction is accurate when only a few absorbing particles are present in the boundary layer. The correction is here effected with the standard aerosol assemblages (no detection of absorption).
- (5) The high percentage of errors within  $\pm 0.002$  confirms that an exact representation of the vertical distribution of aerosols is not crucial when this aerosol is not too much absorbing.
- (6) The same comment as above could be made, except that now the aerosol is strongly absorbing. The rather good results in fact show that some uncertainty in the vertical extension of the absorbing aerosol layer do not lead to large errors if the aerosol in the lookup tables in close enough to the actual one.
- (7) Same comment as for (6)







*Figure 3.19. Histograms of the error in the atmospheric correction at 443 nm, for the peculiar situations described in the text (section 3.1.1.6.1).* 

Results for various geometries and aerosol optical thicknesses are pooled together. The percentages indicate how many errors are within  $\pm 0.002$ .







*Figure 3.20. Histograms of the errors in the retrieved pigment index, corresponding to the errors of the atmospheric correction shown in Fig. 3.19. The nominal value of the pigment index is 0.3 mg Chl m<sup>-3</sup>.* 



### 3.1.1.6.2 Atmospheric pressure

The importance of atmospheric pressure in sizing the Rayleigh reflectances has been already emphasized for the CZCS algorithms (André and Morel, 1989). The lookup tables that are used in the present work (and containing for instance the relationships between  $[\rho_{\text{path}} / \rho_{\text{r}, \tau a=0}]$  and  $\tau_a$ ) have been generated from simulations where the atmospheric pressure is kept to a constant value, namely 1013.25 hPa. If the actual atmospheric pressure is not 1013.25 hPa, then the actual and the tabulated  $[\rho_{\text{path}}(\lambda) / \rho_{\text{r}, \tau a=0}(\lambda)]$  ratios could not coincide.



*Figure 3.21. Relative changes (percents) of the TOA path reflectance, in response to relative changes in atmospheric pressure,*  $\Delta P/P$ *, of*  $\pm 2\%$ *, and displayed as a function of*  $\eta_r$  *(solid curves).* 

The conditions are :  $\theta_s = 40^\circ$ , maritime aerosol (RH = 85%). The three points correspond to the mean error for several geometries ( $\theta_v$  from 0 to 60° each 4°, and  $\Delta \phi = 0$ ,  $\pi/2$  and  $\pi$ ), and the three increasing values of  $\eta_r$  correspond to (1)  $\lambda = 865$  nm and  $\tau_a(550) = 0.3$ , (2)  $\lambda = 443$  nm and  $\tau_a(550) = 0.3$ , and (3),  $\lambda = 443$  nm and  $\tau_a(550) = 0.05$ . The dotted curves show the relative errors in the path reflectance, after Eq. (27) has been used to calculate its value for a standard pressure P = 1013.25 hPa, from its value at P' = P (1 + \Delta P/P).

The relative change  $\Delta \rho_{r, \tau a=0}/\rho_{r, \tau a=0}$  resulting from a relative change  $\Delta P/P$  is close to  $\Delta P/P$ , even if not strictly equal because of multiple scattering effects (Gordon *et al.*, 1988). The situation is different for  $\rho_{path}$ , that is within a compound atmosphere containing molecules (optical thickness  $\tau_r$ ) and aerosols ( $\tau_a$ ). When  $\tau_r$  is increased, the reflectance due to pure Rayleigh scattering<sub>r</sub>, as well as the reflectance corresponding to heterogeneous scattering obviously tend to increase. In the meantime, however, the reflectance due to aerosol scattering only is decreasing : the increase in molecule concentration tends to "mask" the aerosol signal, at least if  $\tau_r$  is large compared to  $\tau_a$ . As a consequence, the repercussion of  $\Delta P/P$  on  $\Delta \rho_{path}/\rho_{path}$  is progressively decreasing when the contribution of molecules ( $\tau_r$ ) to the total optical thickness decreases, *i.e.*, when  $\eta_r (= \tau_r / (\tau_a + \tau_r))$  is





decreasing. For instance, when  $\Delta P/P = +2\%$ ,  $\Delta \rho_{path}/\rho_{path}$  at 443 nm is of about +1.5% when  $\tau_a$  is 0.05 ( $\eta_r \sim 0.8$ ), less than +1% when  $\tau_a$  is 0.3 ( $\eta_r \sim 0.4$ ), and nearly zero at 865 nm when  $\tau_a$  is 0.3 ( $\eta_r \sim 0.05$ ). The following simple and empirical correction is then proposed to account for the changes in atmospheric pressure

$$\rho'_{\text{path}} = \rho_{\text{path}} \left( 1 + (\Delta P/P)\eta_{\text{r}} \right)$$
(27)

where  $\rho_{\text{path}}$  and  $\rho'_{\text{path}}$  are the path reflectances for the standard pressure P and the pressure P' = P (1 +  $\Delta$ P/P). Using Eq. (27) allows to recover the exact value of  $\rho_{\text{path}}$  within ±0.5% (Fig. 3.21). Therefore, if atmospheric pressure significantly differs from the mean value (±5 hPa for instance), Eq. (27) can be used to correct the measured value of  $\rho_{\text{path}}$  in the near infrared, from P' to P, before introducing it into the algorithm. At this stage,  $\tau_a$  is still unknown, and can be taken from the surrounding pixels (a ±20% error on  $\tau_a$  does not appreciably degrades the accuracy of Eq. (27)). The whole scheme is then operated by using the lookup tables generated for the standard pressure, and the values of  $\rho_{\text{path}}$  obtained at the end in the visible domain are again corrected by using Eq. (27), but now from P to P'. This technique has been applied to the same situations as shown in Fig. 3.7, with P = 993 and 1033 hPa (*i.e.*, changing the standard pressure by plus or minus 2%), and the results are shown in Fig. 3.22.

#### 3.1.1.6.3 Inland waters

A peculiar problem is addressed here, and concern the possibility of using the present atmospheric correction algorithm for inland waters (at least if they cover significant areas and are Case 1 waters), and especially if the altitude of these waters is significantly above the 0 level. This problem is connected to the sensitivity to atmospheric pressure, P.

The variations in P due to weather changes above the ocean are of the order of  $\pm 2\%$  (see above), while they are much more important when "moving" a target from the sea level to an altitude of one or several kilometers. In addition, in the case of ocean areas, the small variations in P affect nearly all layers, while in the case of an increasingly elevated target, the layers with the greatest molecule concentration are progressively removed, the aerosol content remaining about the same (the boundary layer and the stratosphere remain unchanged; only the "free troposphere" grow smaller). One can therefore expect that the ratio  $[\rho_{\text{path}} / \rho_{\text{r},\tau a=0}]$  will increase more rapidly with  $\tau_a$  as the number of molecules decreases. It is likely that the coupling between scattering due to aerosol and scattering due to molecules is also affected.



*Figure 3.22.* Error in the retrieved top of atmosphere water leaving reflectance at 443 nm, for the maritime aerosol with RH = 85%, for  $\tau_a(550)$  about 0.03 and 0.30, and for the geometrical conditions indicated.

Solid lines are the results obtained when the actual pressure is the standard pressure. Dashed and dotted lines are for the standard pressure less 20 hPa (*i.e.*, 993 hPa, upper 4 panels), or plus 20 hPa (*i.e.*, 1033 hPa, lower 4 panels), and respectively without or with the correction for the change in pressure (Eq. 27).

Simulations have been carried out to assess these effects, by modifying as follows the vertical atmospheric profiles :





- The boundary layer is still the layer between the altitude of the target and this altitude plus 2 kilometers. It contains the continental aerosol, with an optical of 0.3 at 550 nm.
- The stratosphere is obviously still the layer between altitudes 12 and 50 km, with the  $H_2SO_4$  aerosol (optical thickness of 0.005 at 550 nm).
- The "free troposphere" is the remaining (for instance from 4 to 12 km if the target is at an altitude of 2 kilometers), and contains the continental aerosol. The aerosol optical thickness for this layer results from the integration of the extinction coefficients over less than 10 one-kilometer layers, each with an extinction coefficient of 0.0025 km<sup>-1</sup> (this led to an optical thickness of 0.025 when elevation was 0).
- The vertical profile for molecular scattering (Elterman, 1968) is integrated over the altitudes corresponding to the 3 levels

The ratios  $[\rho_{\text{path}} / \rho_{\text{r},\tau a=0}]$  at 443 and 865 nm are shown in Fig. 3.23, as a function of  $\tau_a$ , and for several altitudes (including the sea level), with an increment of 1 km. Drastic changes appear in the slope of this relationships, clearly preventing from using the present atmospheric correction algorithm as soon as the target is not at the sea level. A simple way to carry out the correction for elevated targets would be to shift to the simple single scattering algorithm (see section 3.1.1.5.6). Yet the problem is not totally solved, as the value of  $\rho_{r,\tau a=0}$  taken from the lookup tables would have to be corrected for the altitude change.



**Figure 3.23.** The relationship  $[\rho_{path} / \rho_{r, \tau a=0}]$  as a function of  $\tau_a$ , at 443 and 865 nm, and for compound atmospheres (aerosols plus molecules) bounded by a Fresnel reflecting interface located at various altitudes, as indicated.

#### 3.1.1.6.4 Wind speed

The relationship  $[\rho_{\text{path}} / \rho_{\text{r,}\tau a=0}]$  versus  $\tau_a$  is probably modified when the sea surface is no longer flat. When wind blows at the sea surface, whitecaps are one cause of changes in the TOA reflectances; their effect on atmospheric correction will be assessed in section 3.1.3.2.5. Sea surface roughness also modifies the sun glint pattern as well as the fate of any diffuse photon interacting with the surface. The latter effect is examined here (see also Gordon and Wang, 1992a, 1992b), by



assuming that the sun glint reflectance has been previously calculated and subtracted from the total reflectance (see section 3.1.3.2.8 for a discussion of this assumption).

Monte Carlo simulations have been carried out for atmospheres bounded by a windroughened ocean, with facet slopes normally distributed, independently of the wind direction. The probability density of surface slopes for the direction ( $\theta_s$ ,  $\theta_v$ ,  $\Delta \phi$ ) is given by (Cox and Munk, 1954)

$$p(\theta_{\rm s}, \theta_{\rm v}, \Delta \phi) = \frac{1}{\pi \sigma^2} \exp\left(\frac{-\tan^2(\beta)}{\sigma^2}\right)$$
(28)

where  $\beta$  is the angle between the local normal and the normal to the facet, and  $\sigma$  is the root mean square of slopes, and is a function of wind speed, W, through (Cox and Munk, 1954)

$$\sigma^2 = 0.003 + 5.12 \ 10^{-3} \ \mathrm{W} \tag{29}$$

The sun glint reflectance at the TOA level is :

$$\rho_{\rm G} = \pi \,\rho_{\rm F} \,\, \mathrm{p}(\theta_{\rm s}, \,\theta_{\rm v}, \,\Delta\phi) \,/ \,(4\cos(\theta_{\rm v})\cos(\theta_{\rm s})\cos^4(\beta))\mathrm{T}(\theta_{\rm v}) \,\mathrm{T}(\theta_{\rm s}) \tag{29'}$$

where  $\beta$  is the angle between the local normal and the normal to the facet  $(\cos(\beta) = (\cos(\theta_V) + \cos(\theta_S)) / 2\cos(\omega))$ , with  $\cos(2\omega) = \cos(\theta_V)\cos(\theta_S) - \sin(\theta_V)\sin(\theta_S)\cos(\Delta\phi))$ , and where  $T(\theta)$  is the direct transmittance of the atmosphere for angle  $\theta$ , and is equal to  $e^{-\tau/\cos(\theta)}$ , with  $\tau$  the total optical thickness (Rayleigh + aerosols + ozone + etc...).

Shadowing effects are not accounted for in the Monte Carlo simulations. The resulting  $[\rho_{\text{path}} / \rho_{\text{r}, \tau a=0}]$  versus  $\tau_a$  curves, obtained at 443 and 865 nm with the maritime aerosol and  $\sigma = 0$  and 0.2, are displayed in Fig. 3.23, for  $\theta_s = 36^\circ$ ,  $\Delta \phi = \pi/2$ , and  $\theta_v = 12^\circ$  (panel (a)) or  $\theta_v = 57^\circ$  (panel (b)). The light field is more and more diffuse as the wavelength decreases, or, for a given wavelength, when  $\theta_v$  increases. The impact of the rough surface on the reflectances is accordingly reduced in the visible, as compared to the near infrared, and also when aiming at the ocean at large viewing angles for  $\lambda = 865$  nm. The curves obtained at  $\lambda = 443$  nm are nearly superimposed when obtained either for  $\sigma = 0$  or for  $\sigma = 0.2$ , because the spatial redistribution of reflected photons cannot further increase the diffuse character of the light field. On the contrary, the redistribution of radiances at 865 nm leads to some changes in the slope of the  $[\rho_{\text{path}} / \rho_{\text{r}, \tau a=0}]$  versus  $\tau_a$  relationship when  $\theta_v = 12^\circ$ .

Two, perhaps three, sets of lookup tables should thus be generated (for the relationship [ $\rho_{\text{path}}$  /  $\rho_{r, \tau a=0}$ ] versus  $\tau_a$ ), in correspondence with W = 0 and with moderate wind speeds, probably around 5 and 10 m s<sup>-1</sup>. Higher wind speeds are not to be considered, because the importance of the changes here examined would become much lower than that due to the reflectance of whitecaps. Switching from one set of lookup tables to another one, or interpolating between them, must rely on the knowledge of wind speed, available either from other sensors, or from meteorological centers.



**Figure 3.24**. The  $[\rho_{path} / \rho_{r, \tau a=0}]$  ratio at 443 and 865 nm is drawn as a function of  $\tau_a$ , and for  $\theta_s = 36^\circ$ ,  $\Delta \phi = \pi/2$ , and  $\theta_v = 12^\circ$  (left) or 57° (right).

The aerosol is the maritime model (RH = 85%). Dotted curves are for a perfectly flat sea surface, and solid curves are for a windroughened interface, characterized by  $\sigma = 0.2$ . Dashed line is as the dotted line, but for the  $[\rho_t / \rho_{r,\tau a=0}]$  ratio (*i.e.*, the sun glint has not been corrected).

#### 3.1.1.6.5 High aerosol optical thickness

Atmospheric correction primarily aims at retrieving the optical properties of the surface ocean, when seen through a scattering and absorbing atmosphere. When using the technique proposed here, however, atmospheric properties are also recovered, as by-products of the algorithm. One of these properties is the aerosol optical thickness,  $\tau_a$ , which is of considerable interest for studies of the earth radiation budget and climate (e.g., Charlson et al., 1992), as well as for ocean biogeochemistry (e.g., Donaghay et al., 1991). When  $\tau_a$  becomes high, say above 0.6-0.8 at 550 nm, it is probably illusory to try an assessment of the oceanic surface properties (at least with the accuracy required here), because the error on  $\tau_a$  would cause prohibitively large errors on  $\rho_w$ . It is however conceivable to recover the value of  $\tau_a$ . Therefore, it is examined in this section whether  $\tau_a$  is still retrievable when it is high. A value of 2 at 550 nm has been chosen; it is probably a maximum, and could correspond for instance to a massive blowing of dust over the ocean. The Lookup tables have been accordingly modified, *i.e.*, the quadratic fits of  $([\rho_{path} / \rho_{r,\tau a=0}]$  versus  $\tau_a)$  have been performed over 6 couples, instead of 5, and including now the couple corresponding to  $\tau_a = 2$ . The error in atmospheric correction at 443 nm, as well as the relative error on the aerosol optical thickness at 865 nm, are displayed in Fig. 3.25 for the four aerosol types. In most cases (i.e., 70 to 90%), atmospheric correction fails, meaning that  $\rho_{\rm w}$  is not recovered with the required accuracy (*i.e.*,  $\pm 0.002$  in reflectance). The retrieval of  $\tau_a$ , however, remains acceptable, with most of the relative errors within  $\pm 30\%$  (*i.e.*,  $\tau_a$  retrieved with an error of about  $\pm 0.3$ ). Therefore, with the MERIS instrument, the retrieval, and thus the global mapping, of the aerosol optical thickness at 865 nm seems possible even for highly turbid atmospheres.



**Figure 3.25.** Upper 4 panels : histograms of the error in atmospheric correction at 443 nm, when  $\tau_a(550) = 2$ , and for several geometries (as in Fig. 3.8).

Lower 4 panels : histograms of the relative errors in the aerosol optical thickness at 865 nm, corresponding to the situations shown in the 4 upper panels.

#### 3.1.1.6.6 Stratospheric aerosols, thin cirrus clouds

The representation adopted in the present work for the stratosphere corresponds to the "background stratospheric aerosol (BSA)" described in WCRP (1986), which is aimed at representing unperturbed conditions (*i.e.*, no recent volcanic eruption). Perturbed stratospheric aerosol profiles may correspond either to the presence of particles of volcanic origin in the lower half of the stratosphere, or to the presence of a thin layer of cirrus clouds at the base of the stratosphere. Based on a few simple and preliminary tests, the impact of such structures on the atmospheric correction has been assessed. As for the volcanic aerosols, 3 profiles have been used, corresponding to the "VSA" profiles described in WCRP (1986), where the stratosphere is divided into 3 levels

- (1) from 30 to 50 km, the aerosol remains unperturbed in any case (H<sub>2</sub>SO<sub>4</sub>), with  $\tau_a = 0.003$  at 550 nm
- (2) from 20 to 30 km, the aerosol type is either  $H_2SO_4$  or volcanic ash. For the  $H_2SO_4$  aerosol,  $\tau_a(550)$  is 0.05 or 0.1, and define respectively the "ancient" and "recent" profiles. For the volcanic ash (absorbing; see Table 3.4, Figs. 3.4 and 3.5), the optical thickness at 550 nm is 0.3, and define the "fresh" profile.





(3) from 12 to 20 km,  $\tau_a$  remains 0.0306 at 550 nm, whatever the aerosol type (either H<sub>2</sub>SO<sub>4</sub> or volcanic ash).

Atmospheric correction has been applied to TOA path reflectances simulated with the 3 peculiar stratospheres and for  $\theta_s = 20$ , 40, and 60°. The results are presented in Fig. 3.26, except for the "fresh" aerosol profile, which lead, as expected, to so large errors (negative errors < -0.01) that it is useless to display them. The errors shown in Fig. 3.26 clearly indicate that the atmospheric correction algorithm proposed here, and implemented as described in this ATBD, cannot successfully apply to TOA reflectances as soon as a significant increase of the concentration of the H<sub>2</sub>SO<sub>4</sub> aerosol occurred (say,  $\tau_a > 0.1$  in the stratosphere; see also Gordon *et al.*, 1997). The situation is even more dramatic when volcanic ash is present. This high sensitivity of the algorithm to products of volcanic origin advocates for a correction of their effect on the TOA reflectances, before atmospheric correction is applied (or, at least, for raising a flag to indicate their possible presence).



Figure 3.26. Error in atmospheric correction at 443 nm, as a function of  $\theta_s$ , and for the viewing geometries indicated.

Upper 2 panels : standard case, *i.e.*, no perturbation of the stratosphere. Middle panels : the "ancient" profile has been used (see text). Lower 2 panels : the "recent" profile has been used (see text).







**Figure 3.27**. Upper panel : single scattering reflectance of a hypothetical pure cirrus layer, as a function of the viewing angle  $\theta_{\nu}$ , and within the principal (anti-solar,  $\Delta \phi = \pi$ , and solar,  $\Delta \phi = 0$ ), and perpendicular  $(\Delta \phi = \pi/2)$  planes (the phase function is shown in insert).

The optical thickness of the cirrus layer is 0.2 at 550 nm. The solar zenith angle is 40°. Solid line is the analytical, exact, calculation; Black diamonds linked by a dashed line are the output of a Monte Carlo simulation. Lower 2 panels : The relationship ( $[\rho_{path} / \rho_{r,\tau a=0}]$  versus  $\tau_a$ ) at 865 nm, and for the geometries indicated. Results are for the standard atmosphere (no cirrus, solid line), and for atmospheres containing a cirrus layer with an optical thickness of 0.05 (dotted lines), 0.1 (dashed lines), and 0.2 (dotted-dashed lines) at 550 nm.

The situation is different for cirrus clouds, which are located a little further down in the atmosphere (say, at the top of the troposphere), are not absorbing, and whose phase function is markedly different from that of stratospheric aerosols (see insert in Fig. 3.27). A prerequisite to any sensitivity study was to examine the possibility of simulating TOA radiances with the Monte Carlo



code in a realistic way, when one of the atmospheric scatterers (*i.e.*, the cirrus) has a strongly peaked, and especially irregular, phase function. The angular discretisation has been accordingly doubled (*i.e.*,  $\Delta \theta = 2.5^{\circ}$ ), and simulations have been performed with a phase function corresponding to hexagonal plates (Brogniez *et al.*, 1995). The single scattering reflectance has been simulated for a pure cirrus layer (the Monte Carlo code is provided with the capability of keeping track of the photon histories, *i.e.*, the number and kind of scattering events they have undergone), and compared to the single scattering reflectance calculated analytically for the same medium with the following equation ( $\tau_c$  is the cirrus optical thickness; see also list of symbols)



*Figure 3.28.* Error in atmospheric correction at 443 nm, as a function of  $\theta_s$ , and for the viewing geometries indicated.



Upper 2 panels : standard case, *i.e.*, no perturbation of the stratosphere. Middle panels : a layer of thin cirrus clouds is introduced between altitudes 10 and 12 km, with  $\tau_c = 0.05$ . Lower two panels :  $\tau_c$  is now 0.1.

The results are displayed in Fig. 3.27 (upper panel), and show that the Monte Carlo technique, despite the inevitable averaging over photon counters, can reproduce most of the features of the primary scattering by cirrus. The peak in the backward direction (rainbow) is a little smoothed, and the double peak in the forward direction (halo) is reduced to a unique peak in the Monte Carlo results. This last result, however, is of no importance, precisely because these peaks scatter in a small angular domain around the forward direction; the involved radiation correspond to the region of maximum sun glint which is anyway discarded when performing the atmospheric correction. A few simulations have been therefore carried out, with a cirrus layer introduced in the standard atmospheric profile between altitudes 10 and 12 km, and for several cirrus optical thicknesses. The impact on the  $[\rho_{\text{path}} / \rho_{\text{r}, \tau a=0}]$  versus  $\tau_a$  relationship is displayed on Fig. 3.27. It seems that the algorithm will be perturbed by the presence of cirrus clouds, as soon as their optical thickness is greater than about 0.05. This is confirmed on Fig. 3.28, where errors of the atmospheric correction at 443 nm are displayed for  $\tau_c = 0.05$  and 0.1. Therefore, a test should be developed, in view of indicating the presence of cirrus clouds, and a correction possibly performed before entering the atmospheric correction. This kind of procedure could be problematic to implement (e.g., see Gordon et al., 1997).

### 3.1.1.7. Ancillary data and aerosol climatology

#### 3.1.1.7.1 Ancillary data : identification and accuracy requirements

The ancillary data needed to perform the atmospheric correction are listed in Table 3.5, along with the reflectance or transmission term(s) that they influence.

#### Extraterrestrial irradiance

The extraterrestrial mean irradiance is taken from the level 1b output.

#### Wind speed at the sea level

This parameter could be accessed through the meteorological and weather forecast centers (*e.g.*, the European Center for Meteorological and Weather Forecast in Readings, ECMWF), or from wind scatterometer measurements. The typical accuracy attached to wind speed is of about 2 m s<sup>-1</sup>. Wind speed is expected to be attached with the input level 1B product (note that wind direction is also needed if it is considered in the definition of the sun glint flag).

#### Atmospheric pressure at the sea level

From the results in 3.1.1.6.2, it seems that about 5-10 mbars could be a reasonable accuracy for the atmospheric pressure. This parameter could be accessed through the meteorological and





weather forecast centers (e.g., ECMWF). Atmospheric pressure is expected to be attached with the input level 1B product.

# Total ozone amount

An accuracy of about 10-20 mAtm-cm (Dobson Units, DU) is a reasonable goal for the total ozone amount of the atmosphere. This parameter could be accessed from the measurements of a Total Ozone Mapping Spectrometer (TOMS). By default, climatological values have to be used. No information is needed about other absorbing gases (H<sub>2</sub>0, O<sub>2</sub>...), because the channels used in the atmospheric correction do not overlap the absorption bands of these gases (if corrections would be needed, however, they would be carried out before entering into the atmospheric correction). Ozone is expected to be attached with the input level 1B product.

# Relative humidity

The relative humidity is not required to operate the algorithm, yet it could provide a useful constraint (or verification) on the aerosol model identification. This parameter could be accessed through the meteorological and weather forecast centers (*e.g.*, ECMWF).

Ancillary data	Affected term(s)
Extraterrestrial irradiance $E_s(\lambda)$	$L_{\text{path}}(\lambda) \longrightarrow \rho_{\text{path}}(\lambda)$
Wind speed at the sea level	$ \rho_{\rm r, \ \tau a=0}(\lambda) $ (also $\rho_{\rm G}(\lambda)$ and $\rho_{\rm wc}(\lambda)$ ) not studied here
Atmospheric pressure at the sea level	$ \rho_{\mathrm{r,}\tau\mathrm{a}=0}(\lambda),\mathrm{t_d}(\lambda) $
Total ozone amount	$ \rho_{\rm r,  7a=0}(\lambda),  {\rm t_d}(\lambda) $
Relative humidity	Aerosol identification

### Table 3.5 : Ancillary data

## 3.1.1.7.2 Aerosol climatology

The use of an aerosol climatology could prove to be useful, in order to avoid totally irrelevant aerosols selections. Regional or global distributions of aerosol types and aerosol optical thickness have been indeed recently generated, either from AVHRR historical observations (e.g., Husar *et al.*, 1997; Stowe *et al.*, 1997; mapping of optical thickness), or from METEOSAT observations (Moulin *et al.*, 1997; mapping of Saharan dust), or from Nimbus-7 TOMS observations (Herman *et al.*, 1997; mapping of UV-absorbing aerosols). Compiling these data, probably along with new data from POLDER, OCTS, and SeaWiFS, could help in generating a tentative aerosol climatology, which would indicate, for instance, the probability of encountering desert dust or other absorbing aerosols. This kind of information, along with a plausible range for optical thickness and for the Ångström exponent, could be defined on a monthly basis and on a regular spatial grid (1°x1° for instance). It would be used to check the aerosol selection made by the algorithm, and then to indicate if this





selection seems realistic or not. This climatology could also be updated as MERIS data are processed.

# 3.1.1.8. Remaining issues

# 3.1.1.8.1. Bidirectionality of the oceanic reflectance and the diffuse transmittance

Yang and Gordon (1997) state that the diffuse transmittance from the pixel to the TOA level is different (by up to 5%) if computed either for a uniform water-leaving radiance distribution, or for a distribution that account for the anisotropic character of the radiance field emerging from the ocean (even for a uniform scene, where all pixels have the same chlorophyll concentration).

# 3.1.1.8.2. The "mixing ratio"

One of the assumptions on which the proposed algorithm relies is : for an aerosol A, bracketed by aerosols A1 and A2 in the near-IR following a "mixing ratio" (called here X) defined by the multiple aerosol scattering terms  $[\rho_{\text{path}} / \rho_{r, \tau a=0}]$ , X remains valid for the visible wavelengths. X actually slightly changes from the near-IR to the visible domain, and this is the main origin of the error in atmospheric correction (when the aerosol type is correctly identified). The possibility of estimating the change in X with wavelength remains to be examined.

## 3.1.2. Mathematical description of the algorithm

The following options are assumed here :

- Atmospheric pressure	: known
	A standard value of 1013.25 hPa has been used when
	generating the lookup tables $[\rho_{\text{path}}(\lambda) / \rho_{\text{r},\tau a=0}(\lambda)]$ versus $\tau_a$
- Wind speed	: known. Two values were considered when generating the
	lookup tables $[\rho_{\text{path}}(\lambda) / \rho_{r,\tau a=0}(\lambda)]$ versus $\tau_a$ .

The following algorithm description concerns clear sky pixels located out of the sun glint area, without whitecaps, and for Case 1 waters. The signals (total radiances) are assumed to be corrected for gaseous absorption, if any (including water vapor, ozone, and oxygen).

The 11 wavelengths are : 412, 443, 490, 510, 560, 620, 665, 681.25, 705, 775, 865 nm.

When operating the atmospheric correction for a given pixel (*i.e.*, for a geometry,  $\theta_s$ ,  $\theta_v$ ,  $\Delta \phi$ ), the successive steps are as follows (angular dependencies are omitted for the sake of clarity, except when needed in peculiar cases):

•0 Input data are taken from the level 1b :





- Total radiance at the instrument entrance for all wavelengths  $(L_t(\lambda))$
- Ancillary data (Wind speed, Atmospheric Pressure, Ozone)
- Geometry ( $\theta_{\rm S}, \theta_{\rm V}, \Delta \phi$ )

•1 Transform total radiance at the sensor level into total reflectance (Eq. (1).

For  $\lambda = 412, 443, 490, 510, 560, 620, 665, 681.25, 705, 775, 865$  nm.

External data :  $\mu_s$ ,  $E_s(\lambda)$ 

•2 Correct the Rayleigh reflectances for possible pressure variations (only for passing them on to the "Case 2 Bright waters flag"):

The Rayleigh reflectance,  $\rho_{r,\tau a=0}(\lambda, \theta_s, \theta_v, \Delta\phi, W)_{TAB}$ , is interpolated within a lookup table for the geometry in question, and then corrected to account for the actual value of the atmospheric pressure, P (only for wavelengths 705, 775, and 865 nm)

$$\rho_{r, \tau a=0}(\lambda) = \rho_{r, \tau a=0}(\lambda)_{TAB} \frac{\left[1 - \exp(-\tau_{r} (P / P_{0}) / \mu)\right]}{\left[1 - \exp(-\tau_{r} / \mu)\right]}$$
(30)

where  $\tau_r$  is the Rayleigh optical thickness at P<sub>0</sub>, and P<sub>0</sub> is 1013.25 hPa, and  $\mu$  is  $\cos(\theta_v)$ .

•3 At 705, 775 and 865 nm,  $\rho_{r, \tau a=0}$  is subtracted from the total reflectance, and the results are passed on to the "Case 2 bright waters flag" and "Case 2 bright waters atmospheric correction" algorithms (ATBDs 2.5 and 2.6). If these schemes return values for the water-leaving reflectances that are not zero, then they are subtracted from the total (path) reflectances (in the 3 channels here considered), before entering the Case 1 waters atmospheric correction.

External data : look-up table of  $\rho_{r,\tau a=0}(\lambda, \theta_s, \theta_v, \Delta\phi, W)$ , W, and P

•4 The ratio  $[\rho_{\text{path}}(\lambda) / \rho_{\text{r,}\tau a=0}(\lambda)]$  (thereafter referred to as  $\Delta \rho_{\text{path}}$ ) is formed at 775 and 865 nm. The values of  $\rho_{\text{path}}$  at 775 and 865 nm have been previously corrected for atmospheric pressure changes, if their actual values are different by at least 5 hPa from the standard value (1013.25 hPa). The correction is done following

$$\rho_{\text{path}} = \rho_{\text{path}} \quad \left(1 + \left(\Delta P / P\right) \eta_{\text{r}}\right) \tag{31}$$

with  $\Delta P = (P_{standard} - P_{actual})$ , and  $\eta_r = \tau_r / (\tau_r + \tau_a)$ . The Rayleigh optical thickness,  $\tau_r$ , is taken from tabulated values, and the aerosol optical thickness,  $\tau_a$ , is taken from the pixels previously processed.

$$\Delta \rho_{\text{path}}(865) = \rho_{\text{path}}(865) / \rho_{\text{r}, \tau a=0}(865)$$
(32)





$$\Delta \rho_{\text{path}}(775) = \rho_{\text{path}}(775) / \rho_{\text{r}, \tau a=0}(775)$$
(32')

where  $\rho_{r, \tau a=0}(775)$  and  $\rho_{r, \tau a=0}(865)$  are for the standard pressure.

•5 For the N aerosol models of the "standard" database (index i), carry out the calculation of  $\tau_a(865)_i$ :

$$\tau_{a}(865)_{i} = \text{func}_{i}(\Delta \rho_{\text{path}}(865)_{i}), i = 1, N$$
 (33)

where func<sub>i</sub> is the relationship between  $\Delta \rho_{\text{path}}$  and  $\tau_a$ , for aerosol model i, for wavelength 865 nm, and interpolated for the geometry in question. This function is a polynomial expression of degree 2, so that 3 coefficients have to be interpolated.

External data : look-up table of func<sub>i</sub>(A,  $\lambda$ ,  $\theta_{s}$ ,  $\theta_{v}$ ,  $\Delta \phi$ , W)

•6 calculate the N values of  $\tau_a(775)_i$ , from the N values of  $\tau_a(865)_i$ , by using the tabulated ratios  $c(775)_i / c(865)_i$  (thereafter referred to as  $\Delta c$ )

$$\tau_{a}(775)_{i} = \tau_{a}(865)_{i} \times \Delta c(775)_{i} i = 1, N$$
(34)

*External data : look-up table of*  $\Delta c(A, \lambda)$ 

•7 For the N aerosol models, carry out the calculation of  $\Delta \rho_{\text{path}}(775)$ 

$$\Delta \rho_{\text{path}}(775)_{i} = \text{func}^{-1}_{i}(\tau_{a}(775)_{i}), i = 1, N$$
(35)

External data : look-up table of func<sub>i</sub>(A,  $\lambda$ ,  $\theta_{s}$ ,  $\theta_{v}$ ,  $\Delta \phi$ )

•8 Select the 2 aerosol models (indices i1 and i2 within the N models) that most closely bracket the actual one, so that :

$$\Delta \rho_{\text{path}}(775)_{i1} < \Delta \rho_{\text{path}}(775)_{\text{actual}} < \Delta \rho_{\text{path}}(775)_{i2}$$
(36)

where  $\Delta \rho_{\text{path}}(775)_{i1}$  is the maximum of the  $\Delta \rho_{\text{path}}$  values that are lower than  $\Delta \rho_{\text{path}}(775)_{\text{actual}}$ , and where  $\Delta \rho_{\text{path}}(775)_{i2}$  is the minimum of the  $\Delta \rho_{\text{path}}$  values that are greater than  $\Delta \rho_{\text{path}}(775)_{\text{actual}}$ .

The aerosol optical thickness at 865 nm is now computed as :

$$\tau_a(865) = \left(\tau_a(865)_{i1} + \tau_a(865)_{i2}\right) / 2 \tag{37}$$

•9 Calculate X, the "mixing ratio", needed to interpolate between the two candidate aerosols





$$X = (\Delta \rho_{\text{path}}(775)_{\text{actual}} \quad \Delta \rho_{\text{path}}(775)_{i1}) / (\Delta \rho_{\text{path}}(775)_{i2} - \Delta \rho_{\text{path}}(775)_{i1})$$
(38)

•10 Carry out the test at 510 and 705 nm :

 $\tau_{a}(510)_{i1} = \tau_{a}(865)_{i1} \times \varDelta c(510)_{i1}$ (39)

$$\tau_a(510)_{i2} = \tau_a(865)_{i2} \times \Delta c(510)_{i2}$$
(39')

$$\Delta \rho_{\text{path}}(510)_{i1} = \text{func}^{-1}{}_{i1}(\tau_a(510)_{i1}) \tag{40}$$

$$\Delta \rho_{\text{path}}(510)_{i2} = \text{func}^{-1}{}_{i2}(\tau_a(510)_{i2}) \tag{40'}$$

$$\Delta \rho_{\text{path}}(510)_{\text{estimated}} = (1 - X) \,\Delta \rho_{\text{path}}(510)_{i1} + X \,\Delta \rho_{\text{path}}(510)_{i2} \tag{41}$$

Then : 
$$\rho_{\text{path}}(510)_{\text{estimated}} = \Delta \rho_{\text{path}}(510)_{\text{estimated}} \ge \rho_{\text{r}, \tau a=0}(510)$$
 (42)

The mean normalized water-leaving reflectance at 510 nm,  $[\overline{\rho_w(510)}]_N$ , is "de-normalized":

$$\rho_{\rm w}(510) = \left[\overline{\rho_{\rm w}(510)}\right]_{\rm N} \left(\varepsilon_{\rm c} \ t_{\theta_{\rm s}}\right) \frac{\Re(\theta')}{\Re_0} \frac{f_1(\theta_{\rm s})}{Q(\theta_{\rm s},\theta_{\rm v},\Delta\phi)} \left[\frac{f_{1,0}(\lambda)}{Q_0(\lambda)}\right]^{-1}$$
(43)

The error in atmospheric correction at 510 nm is therefore obtained as :

$$\Delta \rho(510) = \left[ \left( \rho_{\rm t}(510)_{\rm measured} - \rho_{\rm path}(510)_{\rm estimated} \right) / t_{\rm d}(510) \right] - \rho_{\rm w}(510)$$
(44)

If  $\Delta \rho(510)$  is > 2.5 10<sup>-3</sup>, then the test is again carried out, with  $\rho_w(510)$  increased by 3 10<sup>-3</sup>. If  $\Delta \rho(510)$  is < 2.5 10<sup>-3</sup>, then the test is again carried out, with  $\rho_w(510)$  decreased by 3 10<sup>-3</sup>.

The flag at 510 nm is set to 1 is both tests indicate the presence of absorbing aerosols.

The error in the atmospheric correction at 705 nm is more simply obtained as :

$$\Delta \rho(705) = \rho_{\rm t}(705)_{\rm measured} - \rho_{\rm path}(705)_{\rm estimated}$$
(45)

The flag at 705 nm is raised if the absolute value of  $\Delta \rho(705)$  is > 1.5 10<sup>-3</sup>

The final value of the flag for absorbing aerosols is obtained as :

If both flags (510 and 705) are silent : no absorbing aerosols If at least one flag (either 510 or 705 nm) has been raised : presence of absorbing aerosols.

If the flag has not been raised, then the correction is continued at step •11, by using the couple of aerosol models selected at step •8, and the "mixing ratio" calculated at step •9.




If the flag has been raised, then the correction is carried out five times more, from step 5 to step 9, by selecting other sets of aerosol models. When the relevant groups of aerosol models have been examined, each one providing a couple of possible models, the couple that is retained at the end is the one that leads to the lower  $\Delta \rho_{\rm W}(510)$ . Notice however that, if this final  $\Delta \rho_{\rm W}(510)$  is too large (this is possible if the tests are erroneous), the situation is reset to that of non-absorbing aerosols.

•11 For any wavelength  $\lambda$  in the visible, calculate the 2 values  $\tau_a(\lambda)_{i1}$  and  $\tau_a(\lambda)_{i2}$ , from  $\tau_a(865)_{i1}$  and  $\tau_a(865)_{i2}$ , by using the tabulated ratios  $\Delta c(\lambda)_{i1}$  and  $\Delta c(\lambda)_{i2}$ 

$$\tau_{a}(\lambda)_{i1} = \tau_{a}(865)_{i1} \times \Delta c(\lambda)_{i1}$$
(46)

$$\tau_{a}(\lambda)_{i2} = \tau_{a}(865)_{i2} \times \Delta c(\lambda)_{i2}$$
(46')

*External data : look-up table of*  $\Delta c(A, \lambda)$ 

•12 For the aerosols i1 and i2, carry out the calculation of  $\Delta \rho_{\text{path}}(\lambda)$  for the visible wavelengths :

$$\Delta \rho_{\text{path}}(\lambda)_{i1} = \text{func}^{-1}{}_{i1}(\tau_a(\lambda)_{i1})$$
(47)

$$\Delta \rho_{\text{path}}(\lambda)_{i2} = \text{func}^{-1}{}_{i2}(\tau_a(\lambda)_{i2}) \tag{47'}$$

External data : look-up table of func<sub>i</sub>(A,  $\lambda$ ,  $\theta_s$ ,  $\theta_v$ ,  $\Delta \phi$ )

•13 For any wavelength of the visible domain, calculate :

$$\Delta \rho_{\text{path}}(\lambda)_{\text{estimated}} = (1 - X) \,\Delta \rho_{\text{path}}(\lambda)_{i1} + X \,\Delta \rho_{\text{path}}(\lambda)_{i2} \tag{48}$$

$$\rho_{\text{path}}(\lambda)_{\text{estimated}} = \Delta \rho_{\text{path}}(\lambda) \ge \rho_{\text{r},\tau a=0}(\lambda)$$
(49)

If necessary (*i.e.*, 
$$\Delta P > 5$$
 hPa):  $\rho_{\text{path}}(\lambda)_{\text{estimated}} = \rho_{\text{path}}(\lambda)_{\text{estimated}} (1 + (\Delta P/P)\eta_r)$  (49')  
Where  $\Delta P$  is now ( $P_{\text{octual}} - P_{\text{standard}}$ )

$$t_{d}(\lambda, \theta_{v})\rho_{w}(\lambda) = \rho_{t}(\lambda)_{\text{measured}} - \rho_{\text{path}}(\lambda)_{\text{estimated}}$$
(50)

•14 Finally  $[t_d(\lambda, \theta_v)\rho_W(\lambda)]$  is transformed into  $[t_d(\lambda, \theta_v) L_w(\lambda)]$  (square brackets are used here to indicate that the two terms  $t_d$  and  $\rho_W$  are not separately obtained; the reflectance which is obtained at the end of step 13 is nevertheless equal to this product),  $t_d(\lambda, \theta_v)$  is computed, and the radiance needed to enter the bio-optical algorithms is obtained:

$$[t_{d}(\lambda, \theta_{v})L_{w}(\lambda)] = [t_{d}(\lambda, \theta_{v})\rho_{W}(\lambda)] E_{s} \mu_{s} / \pi$$
(51)

$$\omega_{a}(\lambda) = (\omega_{a}(\lambda)_{i1} + \omega_{a}(\lambda)_{i2}) / 2$$
(52)

$$F_a = (F_a(865)_{i1} + F_a(865)_{i2}) / 2 (F_a \text{ is nearly wavelength independent})$$
(53)





$$t_{d}(\lambda, \theta_{v}) = \exp\left(-\frac{\tau_{oz} + (1 - \varpi_{A} F_{A})\tau_{A} + 0.5\tau_{R}}{\mu}\right) \text{ (see 3.1.1.4.4 for details)}$$
(54)

$$L_{w}(\lambda) = [t_{d}(\lambda, \theta_{v})L_{w}(\lambda)] / t_{d}(\lambda, \theta_{v})$$
(55)

External data :  $E_s(\lambda)$ ,  $\theta_s$ ,  $\theta_v$ , ,  $\tau_r(\lambda)$ ,  $\tau_{oz}(\lambda)$ ,  $\tau_a(\lambda)$ ,  $\omega_a(\lambda)$ ,  $F_a$ 

#### 3.1.3. Error budget estimates

#### 3.1.3.1. Are the aerosol models representative of reality ?

The main assumption upon which the present atmospheric correction scheme relies is that the aerosol models used here are good approximations of the actual aerosols over the oceans; therefore they can be used as inputs of simulations of the radiative transfer in the atmosphere, the results of which being used to generate lookup tables. In principle, this assumption should be valid; the aerosol models used here have been generated after many measurements of aerosol chemical and optical properties, with the aim of defining models as representative as possible of reality. Recent measurements (Schwindling, 1995) of the aerosol optical properties (phase function and spectral optical thickness) have shown for instance that the Shettle and Fenn (1979) aerosol models fairly represent actual aerosols over the Western American coasts. The natural environment is however so variable that a question immediately arises : what kind of improvement the use of an inevitably restricted set of aerosol models brings (restricted as compared to reality) ? In other words : does it help to dispose of a database generated for, say, 30 aerosol models, while hundreds of different aerosol types or aerosol assemblages are possibly encountered over the ocean (even if admittedly they should be similar to those of the database) ?

From the various tests of the algorithm, and also from the results of the sensitivity studies concerning the vertical distribution of aerosols, the answer seems to be positive. In a way, the lookup tables "capture" the essential features of possible aerosol spectral dependencies; as a consequence, when the actual aerosol type or the actual aerosol vertical distribution are not "present" within the database, the correction remains possible, and a reasonable accuracy is preserved. The selected couple of aerosol models is sometimes however unrealistic (this is one of the justifications for using an aerosol climatology).

As a conclusion, the present atmospheric correction should works well, to the extent that we have now some indications that the aerosol models used here are close to reality. It is nevertheless impossible to be fully assertive on this point before the operational use of the algorithm. This observation led us to incorporate the single scattering algorithm into the whole scheme, as a basic and secure "bottom level" algorithm.

3.1.3.2. Other possible error sources 3.1.3.2.1. Aerosol model identification / Correctness of the test at 510 nm





In principle, the tests at 510 and 705 nm ensure that the selected aerosol model is not too different from the actual aerosol : during one step of the correction, if the selected model is totally unrealistic, the error of the atmospheric correction at 510 nm will be large enough to prevent its definitive selection. Ambiguities may subsist, however : for instance a couple of aerosol models can be selected because it is the one which leads to the minimal error at 510 nm, while the similar spectral behavior of this couple of models and of the actual one is fortuitous. This kind of confusion is possible, for instance between a dry maritime aerosol and the mixture of particles of continental origin with a wet maritime aerosol.

#### 3.1.3.2.2. Interpolation within LUTs

The tests of the algorithm presented in this document, as well as the sensitivity analyses, have been carried out with the exact geometry (*i.e.*, the angles  $\theta_s$ ,  $\theta_v$ , and  $\Delta \phi$  selected to test the algorithm correspond to entries of the lookup tables). The linear interpolations that will be necessary during the operational use of the algorithm (because the actual values of  $\theta_s$ ,  $\theta_v$ , and  $\Delta \phi$  will be always intermediate between the entries of the lookup tables) should not introduce significant inaccuracies, provided that each entry of the lookup tables has been adequately sampled. Multiple linear interpolations should recover the exact values at ±0.5% at the maximum, and even much less in many cases.

To meet this requirement, the sampling of the lookup tables indices should of ~5° for  $\theta_s$  and  $\theta_v$ , and of ~7.5° for  $\Delta \phi$  (see MERIS "Table Generation Requirement Document", TGRD, sections 3.6 and 5.6).

#### 3.1.3.2.3. Estimation of the diffuse transmittance, $t_d(\theta_v, \lambda)$

In section 3.1.1.4.4 (computation of  $t_d(\theta_v, \lambda)$ ), it was precised that neighboring effects (adjacent pixels with marked chlorophyll steps), or even the effect of the bidirectionality of the oceanic diffuse reflectance (for a homogeneous scene) were not accounted for. More importantly, it should be reminded that Eq. (17) is valid under the assumption of single scattering, that is when Rayleigh scattering and aerosol scattering are uncoupled (Gordon and Morel, 1983).

Recently, Yang and Gordon (1997) stated that  $t_d(\theta_v, \lambda)$  is not identical if computed either for a uniform water-leaving radiance distribution, or for a distribution that account for the anisotropic character of the radiance field emerging from the ocean (the difference reaching 5%, even for a uniform scene, where all pixels have the same chlorophyll concentration).







**Figure 3.29**. Values of the water-leaving reflectance,  $\rho_W(0^+)$ , and of the "marine reflectance",  $t_d(\theta_v)$ .  $\rho_W$  (TOA), at 560 nm, as a function of the satellite viewing angle, and within the principal plane and perpendicular half plane (left and right panels, respectively).

The sun zenith angle is 35°. Upper and lower panels are respectively for the urban aerosol with RH=80% (absorbing), and for the maritime aerosol with RH=80% (non-absorbing). The dashed and solid lines are, respectively, the values of  $\rho_W(0^+)$  and of  $t_d(\theta_V)$ .  $\rho_W$  (TOA) as obtained via Monte Carlo simulations. The dotted line is the value of  $\rho_W(0^+)$  multiplied by an estimated value of  $t_d(\theta_V)$ . The relative difference between the 2 curves is shown as percents (solid curve on the upper plots of each panel). The dotted lines correspond to a calculation of  $t_d(\theta_V)$  ignoring the effect of aerosols. The conditions are :  $\tau_a = 0.3$  at 550 nm, (Chl) = 0.3 mg m<sup>-3</sup>.





From the above remarks, the ability of Eq. (17) to provide accurate estimates of  $t_d(\theta_v, \lambda)$  is challenged, at least when the turbidity of the atmosphere becomes moderately high. No attempt has been made here to examine possible improvements of Eq. (17). A few calculations have been however carried out, to assess the accuracy to which  $t_d(\theta_v, \lambda)$  can be derived. Monte Carlo simulations have been done, providing simultaneously the values of the water-leaving reflectance,  $\rho_w(0^+)$ , and of the "marine reflectance", which represents the product  $[t_d(\theta_v, \lambda), \rho_w(0^+)]$  at the TOA level.

This estimate of the marine reflectance is then compared to the product  $\rho_w(0^+)$ .  $t_d(\theta_v,\lambda)$ , where the transmittance is computed from Eq. (17), and by using the exact values for optical thicknesses ( $\tau_r$ ,  $\tau_{oz}$ ,  $\tau_a$ ), single scattering albedo ( $\omega_a$ ) and aerosol forward scattering probability (F<sub>a</sub>). Results are given in Fig. 3.29, for two aerosols (the absorbing urban aerosol, and the non-absorbing maritime aerosol, both with RH = 80%), for  $\lambda = 560$  nm, for  $\tau_a = 0.3$  at 550 nm, and for (Chl) = 0.3 mg m<sup>-3</sup>. This figure shows that for a non-absorbing aerosol,  $t_d(\theta_v,\lambda)$  is given within 5% by Eq. (17), and is given within 10% for an absorbing aerosol. The dotted lines in each upper plots, and for each aerosol, correspond to the same relative difference as above, when aerosols, however, are not considered in Eq. (17). Inaccuracies in the parameters of Eq. (17) would even lead to greater errors. Note also that the results presented here are not independent of the adopted angular discretisation. Indeed, as the elementary field of view tends to an infinitesimal point, the diffuse transmittance  $t_d$  tends toward the direct transmittance,  $T = e^{-\tau/\mu} (e.g., Gordon and Morel, 1983)$ .

Clearly, Eq. (17) is not sufficiently precise to preserve the required accuracy for the waterleaving radiances. The development of a more accurate parameterization of  $t_d(\theta_v, \lambda)$  seems inevitable. It is out of the scope of the present ATBD, and is therefore part of the studies that remain to be carried out.

#### 3.1.3.2.4. Uncertainties in the ozone concentration

This section has been deleted, and just kept here for keeping numbering of the document.

#### 3.1.3.2.5. The effect of whitecaps

Whitecaps mainly tend to uniformly increase reflectance in the whole visible-to-near-IR spectrum (*e.g.*, Koepke, 1984), and this effect could alter the atmospheric correction. The Monte Carlo code presently used does not allow the whitecap reflectance to be separately and specifically studied. Therefore, simple tests are carried out here, by adding to total TOA reflectance, as obtained through our simulations, an additional contribution due to whitecaps, as extracted from the outputs of the 6S model (Vermotte *et al.*, 1994). Two parallel simulations are then carried out for the same conditions, except that only the 6S model accounts for the possible occurrence of whitecaps for high wind speeds and of their contribution to the total radiance at the sensor level.

The additional whitecap reflectance is added to the total reflectance, and the atmospheric correction is carried out following three approaches

(1) the classical algorithm is operated to examine the error in the retrieved water-leaving radiances when the whitecaps contribution is ignored,





- (2) a correction for whitecaps reflectance is introduced (see below), and operated with the exact wind speed, and
- (3) the same correction is made with an incorrect value for the wind speed. These two last tests aim at examining the possibility of correcting the whitecaps contribution, and, if proven to be possible, to get an idea about the accuracy needed for wind speed.



Figure 3.30. Reflectance of whitecaps as a function of wind speed (Koepke, 1984).

The 6S model has been run for a wind speed of 15 m s<sup>-1</sup> (about 30 knots), which ensures that whitecaps actually occur and also that visible remote sensing remains possible. The maritime and continental aerosol models used in the 6S model have been selected to run the simulations with optical thicknesses of 0.1 and 0.3 at 560 nm. The correction for whitecaps used in tests (2) and (3) defined above is based on the definitions of Koepke (1984). The whitecaps reflectance,  $\rho_{wc}(\lambda)$ , is (the following expression is used in the 6S model) :

$$P_{\text{path}} = \text{stimate} + (\underline{P} + \underline{P})\eta$$
(56)

where ws is wind speed, and the bracketed expression is the relative area covered by whitecaps.  $\rho_{ef}(\lambda)$  is the effective ocean foam reflectance (accounting for variations in the area and reflectance of individual whitecaps), which is constant (0.22 ±0.11). The change in  $\rho_{wc}(\lambda)$  with wind speed is shown in Fig. 3.30.

The whitecaps reflectance is then multiplied by the diffuse transmittance (without accounting for the transmittance due to scattering and absorption by aerosols), and added to the total reflectance at the TOA level obtained without whitecaps (but with the same wind speed).

So, if the correction for whitecaps is needed, their reflectance, as computed from the above expression, is multiplied by the diffuse transmittance and subtracted from the total radiances before entering the algorithm. The results of the three tests are displayed in Fig. 3.31. When the aerosol scattering is almost independent of wavelength (6S maritime aerosol), ignoring or incorrectly correcting for whitecaps does not lead to serious errors in the retrieved marine reflectances (whitecaps are "seen" as an additional aerosol load). Most of the curves in each of the 4 upper plots of Fig. 3.31 remain between  $\pm 0.002$ . The correction made when the exact wind speed is known is





obviously the more accurate (and its accuracy is about the same than that of the classical algorithm operated over an ocean without foam); it is however out of reach to exactly know the wind speed when operating the routine algorithms.



443 nm (6S maritime aerosol)

**Figure 3.31.** Error in top of atmosphere water-leaving reflectance as a function of the Sun zenith angle  $\theta_s$ . Four upper plots : simulations have been carried out for the 6S maritime model, with  $\tau_a(560) = 0.1$  or 0.3, as indicated. Two lower plots : simulations have been carried out for the 6S continental model, with  $\tau_a(560) = 0.3$ . On each plot, the open circles linked by a dashed line are the results of the correction without whitecaps; the dotted line shows the error  $\Delta \rho$  when the whitecaps contribution is ignored; the dashed line shows the error when the correction for whitecaps is applied with the exact wind speed (15 m s<sup>-1</sup>); the two solid lines show the error when this correction is





applied for an inexact wind speed (*i.e.*, 10 or 17 m s<sup>-1</sup>). Plots on the left (right) column are for viewing at the scan edge (scan center).

In summary, correction for whitecaps should not be attempted for aerosols with small Ångström exponents (< 0.1) (see Gordon and Wang, 1994a; Gordon, 1997). The situation is worse when the aerosol scattering is strongly changing with wavelength (6S continental aerosol) : whitecaps cannot be only "seen" as an additional aerosol load, and produce an apparent, erroneous, spectral behavior for aerosols (the selection of the 2 candidate aerosols can be affected). If whitecaps are ignored, the error in marine radiances becomes too high. The tentative whitecaps correction, as described above, as well is not satisfactory (except for the unrealistic situation of an exact knowledge of wind speed), and can even lead to greater errors than those obtained in absence of whitecaps correction if wind speed is overestimated by only 2 m s<sup>-1</sup>. A more precise algorithm for whitecaps correction is clearly needed (but see Gordon and Wang, 1994b; Gordon, 1997). For the present time, a flag could be introduced, only to indicate that wind actually was blowing during image acquisition, and that whitecaps probably were present.

The present tests have been carried out for a wind speed of 15 m s<sup>-1</sup>, *i.e.*, for  $\rho_{wc}$  about 8-9 10<sup>-3</sup>. The correction could be much more problematic for higher wind speed, when  $\rho_{wc}$  can reach 2-3 10<sup>-2</sup>. The extent to which atmospheric correction remains possible in such conditions is unknown at present time.

The above tests and comments are based on the assumption that the whitecaps reflectance is wavelength-independent. Recent measurements (Frouin *et al.*, 1996) on the contrary show a significant decrease of this reflectance in the near-IR, say beyond 800 nm (and so could concern the channel at 865 nm). The impact on the atmospheric correction of this decrease has not been addressed here (but see Gordon and Wang, 1994a; Gordon, 1997).

#### 3.1.3.2.6. Instrumental errors. 1. : stray light

Instrumental errors (*i.e.*, errors in the instrument calibration) are not a priori predictable. It is therefore impossible to carry out an exhaustive sensitivity analysis about their effect on the accuracy of the atmospheric correction. The sensitivity analyses carried out in the previous sections partly cover the topic here addressed : the spectrally dependent "errors" induced by changes in various environmental factors, as previously examined, could be assimilated to calibration errors, providing then a first quantitative insight into the response of the atmospheric correction to inappropriate calibration of the instrument. The problem actually is more complex, because the sign of calibration errors can change between channels. The loss of accuracy in the atmospheric correction can be anticipated as being more important in this case than when all errors are either positive or negative. A more complete quantification of this problem is provided in section 3.1.3.2.7 below).

A peculiar "instrumental error" originates from straylight in the instrument optics (due to first order scattering events and also to "ghost images"). A first attempt to assess the impact of the additional irradiance due to straylight on the atmospheric correction process is made here, by increasing by a few percents the simulated radiances that would be recorded in absence of instrumental errors (the straylight is proportional to the measured radiance). The increase is not



neutral, and is greater in the near-IR channels than in the visible ones. Percentages of increase, taken from a study of straylight in the MERIS instrument, are 2.3, 2.7 and 3.2% for the wavelengths 410, 620 and 865 nm, respectively. They have been obtained for a homogeneous ocean scene. These values are linearly interpolated for the other wavelengths. The radiances simulated here for the maritime aerosol model with humidity ratios of 70, 80, and 99% are increased following these percentages, and they are introduced in the atmospheric correction procedure. The errors obtained at the end of the correction are shown on Fig. 3.32 (to be compared with Fig. 3.7 for instance). 443 nm (Maritime aerosol, RH = 70, 80, 99%)



**Figure 3.32.** Error in the retrieved top of atmosphere water leaving reflectance at 443 nm, when straylight is added to the "infield" radiance (i.e., the radiance that would be measured in absence of straylight). The solid, dotted, and dashed lines are for the maritime aerosol model, with RH = 70, 80, and 99%, respectively, and with  $\tau(550) = 0.3$ . Results are displayed as a function of the solar zenith angle, either for viewing at the scan edge (left) or at the scan center (right).

The results in Fig. 3.32 show that, over a homogeneous ocean scene, the impact of straylight is not so critical (the  $\Delta \rho$  are due to an apparent spectral variation in the near-IR that is not the actual one). Furthermore, as the gain adjustment would implicitly incorporate the effect of straylight, the spectral variations of the measured radiances could be unchanged, with no impact on the atmospheric correction. The problem is by far more critical over cloudy areas (*e.g.*, small clouds scattered within an ocean scene). The ratio of straylight to in-field radiance can reach 0.5 in such conditions, at a distance of 20 pixels from the cloud edge. Clearly, the atmospheric correction will fail in that case. If straylight cannot be corrected before entering the pixel processing, a distance  $\zeta$  will have to be defined, in terms of a number of pixels from the cloud edge, to discard those pixels which are closer than  $\zeta$  from a cloud edge (note that a correction for straylight is included in the MERIS processing).

#### 3.1.3.2.7. Instrumental errors. 2. : calibration errors

Calibration errors are a second possible source of error in the atmospheric correction and retrieval of the pigment index and atmospheric properties. The comprehensive calibration procedure that is planned for MERIS should provide TOA reflectances with a radiometric accuracy of 2-4%, relative to the sun (Rast and Bézy, 1995). It is as well conceivable that larger errors may occur in some instances. The impact of such errors cannot be fully assessed, precisely because the "pattern" of these calibration errors can vary (it is not predictable), for instance with positive and negative errors randomly distributed among bands, or errors systematically positive or negative for all bands, or for





only a subset of bands, etc... Therefore, only a few situations, presumably representative of possible error combinations, have been examined here. They are similar to those examined by Gordon (1997), while the absolute values of the errors are set to little larger values when they are of opposite signs. The atmospheric correction algorithm is therefore applied to TOA reflectances that are calculated as :

$$\rho_{t}' = \rho_{t} \left( 1 + \alpha(\lambda) \right) \tag{57}$$

where  $\rho_t$  is the "true" TOA reflectance (*i.e.*, the reflectance obtained through the Monte Carlo simulations),  $\alpha(\lambda)$  is the wavelength-dependent calibration error, and  $\rho_t$ " would be accordingly the erroneously registered TOA reflectance. The atmospheric correction errors at 443 nm are displayed in Fig. 3.33, for the maritime aerosol (RH = 85%) when  $\tau_a(550) = 0.1$ , and for the 5 following error combinations :

 $\alpha(\lambda) = 0$  in all bands (reference case)

$$\alpha(443) = 0, \ \alpha(775) = 0.05, \ \alpha(865) = 0.05$$
  
 $\alpha(443) = 0.05, \ \alpha(775) = 0.05, \ \alpha(865) = 0.05$   
 $\alpha(443) = 0, \ \alpha(775) = 0.05, \ \alpha(865) = 0.05$ 

A degradation of the atmospheric correction accuracy obviously occurs when the  $\alpha(\lambda)$  errors are not all zeros, and especially when all errors are +5% at all wavelengths. In all other situations examined, this degradation remains however reasonable (only a few points are outside the ±0.002 limit). It is also less than that obtained by Gordon (1997), who showed errors around ±0.004-0.005 (*i.e.*, at least twice the errors for  $\alpha(\lambda) = 0$  in all bands).

With the present algorithm, which uses the ratio  $[\rho_{\text{path}} / \rho_{\text{r}, \tau a=0}]$ , a relative error  $\alpha$  on  $\rho_{\text{path}}$  directly results in a relative error  $\alpha$  in  $[\rho_{\text{path}} / \rho_{\text{r}, \tau a=0}]$ . With an algorithm based on the  $[\rho_{\text{path}} - \rho_{\text{r}, \tau a=0}]$  difference, the relative error  $\alpha$  on  $\rho_{\text{path}}$  becomes  $\alpha$  ( $\rho_{\text{path}} / [\rho_{\text{path}} - \rho_{\text{r}, \tau a=0}]$ ). The ratio  $(\rho_{\text{path}} / [\rho_{\text{path}} - \rho_{\text{r}, \tau a=0}])$  decreases as the aerosol optical thickness increases. For the wavelength 865 nm, and for  $\theta_{\text{s}} = 60^{\circ}$ ,  $\theta_{\text{v}} = 37^{\circ}$ , and  $\Delta \phi = \pi/2$ , this ratio is 2.56 when  $\tau_{\text{a}} = 0.03$ , 1.76 when  $\tau_{\text{a}} = 0.1$ , 1.28 when  $\tau_{\text{a}} = 0.3$ , and 1.17 when  $\tau_{\text{a}} = 0.5$ . Therefore, in the case of clear maritime atmospheres (*i.e.*,  $\tau_{\text{a}}$  about 0.1), the present algorithm would be twice less sensitive to calibration errors than is an algorithm based on the [ $\rho_{\text{path}} - \rho_{\text{r}, \tau a=0}$ ] difference.







Figure 3.33. Error in the retrieved TOA water leaving reflectance at 443 nm, for the reference case (no calibration errors; upper 2 panels), and for several combinations of calibration errors (see text).Results are displayed as a function of the solar zenith angle, either for viewing at the scan edge (right) or at the scan center (left).



#### 3.1.3.2.8. Residual sun glint

A test, and the associated flag, is planned to identify the sun glint pattern over the ocean (see MERIS ATBD 2.13). This test is based on the Cox and Munk's model (1954) for the distribution of wave slopes, and makes use of a threshold reflectance, above which the pixel is considered as contaminated by sun glint (to be confirmed); this pixel is not further processed. For some pixels that are not identified by this test, the TOA reflectance may still contain a residual sun glint effect (*i.e.*, some photons directly transmitted through the atmosphere, before and after their reflection on a wave facet).



**Figure 3.34**. Panel (a) and panel (b) : ratio of the glint reflectance,  $\rho_G$  (Eq. 29'), to the path reflectance,  $\rho_{path}$ , at 865 nm, and as a function of the viewing angle.

The geometry corresponds to a MERIS scan at 45° north, for an acquisition at the vernal equinox (a), or at the summer solstice (b). Panel (c) and panel (d) : for the geometries in (a) and (b), error in the atmospheric correction at 443 nm, when (1) the actual interface is flat ( $\sigma = 0$ , reference case; solid lines), (2) the interface is roughened, with a wind speed of 7.5 m s<sup>-1</sup> ( $\sigma = 0.2$ ), and the glint reflectance as been calculated exactly, and removed from  $\rho_t$  before entering into the algorithm (dotted lines), and (3) as in (2), whereas the glint reflectance has not been calculated and is therefore not removed from  $\rho_t$  (dashed lines). Note that the lookup tables for  $\rho_r$  and  $[\rho_{path} / \rho_r]$  are for  $\sigma = 0$  in any case.





The sensitivity study to wind speed (surface roughness; section 3.1.1.6.4) assumed that the sun glint reflectance,  $\rho_{\rm G}$ , was correctly estimated, and subtracted from the total reflectance before applying the atmospheric correction. This step is mandatory to the extent that the relationships [ $\rho_{\text{path}}$ /  $\rho_{r,\tau a=0}$ ] versus  $\tau_a$  are deeply modified if they are actually estimated with  $\rho_t$  (i.e.,  $\rho_{path}$  plus a non identified contribution of  $\rho_{\rm G}$ ) instead of  $\rho_{\rm path}$  (dashed line in Fig. 3.23). Even with an exact knowledge of wind speed, existing models cannot actually provide an accurate value of  $\rho_{\rm G}$  in the area of maximum sun glint  $(\Delta \phi \sim \pi, \theta_v \sim \theta_s)$ . The reflectance  $\rho_G$  is there much greater than the path reflectance (see Fig. 3.34, panels (a) and (b)), so that no attempt to perform the correction will be made within this area. For some other geometries, around the maximum sun glint, the TOA total reflectance may still contain some photons directly transmitted through the atmosphere before and after reflection on a wave facet ("residual sun glint";  $\rho_{G}$  is then less than an half of  $\rho_{path}$ ). If the value of  $\rho_{\rm G}$  for these geometries is not calculable accurately, it should be nevertheless computed, at least in view of identifying those pixels possibly affected by specular reflection. The identification could rely on a threshold, either on  $\rho_{\rm G}$  (e.g., Gordon 1997), or on the ratio  $\rho_{\rm G}$  /  $\rho_{\rm path}$  (to be defined). For these pixels, atmospheric correction either would not be performed, or would be carried out and a flag raised. Note finally that ignoring the effect of shadowing on the sun glint pattern, as done in the present work, can only lead to significant errors for grazing viewing direction and sun illumination (simultaneous large  $\theta_s$  and large  $\theta_v$  values), and  $\Delta \phi$  around  $\pi$ ; this geometrical configuration, where  $\rho_{\rm G}$  anyway becomes small, actually does not occur along a MERIS track.

When atmospheric correction is applied to TOA reflectances simulated over a rough ocean ( $\sigma = 0.2$ , corresponding to a wind speed of 7.5 m s<sup>-1</sup>), and if these reflectances have been corrected for the exact value of  $\rho_{\rm G}$ , the results remain correct (*i.e.*,  $\Delta \rho$ (443) within ±0.002) even when lookup tables generated for  $\sigma = 0$  are used (dotted lines in Fig. 3.34, panels (c) and (d)). If  $\rho_{\rm G}$  is not corrected, then atmospheric correction totally fails actually as soon as  $\rho_{\rm G}$  > about 0.0002 (dashed lines in Fig. 3.34; panels (c) and (d)). The conclusions are (1) at least 2 set of lookup tables ([ $\rho_{\rm path} / \rho_{\rm r, \tau a=0}$ ] *versus*  $\tau_{\rm a}$ ) have to be generated, for 2 values of the wind speed, (2) the glint reflectance has to be calculated as exactly as possible, and removed from the TOA reflectance before entering the algorithm.

#### 3.1.3.2.9. Gaseous absorption

When presenting the "detailed mathematical model" (section 3.1.2), the signals (total radiances) were assumed to be corrected for gaseous absorption, if any. Indeed, these absorption are not accounted for when generating lookup tables. In principle, the MERIS channels used for atmospheric correction over Case 1 waters and the pigment index retrieval are exempt from significant gaseous absorptions. The only source of error could originate from neglecting the possible, yet uncertain, effect of the  $H_20$  continuum.



3.1.3.2.10. Non-identified Case 2 waters

The architecture of the MERIS ground segment includes tests dedicated to the identification of Case 2 waters. It is conceivable, however, that in some instances these tests fail in discriminating between Case 1 and Case 2 waters; in such situations, pixels erroneously flagged as Case 1 waters may go through the present algorithm, with expected drawbacks in the processing. This possible cause of failure of the algorithm is examined below.



Figure 3.35. normalized water-leaving reflectances at 510 nm, for oceanic Case 1 waters ( $a_y(440)=0$ ), and for yellow substance dominated Case 2 waters (curves for  $a_y(440) \neq 0$ ). The shaded area correspond to  $\pm 1\sigma$  of [ $\rho_w$ ]<sub>N</sub>(510) when  $a_v(440) = 0$  (see section 3.1.1.4.2 and Fig. 3.3).

#### Case 2 waters dominated by yellow substance

In principle, yellow-substance-dominated Case 2 waters should not lead to any error in atmospheric correction, because the assumption of a black ocean remains valid when an additional absorption (with respect to that of water and phytoplankton) occurs within the water body. The problem lies in the test that is carried out at 510 nm (identification of aerosol absorption), and which is based on a constant value of the normalized water-leaving reflectance at 510 nm; this value of  $[\rho_w]_N(510)$  (1 10<sup>-2</sup>) is only valid for Case 1 waters. When yellow substance actually absorbs, the value of  $[\rho_w]_N(510)$  obviously decreases from its value for Case 1 waters (see Fig. 3.35). The consequence is that yellow substance absorption will be erroneously identified as aerosol absorption. Tests have been performed, where absorption by yellow substance is calculated as (Sathyendranath *et al.*, 1989) :

$$a_{v}(\lambda) = a_{v}(440) e^{-.014(\lambda - 440)}$$
(58)

where  $a_y$  is the absorption coefficient of yellow substance, whose value at 440 nm is, somewhat arbitrarily, fixed to values of 0.1, 0.2, 0.5, 2, and 5 m<sup>-1</sup>. The results of atmospheric correction over yellow substance dominated Case 2 waters are presented in Fig. 3.36, for the maritime aerosol model



(RH = 85%), and  $\tau_a = 0.1$  at 550 nm. The threshold in  $a_y(440)$ , above which atmospheric correction fails because of an erroneous aerosol selection, seems to be around 0.5 m<sup>-1</sup> (*i.e.*, a reasonably high value)



*Figure 3.36.* Error in the retrieved top of atmosphere water leaving reflectance at 443 nm, for the reference case (no yellow substance; dotted lines), and for several values of a<sub>v</sub>(440)

 $(0.1 \text{ and } 0.2 \text{ m}^{-1}, \text{ dotted lines}; 0.5 \text{ m}^{-1}, \text{ yellow line; } 1 \text{ m}^{-1}, \text{ green line})$ . Results are displayed either as a function of the solar zenith angle (upper 2 panels), or as a function of the viewing angle (lower 2 panels).

#### Case 2 waters dominated by suspended matter (sediment) scattering

A test is planned for identifying sediment-dominated Case 2 waters (MERIS ATBD 2.5 : Case 2 turbid water flag, and MERIS ATBD 2.6 : Case 2 (sediment) bright water atmospheric correction). The behavior of the atmospheric correction is examined now, in the case where sediment-dominated Case 2 waters are non-identified and actually observed. The idea is the same as for yellow-substance-dominated Case 2 waters : what is the threshold, here in terms of additional scattering, above which the "Case 1 atmospheric correction" fails. Tests have been performed, where sediment scattering is calculated as (sediments are supposed to be non absorbing particles) :

$$b_{x}(\lambda) = b_{x}(550) \ (\lambda \ / \ 550)^{-n}$$
(59)

where  $b_x(550)$  is the scattering coefficient at 550 nm, and n characterizes the spectral dependency of sediment scattering.  $b_x(550)$  is computed as the product  $[b_x^*(550) \text{ SPM}]$ , where  $b_x^*(550)$  is the specific scattering coefficient of sediments (set to 0.008 m<sup>2</sup> mg<sup>-1</sup>), and SPM is the sediment concentration in mg m<sup>-3</sup>. The concentration SPM has been fixed to values of 0, 0.003, 0.03, 0.1, 0.3,



1, 3, and 10 g m<sup>-3</sup>. The exponent n is set to 0.812, in correspondence with a particle size distribution following a Junge distribution with m = 4, a size range of 0.45 to 20  $\mu$ m, and a refractive index of 1.15. The backscattering ratio, as derived from the particle phase function calculated (MIE theory) with the parameters above, is equal to 1.4%.



*Figure 3.37.* Error in the retrieved top of atmosphere water leaving reflectance at 443 nm, for the reference case (no additional scattering; dotted lines), and for several values of SPM (see text) namely SPM = 0.003 g m<sup>-3</sup> (depp blue curve), 0.03, 0.1, and 0.3 g m<sup>-3</sup> (yellow curve), and 1 and 3 g m<sup>-3</sup> (light blue curve).

namely SPM =  $0.003 \text{ g m}^{-3}$  (depp blue curve), 0.03, 0.1, and  $0.3 \text{ g m}^{-3}$  (yellow curve), and 1 and 3 g m}^{-3} (light blue curve). Results are displayed either as a function of the solar zenith angle (upper 2 panels), or as a function of the viewing angle (lower 2 panels).

In the near infrared, where the effect of phytoplankton on the water-leaving radiance is null, this radiance is calculated as :

$$\rho_{\rm w}(\lambda,\theta,\phi) = \mathcal{E}_{\rm d}(0^+)(\lambda) \quad \Re(\theta) \quad \frac{f_1}{Q}(\lambda,\theta,\phi) \quad \frac{\mathbf{b}_{\rm b}(\lambda)}{\mathbf{a}(\lambda)} \tag{60}$$

where  $b_b(\lambda)$  is the sum of the backscattering coefficients of water itself plus the sediments,  $a(\lambda)$  is absorption by water only, and the  $(f_1/Q)$  ratio, calculated for Case 1 waters, is nevertheless used (for lack of anything else). This last point is not really important when our only aim is to get an idea of the threshold in water-leaving reflectance (in the near infrared) above which atmospheric correction fails (whatever the relevance of the relationship between this water-leaving reflectance and the sediment load).



In the visible, the bio-optical model that we used is the model for Case 1 waters, and the additional backscattering due to sediments is simply added to the backscattering of phytoplankton and water.

Atmospheric correction has been applied to TOA reflectances simulated for these sedimentdominated Case 2 waters, and the results are shown in Fig. 3.37. The same errors in the retrieved marine reflectances are obtained for SPM concentrations of 0.03, 0.1, and 0.3 g m<sup>-3</sup>, and also for concentrations of 1 and 3 g m<sup>-3</sup>. The error in the aerosol selection are indeed identical for several SPM concentrations, because the impact of the additional marine signal in the near infrared evolves in steps. It was not expected that, in some instances, the accuracy of the correction remains acceptable with SPM = 1 g m<sup>-3</sup>. This result indicates, however, that the Case 2 turbid water flag (ATBD 2.5) will be useful if it triggers off for SPM concentrations around 0.3-0.5 g m<sup>-3</sup> (*i.e.*, about 5 10<sup>-4</sup> to 2 10<sup>-3</sup> in terms of reflectance at 865 nm, and about 1.5 10<sup>-3</sup> to 5 10<sup>-3</sup> in terms of reflectance at 775 nm).

#### 3.1.3.2.11. Polarization

The issue of polarization does not interfere with the present development of the atmospheric correction for MERIS. The total and Rayleigh radiances will be changed if polarization is included in the systematic radiative transfer simulations, so that the lookup tables will not contain the same numerical values. The principle of the algorithm and its operation remain however unchanged either with or without including polarization in the simulations. The question of including or not polarization actually is close to that concerning the choice of a method (code) to carry out the systematic simulations (final implementation of the algorithm). A comparison has been made between Rayleigh radiances computed by taking into account polarization (Gordon et al., 1988) : the "Exact Radiative Transfer Equation" is used, where the radiance is replaced by a column vector containing the Stokes parameters describing the state of polarization of the light), and the Rayleigh radiances computed with the Monte Carlo code presently used (without polarization). Differences are observed between the radiances generated by these 2 codes, of a few percent (2-5%), sometimes up to 10%. This preliminary test indicates that polarization should be taken into account (even if MERIS is not sensitive to polarization, the measured radiances can change with polarization). Following Gordon (1997), however, the slight gain in accuracy resulting from the use of the vector theory in computing the lookup tables ([ $\rho_{\text{path}} / \rho_{r,\tau a=0}$ ] versus  $\tau_a$ ]) would be really small, as regards the considerable computational cost when accounting for polarization.

#### 3.1.3.3. Expected global accuracy

Considering the tests and sensitivity studies carried out and presented in this ATBD, the expected global accuracy of the algorithm should be within  $\pm 0.002$  in reflectance; this is slightly greater than the required accuracy (see section 2.3). Errors exceeding this threshold will occur in some cases, corresponding to extreme situations examined here.





#### **3.2. Practical considerations**

#### 3.2.1. Lookup tables

The implementation of a final algorithm (including the generation of complete look-up tables) remains to be carried out. For the present time, suffice it to say that the simulations carried out for the present study will not serve for this purpose. A new set of simulations has to be defined, with an increase in discretisation with respect to geometry. Furthermore, the code to be used to achieve these computations still remains to be selected (see in the TGRD document).

Attention has also to be paid to the storage requirements, which should remain reasonable to allow the algorithm to function properly on various processing platforms.

If the reading of lookup tables and the storage of results is not accounted for, the present implementation can process about 1300 pixels per second on a commonly available workstation (HP 9000, K200 series), when no tests are performed at 510 and 705 nm. When the tests are performed and the aerosol is not absorbing (*i.e.*, probably the most common situation), the number of pixels processed per second is about 1200. When the tests are performed and the aerosol is systematically absorbing, the rate becomes 300 pixels per second. The storage requirement for lookup tables would not exceed 50 Mega bytes for the final algorithm implementation.

3.2.1.1. List of Lookup tables, dimensions, sampling, size

## N.B. : (1) Several tables, of minor importance (or at least of minor interest), are not listed below.

## (2) The indexing and sampling given below are indicative. The numbers given below will change in the final implementation.

3.2.1.1.1 - TOA reflectance for an aerosol-free atmosphere ( $\rho_{r,\tau a=0}$ )

The table contains the values of the TOA reflectance for an aerosol-free atmosphere ( $\rho_{r, \tau a=0}$ ), as computed for various illumination conditions, wavelengths, zenith and azimuth angles, a standard atmospheric pressure (1013.25 hPa), a standard total ozone amount (350 DU), and two wind speeds, namely 0 and 7.5 m s<sup>-1</sup>, corresponding to  $\sigma = 0.055$  and 0.2, respectively (Cox and Munk's model (1954) for the wave slope distribution). Sampling :

	-	
λ	:	11 MERIS channels (412, 443, 490, 510, 560, 620, 665, 681.25, 705, 775, 865)
$\theta_{\rm s}$	:	14 (from 15 to $80^\circ$ , with increment $5^\circ$ )
$\theta_{\rm v}$	:	10 (from 0 to $45^{\circ}$ , with increment $5^{\circ}$ )
$\Delta \phi$	:	25 (from 0 to 180, with increment $7.5^{\circ}$ )
Wind speed	:	2

This table will be generated through radiative transfer computations.

3.2.1.1.2 - TOA total reflectances (Intermediate table)





The table contains the values of the TOA total reflectance for atmospheres with varying aerosol types and aerosol loads, as computed for various illumination conditions, wavelengths, zenith and azimuth angles, a standard atmospheric pressure (1013.25 hPa), a standard total ozone amount (350 DU), and two wind speeds (0 and 7.5 m s<sup>-1</sup>, corresponding to  $\sigma = 0.055$  and 0.2, respectively). Sampling :

Aerosol	:	32
$ au_{\mathrm{a}}$	:	5 values
λ	:	11 MERIS channels (412, 443, 490, 510, 560, 620, 665, 681.25, 705, 775, 865)
$\theta_{\rm s}$	:	14 (from 15 to $80^\circ$ , with increment $5^\circ$ )
$\theta_{ m v}$	:	10 (from 0 to $45^{\circ}$ , with increment $5^{\circ}$ )
$\varDelta \phi$	:	25 (from 0 to 180, with increment $7.5^{\circ}$ )
Wind speed	:	2

This table will be generated through radiative transfer computations.

# 3.2.1.1.3. - the three coefficients of the quadratic relationship between ( $\rho_{path}$ / $\rho_{r,\tau a=0}$ ) and $\tau_a$

This table contains the 3 coefficients of the second order polynomial representing the relationship between the relative increase in the path reflectance (from an aerosol-free atmosphere to an atmosphere containing a given amount of aerosols) and the total aerosol optical thickness ( $\tau_a$ ). The coefficients are stored for several values of (i) aerosol model, (ii) wavelength, (iii) geometry (sun zenith angle, viewing angle, and azimutal difference), (iv) wind speed. The coefficients are obtained by fitting five points to a second-order polynomial. Four of these points are obtained from simulations for 4 values of the aerosol optical thickness, and the fifth one is simply (0,1), corresponding to a ratio of 1 for an aerosol-free atmosphere. Sampling :

Aerosol	:	32
λ	:	11 MERIS channels (as for the Rayleigh Table).
$\theta_{\rm s}$	:	14
$\theta_{\rm v} \ge \Delta \phi$	:	10 x 14 (= 140)
W	:	2

Method to extract values from the tables : multiple linear interpolations

## 3.2.1.1.4 - The spectral optical thicknesses for various aerosols, normalized to $\lambda = 865 \text{ nm}$ (Operational table)

This table contains the aerosol spectral optical thicknesses for the N assemblages of aerosols, and normalized at 865 nm. The extinction (absorption + scattering) coefficients are computed via the Mie theory, as a function of the aerosol size distribution and refractive index. The spectral optical thicknesses are given for four nominal values at 550 nm (this is necessary because the proportion of various aerosol models in each assemblage is defined at this wavelength, and may become different at other wavelengths, depending on the spectral characteristics of each aerosol model. The spectral





change in optical thickness of a given assemblage is therefore dependent on the optical thickness specified at 550 nm).

Aerosol	:	32
λ	:	10 MERIS channels (865 being useless here)
$ au_{a}$	:	5 values

#### 3.2.1.2. Possibilities for reducing data storage

Concerning the  $(\rho_{\text{path}} / \rho_{\text{r},\tau a=0})$  versus  $\tau_a$  lookup table, a solution for reducing storage is to expand the coefficients of this relationship in Fourier series in  $\Delta \phi$ , and store the Fourier coefficients (Gordon, 1997). We found, however, that the gain in disk storage, even if significant (about a factor of 2), results, when using these tables, in a significant increase in computational time. Therefore, we decided to store the coefficients themselves, and to abandon the Fourier expansions. Note that the  $(\rho_{\text{path}} / \rho_{\text{r},\tau a=0})$  versus  $\tau_a$  relationship is used in both "directions", meaning that sometimes the ratio is calculated from  $\tau_a$ , while in other cases  $\tau_a$  is inferred from the ratio. The relationship is only stored for one of these two possibilities (*i.e.*, coefficients to calculate ( $\rho_{\text{path}} / \rho_{\text{r},\tau a=0}$ ) from  $\tau_a$ ), and the coefficients are inverted through simple mathematical methods when necessary.

#### **3.2.2.** Calibration and validation

Before the routine operation of the instrument, the MERIS system simulator (MERSS; in a future release, including the present atmospheric correction algorithm), as well as the MERIS ground segment prototype, will be used to explore the response of the atmospheric correction scheme when various situations are faced (regarding either the environment or the instrument itself).

It is also planned to carry out tentative atmospheric correction of SeaWiFS data. Such tests require, however, that the lookup tables are adapted to the position and spectral width of the MERIS channels. These tests will form the first assessment of the performance of the algorithm presented in this ATBD. Preliminary results are presented in section 5 of this ATBD.

When the instrument will be in flight : joint measurements of water-leaving radiances, auxiliary data, and of aerosol properties could help in calibrating the algorithm-plus-instrument system. Such experiments remain to be defined. The calibration/validation operations are critical for the success of the MERIS mission, as for any other color sensor; they cover a wide range of *in situ* measurements, and would justify by themselves a specific ATBD (*e.g.*, see Clark *et al.*, 1997; Kishino *et al.*, 1997). They are not the scope of the present ATBD.

An integrated project, including all necessary measurements, and whose central part is the development of an optical buoy and its deployment in the Mediterranean sea, has been prepared and submitted to ESA and other funding agencies and administrative entities. This project, called "BOUSSOLE", would allow a permanent monitoring of the MERIS instrument and algorithms, in order to ensure the generation of a coherent and reliable long-term global data base of ocean color.

#### **3.2.4.** Exception handling





Criteria are to be defined, with the corresponding flags, to identify the pixels for which the atmospheric correction has failed, or has been carried out in non-optimal conditions. The following are proposed :

- (1) The "CZCS like" algorithm has been used.
- (2) The tests at 510 and 705 nm were not performed.
- (3) The atmospheric pressure value has been taken from a climatology.
- (4) The total ozone amount value has been taken from a climatology.
- (5) Wind speed was greater than  $20 \text{ m s}^{-1}$ .
- (6) Correction for stratospheric aerosols has been carried out.
- (7) The selection of the aerosol model is in contradiction with the climatology.
- (8) Absorbing aerosols have been detected.
- (9) The actual aerosol is out from the extreme aerosols of the LUTs.
- (10) The aerosol mixing ratio was equal to 1.
- (11) The aerosol optical thickness is greater than 0.6.
- (12) The atmospheric correction has been actually carried out over Case 2 bright waters.
- (13) The minimum absolute value of  $\Delta \rho 510$  was greater than 2.5 10<sup>-3</sup>.
- (14) Total reflectances at the TOA level were out of possible values.
- (15) The sun zenith angle was greater than  $70^{\circ}$ .
- (16) Negative water-leaving radiances have been derived.

#### 3.2.5. Outputs of the atmospheric correction

The outputs of the atmospheric correction will be

- (1) the water-leaving reflectances in the MERIS bands 1 to 8, for cloud-free pixels (the water-leaving reflectances are not a MERIS product, but an intermediate quantity needed to derive the pigment index, which is the MERIS product)
- (2) the aerosol optical thickness at 865 nm
- (3) information about the two "bracketing" aerosol models
- (4) flag(s) indicating the level of confidence of the atmospheric correction (see section 3.2.4)

Note that from the knowledge of the aerosol models, the aerosol optical thickness can be calculated at any wavelength from its value at 865 nm.

### 4. Assumptions, constraints, and limitations

#### **4.1.** Assumptions

• The aerosol models used in the simulations (to generate the lookup tables) are assumed to be good approximations of the actual aerosols over the oceans. This point has been discussed in 3.1.3 (Error budget estimates).





- The "mixing ratio" is wavelength-independent. This point has been discussed in section 3.1.1.8 (remaining issues).
- The oceanic diffuse reflectance at 510 nm is roughly constant whatever the chlorophyll concentration, and is equal to 2% (section 3.1.1.4.2).
- The TOA total reflectance in the visible is adequately represented by summing the atmospheric path reflectance, obtained through radiative transfer simulations over a black, Fresnel-reflecting, ocean, and the product t. $\rho_w$ , calculated independently (section 3.1.1.1).
- The plane-parallel atmosphere is a good approximation of the real atmosphere for radiative transfer simulations, at least when the remote sensing configuration is concerned (see Ding and Gordon, 1994).
- It has been assumed here that the algorithm is applied to TOA reflectances that have been previously corrected for gaseous absorption, if any (including ozone).

#### **4.2.** Constraints, limitations

- The algorithm is designed to be operated over Case 1 waters. Its application over coastal turbid Case 2 waters (in a situation where pixel classification would have failed) either would not be possible (abnormal results) or should produce artifactual high pigment concentrations, greater than the actual ones (see section 3.1.3.2.10).
- Problems could also be encountered over open ocean, when highly reflecting detached coccoliths are present (*e.g.*, Balch et al., 1989, 1991; Gordon and Balch, 1997), and more generally for any departure of the optical properties from those typical of Case 1 waters (if not identified).
- The algorithm obviously works over cloud free pixels, off the sun glint area (section 3.1.3.2.8).
- The algorithm development heavily relied upon aerosol models, radiative transfer models, as well as bio-optical models. The algorithm reliability is therefore connected to the quality of these models.





### 5. Test of the algorithms with SeaWiFS data

Specific LUTs have been generated for the peculiar set of bands and bandwidths of SeaWiFS (412, 443, 490, 510, 555, 670, all with 20 nm width, and 765, 865 with 40 nm width). Oxygen has been considered for the 765 nm band (*i.e.*, incorporated into the radiative transfer simulations to generate the LUTs), for an atmospheric pressure of 1013.25 hPa. When performing the atmospheric correction of real data, no correction is attempted if atmospheric pressure is significantly different from this standard value. The test for absorbing aerosols is obviously only performed at 510 nm since the 705 nm band is absent. There is no other significant modifications of the algorithm and of its implementation as compared to the nominal MERIS algorithms.

#### 5.1. General tests

#### 5.1.1. Data and procedures

Level 1B files have been generated from SeaWiFS level 1A files, by using the SeaDAS software package (SeaDAS v3.2). Calibrated radiances are then extracted from the level 1B (HDF format), along with geometrical and other required information, and then transformed into reflectances before being introduced into the MERIS breadboard prototype. Results are presented here as color plates (Appendix 3) and histograms of SeaWiFS and MERIS outputs. As such, the results of these tests only represent a "cross-validation", assuming that the SeaWiFS algorithms and products are fully validated (the commissioning phase of SeaWiFS has been completed around August 1998). The tests performed here deal with the retrieval of the normalized water-leaving radiances (Figs. 5.1, 5.2, and 5.6), of the aerosol optical thickness (Fig. 5.4), and of the chlorophyll concentration (Fig. 5.5). They have been performed on two scenes, acquired above the Mediterranean sea (7 may 1998, left panels on figures cited above; plate 1 in Appendix 3) and above the Mauritanian upwelling (5 march 1998, right panel on the figures; plate 2 in Appendix 3). Red and black curves correspond to the SeaWiFS and MERIS processing, respectively.

#### 5.1.2. Results

The mean value of the normalized water-leaving radiance at 550 nm,  $[L_w]_N$ , is 0.3 mW cm<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup> in clear Case 1 waters (Gordon and Clark, 1981). Both histograms (MERIS and SeaWiFS processing) are indeed centered around this value for the Mediterranean sea image (figure 5.1). The situation is totally different for the Mauritanian scene, where the SeaWiFS algorithm totally fails (over-correction) because of the presence of a significant amount of desert dust in the atmosphere (see also the next section and Appendix 2). In the same situation, the MERIS algorithm still function





well for about half the pixels ( $[L_w]_N$  about 0.3 mW cm<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup>), with, however, a second peak in the histogram with a mode at about 0.65 mW cm<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup>. This second mode corresponds to those pixels where atmospheric correction, even if completely performed, has been incapable of retrieving the marine signal correctly (too much aerosol in the atmosphere). At 443 nm (Fig. 5.2), the pattern in  $[L_w]_N$  is quite different for the Mediterranean scene, where the modes are about 1 and 1.5 for the SeaWiFS and MERIS processing, respectively. Considering the chlorophyll concentration in this image, around 0.1-0.2 mgChl m<sup>-3</sup>, the typical value of  $[L_w]_N$  should be within the range 0.8-1.6 mW cm<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup>, so that it is impossible to decide between both algorithms, except if we think that SeaWiFS is now sufficiently validated to provide the right answer (but see below). For the Mauritanian upwelling, the situation observed at 555 nm is reinforced, and still demonstrate that MERIS algorithms would be more effective than SeaWiFS algorithms in this case. Figure 5.3 shows the 443-to-555 radiance ratio corresponding to the radiances shown in Figs. 5.1 and 5.2.

Concerning the retrieval of  $\tau_a(865)$  (Fig. 5.4), the frequency distributions are quite similar for both algorithms, yet the MERIS processing allows higher  $\tau_a$  (865) values to be retrieved. This is due, in particular, to the detection of desert dust, and also to the difference in the aerosol LUTs.

For the retrieval of the chlorophyll concentration, an additional curve is displayed (in green; Fig. 5.5), which corresponds to the use of the SeaWiFS chlorophyll algorithm, when applied to the marine reflectances obtained with the MERIS atmospheric correction. For the Mauritanian region, the results only show that MERIS should be able to process more pixels than SeaWiFS does, because of the detection of desert dust. A problem that still remains, however, is the bad retrieval of the marine signal below the dust plume (see Plates 1 and 2, where the "images" of the dust plumes are obvious in the chlorophyll maps). For the Mediterranean sea, the results are in nearly perfect agreement (note, however, that this perfect agreement is somewhat fortuitous when considering the large differences in the retrieved values of the normalised water-leaving radiances; this is probably a strong argument in favour of the band ratio algorithms, which are at present time often criticised).

The comparison has been extended to spectra of  $[L_w]_N$ , and the results are shown in Fig. 5.6, for four pixels extracted from the image of the Mediterranean sea (plate 1). The solid red curves are the spectra of  $[L_w]_N$  obtained via the SeaWiFS processing (SeaDAS v3.2), and the solid black curves are the spectra obtained when the MERIS atmospheric correction is applied to the same SeaWiFS TOA reflectances. The dotted red and black curves are obtained via a reflectance model (Morel, 1988), which is fed with the chlorophyll concentration obtained through the SeaWiFS or MERIS algorithms, respectively. These modeled spectra are just an indication of what spectra should have been retrieved for "nominal" Case 1 waters with the same chlorophyll concentration; they should not be considered as the truth.





The clearest waters and atmospheres are found in the Sicily straight and East of the Balearic islands, with spectra typical of "blue waters". It seems that the shape of the spectra obtained via the MERIS atmospheric correction are closer to what is expected for Case 1 waters (*i.e.*, closer to the modeled spectra), even if the magnitude is different for the station located east of Balearic islands (but remind that the modeled spectra are not the truth). The spectra obtained by SeaWiFS exhibit a systematic decrease from 443 to 412 nm, which does not correspond to what is usually observed. The decrease even starts at 490 nm for waters with higher chlorophyll concentrations, as encountered at the 2 stations in the North Adriatic sea and in the gulf of Lion. In this case neither the SeaWiFS nor the MERIS processing provide the same values for  $[L_w]_N$  than the model (again, remind that these modelled spectra are not the truth), yet the shape of the spectra is still better with the MERIS processing. Note also that the values retrieved for  $[L_w]_N$  at 555 nm for the Adriatic station, if correct, are nearly at the limit between Case 1 and Case 2 waters.

#### 5.1.3. Conclusions

A true validation is only possible when parameters determined *in situ* are available. The present exercise with SeaWiFS data cannot provide definitive answers, because these data are themselves still unconfirmed, as demonstrated here by the relatively strange and unexpected shape of the radiance spectra. Nevertheless, the results shown in Figs. 5.1 to 5.6 are clearly satisfactory. The coherence between the spectra derived from the MERIS atmospheric correction and those computed from the Case 1 water model is a strong argument in favor of the MERIS algorithms, even if the inescapable refinements and tuning of the algorithms will have to be carried out after launch, during the commissioning phase.



*Figure 5.1* : Frequency distributions of the normalized water-leaving radiance at 555 nm, as obtained through the SeaWiFS processing (red curves) and the MERIS processing (black curves).

The left panel is for an image acquired above the Mediterranean sea on the 7<sup>th</sup> of may, 1998 (plate 1 in Appendix 3). The right panel is for an image acquired above the Mauritanian upwelling on the 5<sup>th</sup> of march, 1998 (plate 2 in Appendix 3). All pixels flagged in the SeaWiFS level 2 data (*i.e.*, land, clouds, and various failures of the algorithms) have been discarded from the analysis.



Figure 5.2 : As figure 5.1, but for the normalized water-leaving radiance at 443 nm.



*Figure 5.3* : As figure 5.1, but for the ratio of the normalized water-leaving radiance at 443 nm to the normalized water-leaving radiance at 555 nm (the "blue-to-green" ratio).



Figure 5.4 : As figure 5.1, but for the aerosol optical thickness at 865 nm.





The green curve, that was not drawn in the previous figures, corresponds to the computation of the chlorophyll concentration by using the pigment algorithm of the SeaWiFS project, when applied to the water-leaving radiances generated with the MERIS atmospheric corrections.





and as extracted from a SeaWiFS scene acquired over the Mediterranean sea (7 may 1998; plate 1). The solid red curves are the spectra of  $[L_w]_N$  obtained via the SeaWiFS processing (SeaDAS v3.2), and the solid black curves are the spectra obtained when the MERIS atmospheric correction is applied to SeaWiFS TOA reflectances. The dotted red and black curves are obtained via a reflectance model (Morel, 1988) which is fed with the chlorophyll concentration obtained through the SeaWiFS or MERIS algorithms, respectively (other information relevant to the calculation of  $[L_w]_N$  are also given on the figure).





#### 5.2. Tests dedicated to the detection of desert dusts

#### 5.2.1. Data and procedures

An important aspect of the MERIS atmospheric corrections is their ability to separately identify, at least in principle, several kinds of aerosols, among which the desert dust whose climatic and geo-chemical impact is well established, if not well quantified. Specific tests have been performed to test this peculiar point of the algorithms, by applying it to images of the Mediterranean sea and of the Mauritanian coasts, which are two regions where Saharan dust is often transported. Level 1A data have been examined, and some were selected when dust plumes, or at least what looks like a dust plume, were observed.

#### 5.2.2. Results

This study and its results are discussed in Appendix 2 (Paper presented at the Ocean Optics XIV conference (SPIE), Kailua Kona, Hawaii, 10-13 November 1998). They show that dust is well identified (as soon as  $\tau_a > 0.10$ ). There was no possibility, however, to validate the retrieved optical thickness (no ground measurements, and no other satellite providing similar measurements). It is also obvious that the water-leaving radiances are not well retrieved below the dust plumes, because (1) the marine signal is in this case less than 1% of the total so that it is illusory to retrieve it whatever the technique that may be used, (2) the dust model used in the algorithm is not enough representative of the actual dust. The "feeling" of the algorithm failure is even reinforced, when looking to an image of pigments, because the border of the plume is delineated by a band of underestimated concentrations : when approaching the plume, the algorithm more and more fails in retrieving the radiance spectrum (until the correct aerosol, *i.e.*, dust, is finally detected), resulting in an increasing underestimation of the blue-to-green ratio, hence a decrease of Chl. This degradation of the atmospheric correction was already pointed out in this ATBD (see section 3.1.1.5.4, Figs. 3.11 to 3.14). This problem is particularly difficult to deal with, because "desert aerosol experiences the largest variability of all aerosol types by virtue of its physical and optical properties" (D'Almeida et al., 1991). It is conceivable that future improvements of the MERIS algorithms incorporate at least 2 different kinds of desert aerosols, namely the Saharan and Asian dusts, or that we keep only one model, which would be improved in terms of optical properties, however. Accounting for the wind speed dependence of the dust properties could also be a possible way.





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## 7. Symbols

Symbol	definition	Dimension / units		
Geometry, wavelengths				
λ	Wavelength	nm		
$\theta_{\mathrm{s}}$	Sun zenith angle ( $\mu_{s} = \cos(\theta_{s})$ )	degrees		
$ heta_{ m v}$	Satellite viewing angle ( $\mu_v = \cos(\theta_v)$ )	degrees		
$arDelta \phi$	Azimuth difference between the sun-pixel and pixel-sensor	degrees		
	half vertical planes			
Atmospher	re and aerosol properties			
$F_0(\lambda)$	Mean extraterrestrial spectral irradiance	W m <sup>-2</sup> nm <sup>-1</sup>		
$\mathcal{E}_{c}$	Eccentricity of the Earth orbit	dimensionless		
$F_a(\lambda)$	Aerosol forward scattering probability	dimensionless		
$F_r(\lambda)$	Rayleigh forward scattering probability	dimensionless		
$ au_{\rm a}(\lambda)$	Optical thickness due to aerosol scattering	dimensionless		
$\tau_{\rm r}(\lambda)$	Optical thickness due to Rayleigh scattering	dimensionless		
$\eta_{ m r}$	Contribution of molecules to the total optical thickness	dimensionless		
	$(=\tau_{\rm r} / (\tau_{\rm r} + \tau_{\rm a}))$			
$\tau_{\rm ag}(\lambda)$	Optical thickness due to gaseous absorption	dimensionless		
$\varpi_{a}(\lambda)$	Aerosol single scattering albedo	dimensionless		
$\varpi_{\rm r}(\lambda)$	Rayleigh single scattering albedo	dimensionless		
$P_r(\lambda, \gamma)$	Rayleigh phase function	sr <sup>-1</sup>		
	$\mathbf{p}_{r}(\boldsymbol{\gamma} \pm) =  \mathbf{P}_{r}(\boldsymbol{\lambda}, \boldsymbol{\gamma} \pm) +  \left[ \boldsymbol{\rho}_{F}(\boldsymbol{\theta}_{s}) + \boldsymbol{\rho}_{F}(\boldsymbol{\theta}_{v}) \right] \mathbf{P}_{r}(\boldsymbol{\lambda}, \boldsymbol{\gamma} \pm)$			
	where $\gamma \pm$ is the scattering angle			
	$\cos(\gamma \pm) = \pm \cos(\theta_0) \cos(\theta_v) - \sin(\theta_0) \sin(\theta_v) \cos(\Delta \phi)$			
$P_a(\lambda, \gamma)$	Aerosol phase function	sr <sup>-1</sup>		
	$\mathbf{p}_{a}(\boldsymbol{\gamma} \pm) = \mathbf{P}_{a}(\boldsymbol{\lambda}, \boldsymbol{\gamma} \pm) + \left[ \boldsymbol{\rho}_{F}(\boldsymbol{\theta}_{s}) + \boldsymbol{\rho}_{F}(\boldsymbol{\theta}_{v}) \right] \mathbf{P}_{a}(\boldsymbol{\lambda}, \boldsymbol{\gamma} \pm)$			
V	Exponent of the Junge law for the distribution of aerosol	dimensionless		
	particles (sensitivity studies)			
$c(\lambda)$	Attenuation coefficient for wavelength $\lambda$	m <sup>-1</sup>		
$t_{\theta_s}(\lambda, \theta_s)$	Irradiance transmittance for a sun zenith angle $\theta_{\rm s}$	dimensionless		
	$t_{\theta_s}(\lambda, \theta_s) = E_d(0^+) / (\mu_s \varepsilon_c F_0)$ , where $E_d(0^+)$ is the			





	downwelling irradiance just above the sea surface	
$t_d(\lambda, \theta)$	Diffuse transmittance for angle $\theta$	dimensionless
	$t_{d}(\lambda, \theta) = L_{\text{TOA}}(\lambda, \theta_{s}, \theta_{v}, \Delta\phi) / L_{0+}(\lambda, \theta_{s}, \theta_{v}, \Delta\phi)$	
$L(\lambda, \theta_{s}, \theta_{v}, \Delta \phi)$	Radiance	W m <sup>-2</sup> nm <sup>-1</sup> sr <sup>-1</sup>
	Subscripts : TOA $\rightarrow$ top of atmosphere	
	$0^+ \rightarrow$ just above the sea surface	
	w for water-leaving radiance, just above the sea	a surface
	u for upwelling radiance, just below the sea sur	face
Р	Atmospheric pressure at sea level	hPa
RH	Relative humidity	percents
$\rho(\lambda, \theta_{\rm s}, \theta_{\rm v}, \Delta \phi)$	Reflectance $(\pi L / F_0 \mu_s)$	dimensionless
	where the product $\pi$ .L is the TOA upwelling irradiance if upwelling radiances are equal to $L(\lambda, \theta_s, \theta_v, \Delta \phi)$ for any values	of $\theta_{\rm v}$
	within $0 - \pi/2$ and any $\Delta \phi$ within $0 - 2\pi$ .	
	Subscripts t: total reflectance	
	w : water-leaving reflectance	
	path : path reflectance	
	r : Rayleigh reflectance	
	rs: Rayleigh reflectance (single scattering only)	
	a: aerosol reflectance	
	as: aerosol reflectance (single scattering only)	
	ra: heterogeneous aerosol-molecule scattering	
	G : sun glint reflectance	
	wc : whitecaps reflectance	
$\rho^*(\lambda, \theta_{\rm s}, \theta_{\rm v}, \Delta\phi)$	b)Reflectance within a compound atmosphere, containing molecu	ales dimensionless
	and aerosols (subscripts as for $\rho$ )	
$\varepsilon(\lambda_1,\lambda_2)$	Ratio $\rho_{\rm as}(\lambda_1) / \rho_{\rm as}(\lambda_2)$	dimensionless
$\varepsilon'(\lambda_1,\lambda_2)$	Ratio $[\rho_{\text{path}}(\lambda_1) - \rho_{\text{r}}(\lambda_1)] / [\rho_{\text{path}}(\lambda_2) - \rho_{\text{r}}(\lambda_2)]$	dimensionless
$f(\tau_{\rm a})$	Relationship between the ratio $[\rho_{\text{path}} / \rho_{\text{r}}]$ and $\tau_{\text{a}}$	dimensionless
Water prope	rties	
Chl	Chlorophyll concentration	mg m <sup>-3</sup>
$a(\lambda)$	Total absorption coefficient (due to water and algae)	m <sup>-1</sup>
$b_b(\lambda)$	Total backscattering coefficient (due to water and algae)	m <sup>-1</sup>
$\Lambda_{\lambda_1,\lambda_2}$	Ratio of $(b_b/a)$ at $\lambda_1$ to $(b_b/a)$ at $\lambda_2$	dimensionless




R( <i>λ</i> , 0⁻)	Diffuse reflectance of oceanic Case 1 waters, at null depth	dimensionless
f	Ratio of R(0 <sup>-</sup> ) to ( $b_b/a$ ); subscript 0 when $\theta_s = 0$	dimensionless
$Q(\lambda, \theta_{\rm s}, \theta_{\rm v}, \Delta \phi)$	b) Factor describing the bidirectional character of the	sr
	diffuse reflectance of oceanic Case 1 waters; subscript 0 when $\theta_s = \theta_v = 0$	
$[\rho_{\rm w}]_{\rm N}(\lambda)$	Normalised water-leaving reflectance (i.e., the reflectance if	
	there were no atmosphere, and for $\theta_{\rm s} = \theta_{\rm v} = 0$ )	dimensionless
Air-water in	terface	
$\Re( heta)$	Geometrical factor, accounting for all refraction and reflection	dimensionless
	effects at the air-sea interface (Morel and Gentili, 1996)	
	$\Re(\theta') = \left[\frac{(1-\overline{\rho})}{(1-\overline{r}R)} \frac{(1-\rho_{\rm F}(\theta'))}{n^2}\right] \text{ (subscript 0 when } \theta' = 0\text{)}$	
	where	
	n is the refractive index of water	dimensionless
	$\rho_{\rm F}(\theta)$ is the Fresnel reflection coefficient for incident angle $\theta$	dimensionless
	$\overline{\rho}$ is the mean reflection coefficient for the downwelling	dimensionless
	irradiance at the sea surface	
	$\overline{\mathbf{r}}$ is the average reflection for upwelling irradiance at the	dimensionless
	water-air interface	
	$\theta$ is the refracted viewing angle ( $\theta = \sin^{-1}(n.\sin(\theta_v))$ )	degrees
$\sigma$	Root-mean square of wave facet slopes	dimensionless
β	Angle between the local normal and the normal to a facet	
р	Probability density of surface slopes for the direction ( $\theta_s$ , $\theta_v$ , $\Delta \phi$ )	dimensionless
Miscellaneo	us	
W	Wind speed	dimensionless
Х	Aerosol mixing ratio defined on the basis of the [ $\rho_{\text{path}}$ / $\rho_{\text{r}}$ ] ratio	dimensionless
	At 775 nm.	





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# 8. Appendix 1 : paper published in *"Applied Optics"*, 34, 1998. Relative importances of multiple scattering by air molecules and aerosols in forming the atmospheric path radiance in the visible and near infrared parts of the spectrum.

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Abstract. Single and multiple scattering by molecules or atmospheric aerosols only (homogeneous scattering), and heterogeneous scattering by aerosols and molecules, are recorded in Monte Carlo simulations. It is shown that heterogeneous scattering (1) always significantly contributes to the path reflectance ( $\rho_{path}$ ), (2) is realized at the expense of homogeneous scattering, (3) decreases when aerosols are absorbing, and (4) introduces deviations in the spectral dependencies of reflectances as compared to the Rayleigh exponent and aerosol Ångström exponent. The ratio of  $\rho_{path}$  to the Rayleigh reflectance for an aerosolfree atmosphere is linearly related to the aerosol optical thickness. This result affords the basis of a new scheme for atmospheric correction of remotelysensed ocean color observations.

#### 1. Introduction

When correcting for atmospheric effects Earth observations taken from satellite sensors, or when inverting ground-based measurements of sky radiances, one must estimate the "path radiance", or the "path reflectance" if the following transformation is used (symbols and definitions in Table 1)

 $\rho(\lambda, \theta_{v}, \theta_{0}, \Delta\phi) = \pi L(\lambda, \theta_{v}, \theta_{0}, \Delta\phi) / F_{0}(\lambda) \cos(\theta_{0})$ 

Except if expressly needed, wavelength and angular dependencies will thereafter be omitted for clarity. In the case of a satellite sensor aiming at the ocean, the path radiance at the top of the atmosphere (TOA) originates from single and multiple scattering by molecules and aerosols, which affect photons traveling downward through the atmosphere and also photons traveling upward after they have been reflected at the air-water interface. Therefore, estimating the path radiance requires that the combined effects of aerosols and molecules on the radiative field are understood and assessed.

According to previously adopted assumptions, radiances due to Rayleigh and aerosol scattering are separable<sup>1</sup>, so that they would be calculable for single component atmospheres, and then summed up to simulate the path radiance. In this case, the determination of that part of the path radiance originating from molecular scattering (Rayleigh scattering) is easily dealt with, for only the illumination and observation conditions have to be known. In contrast, the numerical density of aerosol particles, their chemical nature and vertical distribution are greatly varying, so that they are *a priori* unknown in most situations. By assuming however that the radiance due to aerosol scattering is calculable (under some assumptions), the approach then consists in adding this radiance to the Rayleigh radiance (both being obtained for single component atmospheres), and finally in introducing a corrective term, which accounts for the non additive character of the radiances (which are apparent optical properties). This term is usually referred to as the "coupling term" between aerosol and molecule scattering, and involves heterogeneous multiple scattering. The attribute "heterogeneous" is used here to identify the molecule-particle scattering, as opposed to "homogeneous" molecule-molecule or aerosol-aerosol multiple scattering. In fact, the validity of the above approximations is not firmly established, mainly because the heterogeneous scattering, which necessarily occur in the atmosphere, has not been clearly studied. As far as we know, the creation of a flux resulting from multiple molecule-aerosol scattering events, the spatial rearrangement of the scattered flux, and the relative importance of multiple scattering when the aerosol load increases have not yet been thoroughly examined nor quantified. The study presented in this paper aims at filling this gap.

In the present work, Monte Carlo simulations have been carried out in compound (molecules plus aerosols), multilayered, atmospheres, so that all kinds and orders of scattering are considered. In addition, the code is provided with the capacity of keeping track of the photons, allowing the total radiance to be decomposed into three "partial radiances", corresponding to the contributions of (1) single and multiple scattering by molecules only (in presence of aerosols, however) (2) single and multiple scattering by aerosols only (in presence of molecules) and finally (3) heterogeneous scattering by both aerosols and molecules. The addition of these three "partial radiances" is strictly valid, contrary to the sum of radiances separately computed for single component atmospheres.

A detailed study of the three terms has been undertaken, allowing a better understanding of their changes in response to changes in (1) the vertical structure of the atmosphere, (2) the





aerosol optical thickness, and (3) the ratio of aerosol to total optical thicknesses. The partial radiances have been first examined for specific geometries, and then their contribution to the global flux assessed. The spectral dependencies of the three terms have been also analyzed and compared to the Rayleigh exponent and the aerosol Ängstrøm exponent. The impact of aerosol absorption on results obtained for nonabsorbing aerosols has been assessed. It is also shown that, for a given aerosol, the relative change of the path radiance in response to increasing aerosol optical thickness is monotonously and unambiguously related to the aerosol optical thickness. This results has been applied to the problem of atmospheric correction of ocean color observations from space, and a new scheme is presented, which implicitly accounts for the three terms exposed above.

# 2. Decomposition of the top-of-atmosphere signal

The TOA atmospheric signal includes three terms, as follows : (1) The photons specularly reflected at the air-water interface, after a direct path from the sun, and then traveling back to the top of the atmosphere without scattering; they form the sun glint term and are not considered here.

(2) The contribution of white caps and foam, which return toward the top of the atmosphere a fraction of the direct sun light and of diffuse sky light; this term neither is examined.

(3) The path reflectance, which is the term specifically studied here; it is generated along the two-way path through the atmosphere, mainly by backscattering along the downward path, and mainly by forward scattering along the upward path, after reflection of the skylight at the interface.

A first approximation has consisted in simply expressing the path reflectance for a given compound atmosphere,  $\rho_{\rm path}$ , as the  ${\rm sum}^{1,2}$ 

$$\rho_{\text{path}} = \rho_{\text{rs}} + \rho_{\text{as}} \tag{1}$$

where  $\rho_{\rm rs}$  is the Rayleigh reflectance of the same atmosphere in absence of aerosol, and  $\rho_{\rm as}$  the aerosol reflectance in absence of air molecules, and when both reflectances result from single scattering (as indicated by the subscript s). This equation, strictly valid only under the assumption of single scattering, implies that the optical thicknesses  $\tau_{\rm r}$  and  $\tau_{\rm a}$ , for Rayleigh and aerosols respectively, are small enough (*i.e.*, below 0.1). In this approximation, and with a flat sea surface,  $\rho_{\rm rs}$  and  $\rho_{\rm as}$  can be expressed from the corresponding phase functions as

$$\rho_{as[rs]}(\lambda,\theta_{s},\theta_{v},\Delta\phi=\tau_{a[r]}(\lambda)\,\omega_{a[r]}(\lambda)\,p_{a[r]}(\lambda,\theta_{s},\theta_{v},\Delta\phi)$$

$$/4\,\mu_{s}\,\mu_{v}$$
(2)

where

$$p_{a[r]}(\lambda, \theta_{s}, \theta_{v}, \Delta \phi) = P_{a[r]}(\lambda, \gamma_{-}) \left[ \rho_{F}(\theta_{s}) + \rho_{F}(\theta_{v}) \right] P_{a[r]}(\lambda, \gamma_{+}) (2)$$

with

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 $\cos(\gamma \pm) = \pm \cos(\theta_0) \cos(\theta_v) - \sin(\theta_0) \sin(\theta_v) \cos(\Delta \phi)$ 

where  $\varpi_a$  and  $\varpi_r$  are the aerosol and Rayleigh single scattering albedos (ratio of scattering to attenuation, close to 1 for most oceanic aerosols, and unity for air molecules, at least at the wavelengths considered here),  $p_a$  and  $p_r$  are related (through (2')) to the aerosol and Rayleigh phase functions,  $P_a$ and  $P_r$  respectively, via  $\rho_F(\theta)$ , the Fresnel reflection coefficient at the interface.

Even for a clear atmosphere (*i.e.*, small  $\tau_a$ ),  $\tau_r$  is never small in the short wavelength domain, so that a first improvement, introduced by Gordon *et al.*<sup>3</sup>, has consisted in computing the reflectance due to Rayleigh scattering as a result of multiple scattering events between molecules. Another improvement has consisted in considering all kinds of multiple scattering, and Deschamps et al.<sup>4</sup> proposed to split  $\rho_{path}$  into three terms as follows

$$\rho_{\text{path}} = \rho_{\text{r}} + \rho_{\text{a}} + C_{\text{ra}} \tag{3}$$

where  $\rho_r$  is the reflectance due to multiple scattering by air molecules (Rayleigh reflectance) in an aerosol-free atmosphere,  $\rho_a$  is the reflectance due to multiple scattering by aerosols in a hypothetical atmosphere containing exclusively aerosols (no molecules), and  $C_{ra}$  is defined as a "coupling term" describing the interactions between molecular and aerosol scattering; in most cases it is found to be negative<sup>4,5</sup>. The term  $C_{ra}$  is denoted  $C^{R,P}$  in Ref. 4, and  $\rho_{ra}$  in Gordon and Wang<sup>6</sup>.

Another type of decomposition has also been proposed<sup>7</sup>, where both heterogeneous and homogeneous multiple scattering (by aerosols or molecules) are accounted for as a whole in a "correction term", CT, according to

$$\rho_{\text{path}} = \rho_{\text{s}} + \text{CT} \tag{4}$$

Here  $\rho_{\rm s}$  represents the single scattering reflectance computed from Eq. (2), with, however, a single compound phase function for the mixture of aerosols and molecules. The correction term CT can then be expanded as the sum of a Rayleigh correction term and of a correction for aerosol scattering, which is proportional to  $\tau_{\rm a}$ . This decomposition scheme will not be examined here and the two phase functions, for molecules and aerosols, will always be separately considered and introduced in the following computations with their appropriate weights.

When aerosol particles are added to a given amount of molecules, so that a compound atmosphere is built, the radiative regime changes. It can thus be expected that  $\rho_r$  does not remain unchanged. Similarly the hypothetical  $\rho_a$  is likely affected by the additional presence of molecules. The additivity that is suggested by Eq. (3) is formal to the extent that the 2' coupling term C<sub>ra</sub> includes several phenomena. In addition to the effect of heterogeneous scattering, it reflects the changes in the radiative regime, namely the changes in the previously defined reflectances,  $\rho_r$  and  $\rho_a$ , when molecules and aerosols are simultaneously present. These changes and therefore the



magnitude of  $C_{ra}$  (hereafter named "corrective" term) are not simply predictable.

A strict additivity can be restored provided that the definitions of the three terms are accordingly modified. Let  $\rho_r^*$  be the reflectance which originates from scattering (single and multiple) by molecules only, but *in presence of aerosols*,  $\rho_a^*$ , the equivalent term for aerosols, also *in presence of molecules*, then

$$\rho_{\text{path}} = \rho_{r}^{*} + \rho_{a}^{*} + \rho_{ra}^{*}$$
(5)

where now  $\rho_{\rm ra}^*$  stands for that part of  $\rho_{\rm path}$  which strictly results from heterogeneous scattering (from double to multiple collisions). From Eqs. (3) and (5), it comes that

$$C_{ra} = \rho_{ra}^{*} + [\rho_{r}^{*} - \rho_{r}] + [\rho_{a}^{*} - \rho_{a}]$$
(6)

which expresses that the corrective term  $C_{ra}$  includes a necessarily positive term  $\rho_{ra}^*$ , to which are added two terms corresponding to the changes in the radiative regime, from single component atmospheres to the two-component atmosphere. If these changes, represented by the differences between brackets, reveal to be negative, and not compensated by the magnitude of  $\rho_{ra}^*$ ,  $C_{ra}$  may become negative<sup>4</sup> (see also Appendix in Gordon et al.<sup>8</sup>).

The practical way for estimating each of the terms in Eq. (5), as well as of  $C_{ra}$  in Eq. (6), is to keep track of the photons in a Monte Carlo simulation, and to sort them according to their histories, *i.e.*, according to the nature and number of scattering events they have undergone. This is done here by using a Monte Carlo code already described elsewhere<sup>9,10</sup> and validated against other radiative transfer codes<sup>11</sup>. The practical way of operating this code is detailed in Appendix, along with a description of the parameters selected to simulate the path reflectance.

#### 3. Results

#### A. Two-Layer and multilayer atmospheres

Before entering into an analysis of the terms appearing in Eq. (6), a prerequisite is to assess the effect of the vertical stratification of aerosols on the total reflectance. In previous studies<sup>4,6,12</sup>, and with a view to sparing time in extensive computations, simplified atmospheres were considered; aerosols were confined within the lower boundary layer, and only molecules were present above this layer. According to previous tests<sup>4</sup>, such a simplification would be reliable when  $\theta_{\rm u}$  < 30°, and the reflectances computed for a two-layer atmosphere remained in agreement (to better than 10<sup>-3</sup>) with those obtained when a more realistic aerosol vertical distribution<sup>13</sup> was used. With regard to Eq. (5), this agreement means that the  $\rho_{\rm path}{\rm 's}$  coincide for the simplified and the more realistic vertical distributions, notwithstanding the possible variations in the three constitutive terms. This last point, and more generally the validity of the two-layer approximation, deserve examination when  $\theta_v$  exceeds 30°.

With this aim, fifty 1km-thick atmospheric layers (from 0 to 50 km) have been considered with specified values for Rayleigh scattering coefficient, aerosol content (without aerosol absorption) and ozone absorption<sup>14</sup>. For comparison with the associated two-layer atmosphere, the same aerosol has been distributed along the vertical, with an equal resulting optical thickness (Fig. 1). Such modeled, stratified, atmospheres admittedly differ from natural ones, as differing aerosols actually are present in the boundary layer, the troposphere and the stratosphere. This choice of a unique aerosol type along the vertical was mandatory for the sake of comparison with the corresponding two-layer atmosphere, which obviously contains only one aerosol type.

Examples of  $\rho_{\text{path}}$  computed for 50 and 2 layers are displayed in Fig. 2(a), with four increasing aerosol loads (maritime type<sup>15</sup>). Between the two kinds of curves the differences are minute and below 0.5% on the average, that is within the weak stochastic noise inherent to Monte Carlo simulations. The absence of significant differences has been systematically verified for other aerosol types and illuminationviewing geometries (see Table 2; Figures not shown). It can therefore be concluded that, for a given aerosol optical thickness, the TOA total reflectances are safely computed by using a two-layer system, even for viewing angles exceeding 30°, actually up to 70°, and provided that aerosols are not absorbing.

This result is nonetheless surprising to the extent that the reflectances  $\rho_{a}^*$ ,  $\rho_{r}^*$ , and  $\rho_{ra}^*$  are all changing when the aerosol vertical distribution is changed (Fig. 2(b), 2(c), and 2(d)), whereas their sum remains unchanged. By comparing the results for the two distributions (subscripts 2 and 50, respectively), it can be seen that for the (dominant) Rayleigh component,  $\rho_{r,50}^*$  is always inferior to  $\rho_{r,2}^*$ , while the contrary holds true with respect to the two other terms,  $\rho_{a,50}^*$  and particularly  $\rho_{ra,50}^*$ , always above  $\rho_{a,2}^*$  and  $\rho_{ra,2}^*$ .



**Figure 1.** Vertical profiles used in the present work for molecules, ozone, and aerosols. (a) Vertical repartition of the attenuation coefficients at 550 nm, taken from Elterman<sup>14</sup>. The four solid curves correspond to  $\tau_a = 0.05$ , 0.1, 0.3 and 0.5. For the last three values, only the bottom layer aerosol contents (< 5 km) are changed, while the whole profile is shifted to obtain an optical thickness of 0.05. The profile with steps at 2 and 12





km is used for sensitivity studies (see text) (b) For molecules and ozone, the optical thicknesses over the 0-2 and 2-50 km layers, computed from the vertical profiles shown in (a), have been homogeneously distributed in the same layers, to construct an equivalent simplified atmosphere. For aerosols, their whole content (0-50 km in A) has been confined within the 0-2 km boundary layer.

The more noticeable change affects the heterogeneous scattering, which is enhanced by 40-60% when aerosols are spread over the 50 layers, instead of being confined within the 2km-thick lower layer.

As a consequence, it must be stressed for what follows that a vertically resolved atmosphere is needed if an analysis of the partial reflectances is to be undertaken, even if aerosol absorption is not considered. Consequently, it was necessary to verify that realistic changes in the aerosol vertical distribution do not significantly modify the partial reflectances shown in Fig. 2. With this purpose, simulations were performed by using another vertical distribution, namely that proposed in WCRP<sup>16</sup>, and keeping the Rayleigh scatterers and ozone absorption distribution as in Fig. 1(a). The total aerosol optical thickness is the same as in previous simulations, but only three layers are considered, the boundary layer (0-2 km), the free troposphere (2-12 km), and the stratosphere (12-50 km), each with its specific mean extinction coefficient. The mean differences in  $\rho_{a}^{*}, \rho_{r}^{*}$ , and  $\rho_{ra}^{*}$  resulting from the use of these two different profiles, and computed for all azimuth angles and for viewing angles less than 70 degrees (see Appendix), are respectively of +2.7, -3.8, and +5%, with standard deviations of 2.5, 3.2, and 2.8%. It is therefore believed that (1) the partial reflectances are simulated in a realistic way when the aerosol is vertically distributed as shown in Fig. 1(a), and (2) for real atmospheres which necessarily differ in vertical structure from the 50-layer atmosphere in Fig. 1(a), the reflectances remain close enough to those simulated here to allow a generalization of the results discussed hereafter.

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**Figure 2.** TOA reflectances for  $\lambda = 445 \text{ nm}$ ,  $\theta_0 = 60^\circ$ , and four values of  $\tau_a(550)$  (0.05, 0.1, 0.3 and 0.5). The aerosol is the maritime model with a relative humidity of 70%. Reflectances are displayed as a function of the viewing angle,  $\theta_v$ , throughout the sun and antisun half vertical planes ( $\Delta \phi = 0$  and  $\pi$ , respectively), and in the perpendicular half plane ( $\Delta \phi = \pi/2$ ). Viewing angle,  $\theta_v$ , is limited to 70°. Solid curves are the results for the 50-layer structured atmosphere, and dotted curves are for the simplified, two layers, atmosphere. (a) Global path reflectances,  $\rho_{\text{path}}$ , (b) reflectances due only to multiple Rayleigh scattering,  $\rho_{\text{ra}}^*$ , (c) reflectance due to heterogeneous scattering,  $\rho_{\text{ra}}^*$ .







**Figure 3.** TOA reflectances for a vertically structured (50 layers) atmosphere, as a function of wavelength, when  $\theta_0 = 40^\circ$ ,  $\theta_v = 30^\circ$ , and  $\Delta \phi = \pi/2$ . The aerosol is the maritime model with a relative humidity of 70%, and an optical thickness of 0.3 at 550 nm. The various reflectances as indicated are described in the text.

#### B. Analyzing the terms of the total signal decomposition

Scattering in single component versus two-component atmospheres. The aerosol-free and the molecule-free "atmospheres" have been considered with a view to computing the reflectances  $\rho_{\rm a}$  and  $\rho_{\rm r}$  (Eq. 3). Then, the same global amount of molecules and aerosols was vertically distributed amongst the 50 layers as described above, to build the related compound atmosphere and compute the three terms appearing in Eq. (5). The comparison between the three atmospheres allowed C<sub>ra</sub> (in Eq. 6) to be derived. To the extent that the molecular phase function is unique, such a triplet of atmospheres is determined by three modifiable parameters, namely the aerosol phase function and the optical thicknesses  $\tau_a$  and  $\tau_r$ . Modifications can be made as a purely numerical experiment, or as well by changing the wavelength, as far as the aerosol nature is kept unchanged. The sun zenith angle  $\theta_0$ is an additional (external) parameter. All the results have to be analyzed in their dependence with respect to the viewing zenithal angle,  $\theta_v$ , and azimuth difference,  $\Delta \phi$ .

The 7 terms appearing in Eqs. (3) and (5) are plotted as a function of wavelength for a particular aerosol load and nature, and a specific geometry (Fig. 3). The trends shown by this figure remain valid in all circumstances, whereas they are quantitatively varying according to the geometrical and aerosol conditions (discussed later on). From this particular example, some general trends and behaviors can already be put in evidence and are summarized as follows





**Figure 4.** TOA reflectances, as a function of  $\theta_v$ , and in the vertical planes as in Fig. 2, when  $\lambda = 445$  nm and  $\theta_0 = 40^\circ$ , for a vertically structured (50 layers) atmosphere, either containing both aerosols and molecules (dotted and dashed curves) or for the two atmospheres containing only one of these two scatterers (solid curves). The aerosol is the maritime model with a relative humidity of 70% and for  $\tau_a(550) = 0.3$ . The path reflectance, and the reflectances due to multiple scattering by aerosols ( $\rho_a^*$  and  $\rho_a$ ) or molecules ( $\rho_r^*$  and  $\rho_r$ ) are shown in (a); the reflectance due to heterogeneous scattering,  $\rho_{ra}^*$ , and the "correction term",  $C_{ra}$ , are shown in (b).

1- In the compound atmosphere,  $\rho_r^*$  and  $\rho_a^*$  are systematically below their germane terms,  $\rho_r$  and  $\rho_a$ , specific of the single component atmospheres, so that the bracketed differences in Eq. (6) are systematically negative.

2- The heterogeneous reflectance  $\rho_{ra}^*$  is apparently created at the expense of the homogeneous multiple scattering of both kinds.

3- The spectral dependencies of  $\rho_r$  and  $\rho_a$  approximately follow the  $\lambda^{-4.09}$  and  $\lambda^{-0.4}$  laws, as the corresponding scattering coefficients (see later on). For  $\rho_a$  the approximate maintenance of the Ängstrøm exponent is possible because the shape of the phase function for this particular aerosol is practically insensitive to wavelength.

4- The spectral variations in  $\rho_a^*$  depart from those in  $\rho_a$  and, in this instance, the exponent becomes clearly positive. The spectral selectivity of  $\rho_r^*$  remains close but not equal to that of  $\rho_c$ .

 $\rho_{\rm r}$ . 5- The heterogeneous scattering reflectance  $\rho_{\rm ra}^*$  is rather important in magnitude, occasionally exceeding  $\rho_{\rm a}^*$ , and amounting to about half of the Rayleigh term in this example.



Its spectral dependence seems, somewhat surprisingly, mainly governed by that of molecular scattering.

6-Finally, the correction term  $C_{ra}$  is much smaller than  $\rho_{ra}^*$ , as expected from the negative terms, as already identified in the first remark. Here  $C_{ra}$  is positive, yet this result is not general. When examining various results, and figures like Fig. 3,  $C_{ra}$  actually appears to be the most changing term, and is not always with values as small as those shown in Fig. 3.

The respective magnitudes of all the terms, as described above, are not modified when various  $\theta_{v}$  directions are considered at a single wavelength (Fig. 4). The inequalities  $\rho_{r}^{*}$  $< \rho_{\rm r}$  and  $\rho_{\rm a}^* < \rho_{\rm a}$  are maintained everywhere (Fig. 4(a)). The forward lobe of the aerosol phase function results in forming a peak, centered on the direction corresponding to the reflected sunrays ( $\Delta \phi = \pi$ ). Despite the asymmetrical disposition of  $\rho_{r}^{*}$ and  $\rho_{a}^{*}$ , the heterogeneous scattering reflectance  $\rho_{ra}^{*}$  is practically symmetrical with respect to nadir (Fig. 4(b)), and this symmetry is not significantly altered when  $\theta_0$  is changed (up to  $60^{\circ}$ , not shown). With such an angular distribution, the  $\rho_{\rm ra}^{*}$  values are higher than those for the pure aerosol term ( $\rho_{\rm a}^{*}$ ) in almost all azimuthal directions, except around the anti-sun direction ( $\Delta \phi$  near  $\pi$ ). The behavior of  $C_{ra}$  (Fig. 4(b)), either positive or negative, is rather complex, although numerically understandable from Eq. (6).

Evolution of the three partial reflectance for increasing aerosol optical thickness. When the aerosol load is progressively increased, the directly related term,  $\rho_a^*$  (Fig. 5(a)), increases almost linearly with  $\tau_a$ , with differing slopes according to the wavelength and also to the geometry ( $\theta_v$  and  $\theta_0$ , not shown). The slopes of the  $\rho_a^*(\tau_a)$  curves are always lower than that of the unique  $\rho_a(\tau_a)$  curve, and the differences  $[\rho_a^* - \rho_a]$  are accordingly always negative. As expected from Fig. 3, the lower  $\rho_a^*$  slopes occur at the shortest wavelength (445 nm in Fig. 5(a)). The molecular reflectance,  $\rho_r^*$  (Fig. 5(b)) decreases abruptly from its initial value  $\rho_r$ , as soon as aerosols are present, and then more slowly when  $\tau_a > 0.1$ . The strong depression that affects the initial part of the  $\rho_{r}^{*}$  curve is related to the steep rise of the heterogeneous scattering,  $\rho_{\rm ra}$ (Fig. 5(c)). The introduction of a small amount of aerosol is more efficient in creating  $\rho_{ra}^*$  than are further additions (*i.e.*, when  $\tau_a > 0.1$ ). For the geometry selected in Fig. 5 and  $\lambda = 445$ nm,  $\rho_{ra}^{*}$  is always greater than  $\rho_{a}^{*}$ . The addition of the three partial reflectances leads to  $\rho_{\text{path}}$  (Fig. 5(d)) which varies with  $\tau_a$  in a nearly linear way because of compensating effects, and with slopes only slightly different for  $\lambda = 445$  nm (slope is about 0.09) and  $\lambda = 865$  nm (about 0.08). This simple result offers a possibility of developing an atmospheric correction scheme, as examined later.

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The above results for a particular aerosol and a given illumination/viewing geometry remain essentially valid for other configurations. Because of the weak anisotropy of the Rayleigh scattering phase function,  $\rho_r^*(\lambda, \tau_a)$ , and to a lesser extent  $\rho_{ra}^*(\lambda, \tau_a)$ , are weakly changing when  $\theta_0$  and  $\theta_v$  are changed. With a much more asymmetrical pattern, the phase function of aerosols induces significant variations in the  $\rho_a^*(\lambda, \tau_a)$  values according to the geometrical configuration. These rather complex, albeit understandable, variations (particularly those in  $C_{ra}$ ), cannot be discussed in full detail.

Relative proportions of the three partial reflectances in the global upward flux. In a first attempt to embrace the global phenomenon and to condense the results, the upward radiance field has been integrated over all azimuth angles and over zenith angles from 0 to only 70°. This limitation was adopted because the earth's sphericity is not represented in the modeling. The corresponding solid angle is 4.4 sr, and these integrated reflectances are denoted with an overbar.

$$\overline{\rho} = \int_{\Delta\phi=0\theta_{\rm v}=0}^{2\pi} \int_{0}^{70} \rho(\theta {\rm v}, \Delta\phi) \cos(\theta_{\rm v}) \sin(\theta_{\rm v}) \,\mathrm{d}\theta_{\rm v} \,\mathrm{d}\phi \tag{7}$$

The flux within this solid angle actually represents at least 70% of the total flux integrated over  $2\pi$  sr (in the unrealistic plane-parallel system). The spatially integrated values of the three partial reflectances (right hand side of Eq. 5) are then transformed into relative contribution to  $\rho_{\text{path}}$ , hereafter denoted  $<\rho_x >$ , and computed as  $<\rho_x > = \rho_x / \rho_{\text{path}}$ , where x is either r, a or ra. Their changes have been examined as a function of the mixing ratio  $\eta_a$ , which is defined as

$$\eta_{\rm a} = \tau_{\rm a} / \left(\tau_{\rm a} + \tau_{\rm r}\right) \tag{8a}$$

and the opposite term, for molecular scattering, denoted  $\eta_r$ , is

$$\eta_{\rm r} = 1 - \eta_{\rm a} \tag{8b}$$

In such a compound atmosphere, the radiative regime is not univocally determined by the value of  $\eta_a$ . Simultaneous changes in  $\tau_a$  and  $\tau_r$  can lead to the same  $\eta_a$  value, while the radiative field is modified. In what follows, the descriptor  $\eta_a$  is made varying either by changing  $\tau_a$  (with  $\tau_r$  constant) or  $\tau_r$ (with  $\tau_a$  constant). The relative proportions of the partial reflectances are displayed for particular cases in Figs. 6(a) and 6(c), the reflectances themselves in Figs. 6(b) and 6(d), and a generalization of these results is proposed in Fig. 7.



**Figure 5.** Reflectances as a function of  $\tau_a$ , for the wavelengths indicated, and when  $\theta_0 = 40^\circ$ ,  $\theta_v = 30^\circ$ , and  $\Delta \phi = \pi/2$  (the aerosol is the maritime model, with RH = 70%). (a) Reflectances due to multiple scattering by aerosols only : the dotted curve is for  $\rho_a$  and is therefore unique; the solid curves are for  $\rho_a^*$  (b) reflectances due only to multiple Rayleigh scattering,  $\rho_r^*$ , (c) reflectance due to heterogeneous scattering,  $\rho_{ra}^*$ , (d) path reflectance,  $\rho_{path}$ . The black diamonds correspond to the simulations carried out for  $\tau_a(550) = 0.05, 0.1, 0.3, and 0.5$ .

In Fig. 6(a),  $\tau_r$  is let equal to 0.05, whereas  $\tau_a$  is made varying from 0 to 2. In Fig. 6(c),  $\tau_a$  is kept constant (0.05) and  $\tau_r$  varies from 0.02 (corresponding to  $\lambda \sim 850$  nm when atmospheric pressure is 1013 hPa) to 0.35 ( $\lambda \sim 400$  nm). In these graphs, the two relative contributions  $\langle \rho_a \rangle$  and  $\langle \rho_r \rangle$  exhibit inverse variations and roughly behave like quantities governed by a mixing rule. A slight departure from this rule however occurs, and originates from the presence of the third term,  $\langle \rho_{ra} \rangle$ , which can reach about 15% of  $\rho_{path}$ . The crossing point where  $\langle \rho_a \rangle \langle \rho_r \rangle$  (about 45%) occurs at a  $\eta_a$  value which seems roughly independent from the way of having varied  $\eta_a$  (by changing either  $\tau_a$  or  $\tau_r$ ).

In contrast, this crossing point moves with the value given to  $\theta_0$ . It is around  $\eta_a = 0.66$  when  $\theta_0 = 60^\circ$  (not shown), instead of 0.78 for  $\theta_0 = 0^\circ$ . The relative contribution of heterogeneous scattering, identified as  $\langle \rho_{ra} \rangle$ , is necessarily zero at both ends of the  $\eta_a$  scale and must exhibit a maximum somewhere inside the  $\eta_a$  (or  $\eta_r$ ) range. The maximal  $\langle \rho_{ra} \rangle$  value lies around  $\eta_a$ = 0.8, when the heterogeneous scattering is "aerosol-regulated" as in panel A ( $\tau_r$  constant), and in this case  $\langle \rho_{ra} \rangle$  may exceed  $\langle \rho_r \rangle$  at the extreme end of the  $\eta_a$  range. In a symmetrical manner,  $\langle \rho_{ra} \rangle$  experiences a maximum at  $\eta_r = 0.8$  when it is "molecule-regulated" (panel C,  $\tau_a$  constant), and it exceeds  $\langle \rho_a \rangle$  in the domain of low  $\eta_a$  values. The corrective term  $\langle C_{ra} \rangle$ , expressed relatively to  $\rho_{path}$ , is also shown on Figs. 6(a) and 6(c). It is small, except at both ends of the  $\eta_a$  range, is often negative, and may be zero; in this particular case the global flux for the compound atmosphere is simply the sum of the global fluxes for the two single component atmospheres ( $\rho_{path} = \rho_a + \rho_r$ ).



**Figure 6.** Relative proportions  $\langle \rho_r \rangle$ ,  $\langle \rho_a \rangle$ ,  $\langle \rho_{ra} \rangle$  and  $\langle C_{ra} \rangle$  (as %), displayed as a function of  $\eta_a$  (see text); (a) when changing  $\tau_a$  (from 0 to 2) and keeping  $\tau_r$  fixed, or (c) when changing  $\tau_r$  (from 0.02 to 0.35) while  $\tau_a$  is fixed (the aerosol phase function is that of the maritime model, with RH = 70%, and the sun is at the zenith). Diamonds indicate the entries of the computations, namely  $\tau_a = 0, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 2.0$  when  $\tau_r$  is 0.05, and  $\tau_r = 0, 0.02, 0.05, 0.1, 0.2, 0.3, 0.35$  when  $\tau_a$  is 0.05. The corresponding variations of  $\rho_{path}$ ,  $\rho_r$ ,  $\rho_a$ ,  $\rho_{ra}$  are displayed in panels B and D.

As already said, the single parameter  $\eta_a$  is insufficient to explore the whole domain of possible variations in the radiative regime, even if  $\theta_0$  and the aerosol type are fixed. Curves like those in Fig. 6, representing the  $\langle \rho_r \rangle$ ,  $\langle \rho_a \rangle$ , and  $\langle \rho_{ra} \rangle$  terms, actually are not unique and depend on the selected  $\tau_a - \tau_r$  or  $\tau_a - \eta_a$  couples.

In Fig. 7, as an attempt to generalize the results of Fig. 6, the problem is scaled by introducing  $\tau_a$ . In the  $\tau_a - \eta_a$  space, the loci corresponding to constant  $\tau_r$  are hyperbolae such as those drawn to delimit the domain considered ( $0.02 < \tau_r < 0.35$ ). The three curves shown in Fig. 6(a) actually explore the  $\tau_a - \eta_a$  domain along the hyperbola corresponding to  $\tau_r = 0.05$ . Similarly, the three curves shown in Fig. 6(c) deal with situations found along a transect of the  $\tau_a - \eta_a$  domain represented by the vertical line in Fig. 7, with  $\tau_a = 0.05$ . The relative proportions of pure aerosol and pure molecule scattering (panels A and B) in forming  $\rho_{\text{path}}$  are mainly controlled by the mixing ratio, depicted by  $\eta_a$ . As an example,

equal contributions (about 40% each) are found when  $\eta_a \sim 0.8$ , whatever  $\tau_a$  (at least when  $\tau_a > 0.1$ ). Whatever the aerosol load, the Rayleigh contribution  $< \rho_r >$  exceeds 50% of  $\rho_{path}$  as long as  $\eta_a$  is < 0.7 (approximately as long as  $\tau_a < 2 \tau_r$ ). The aerosol contribution  $< \rho_a >$  exceeds 40% above the same threshold in  $\eta_a$  ( $\tau_a > 2 \tau_r$ ). The roughly horizontal arrangement of the isolines of  $< \rho_r >$  and  $< \rho_a >$ , and their inverse evolutions (*i.e.*, increasing for  $< \rho_a >$  and decreasing for  $< \rho_r >$  with increasing  $\eta_a$ ) reflect the mixing rule above mentioned. The approximately horizontal ordering is disturbed in the domain of small  $\tau_a$  values, more precisely when the  $< \rho_{ra} >$  isolines undergo a drastic change in their orientation. In fact,  $< \rho_{ra} >$  is determined by  $\tau_r$  as long as  $\tau_a > 2 \tau_r$ , and otherwise by  $\tau_a$ .





**Figure 7.** Isolines of the relative proportions  $\langle \rho_r \rangle$ ,  $\langle \rho_a \rangle$ and  $\langle \rho_{ra} \rangle$  expressed as percent of  $\rho_{path}$  (panels A, B, and C, respectively), within the  $\eta_a$ - $\tau_a$  plane. The hyperbolic envelopes correspond to the extrema of  $\eta_a$  for a given  $\tau_a$  value, and delimit the domain inside which  $\tau_r$  varies between 0.02 and 0.35 (*i.e.*, near infrared to ultraviolet). The aerosol is the maritime model, for RH = 70%, and the sun is at the zenith.

The maximal relative contribution of heterogeneous scattering (up to 20-30%) lies in the middle of the  $\eta_a$  range, that is when  $\tau_a$  and  $\tau_r$  are roughly similar, and both of sufficient magnitude (each of about 0.2, with  $\langle \rho_{ra} \rangle$  above 20%). It has been also found that the relative change in the aerosol reflectance (*i.e.*,  $[\rho_a - \rho_a] / \rho_a$ ) is mostly determined by the Rayleigh optical thickness  $\tau_r$ , whatever  $\tau_a$ .

**Spectral aspects.** The Rayleigh exponent for air molecules (-4.09), as well as any Ångstrøm exponent for aerosols describe the spectral variations of the respective scattering coefficients. These exponents apply directly to reflectances only if these reflectances result from single scattering (namely when the optical thickness is low enough, so that Eq. (2) is valid), and if the shape of the phase function is not wavelength dependent. If multiple scattering events occur,  $\rho(\theta_v, \theta_0, \Delta\phi)$  is no longer a simple reproduction of a portion of the phase

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function (as implied by Eq. 2); thence the above exponents cannot be simply transferred to the spectral variations in reflectances. The spectral dependency of the path reflectance, or other partial reflectances, can be operationally expressed through an exponent defined as

$$n = \frac{\ln[\rho(\lambda_i) / \rho(\lambda_j)]}{\ln[\lambda_i / \lambda_i]}$$
(9)

where  $\rho$  is any of the reflectances already discussed. The star and subscripts used with the  $\rho$ 's are transferred to the n's with the same meaning. In what follows, reflectances integrated over the solid angle previously used (*i.e.*, 4.4 sr) have been used to calculate the n's, for  $\lambda_i = 445$  and  $\lambda_j = 865$  nm.

In a conservative atmosphere (no absorption), multiple scattering events result only in re-arranging the radiance field originating from singly scattered radiation. The backscattered radiation is predominantly involved in the present problem. Radiances reflected at the interface, however, act as an additional source, located at the bottom of the atmosphere, and thus forward scattering is also involved. The exponent defined above will depend on the change of the global optical thickness ( $\tau_a + \tau_r$ ) between the two wavelengths in question, as well as on the respective weight of the phase functions with their specific asymmetry, which govern the radiance distribution.

The "operational" exponents have been computed for single component atmospheres (molecules, maritime aerosol, or rural aerosol), and then for the two corresponding compound atmospheres. The results for the n's are shown as a function of the sun zenith angle in Figs. 8(a) and 8(b). Their interpretation rests on the relative contributions to the total signal of the various types of scattering (single-multiple, homogeneous-heterogeneous) shown in Fig. 9, and generated as described in Appendix. The behavior of the exponents can be summarized as follows :

(1) In the aerosol-free atmosphere (shown in Figs. 8(a) and 8(b)), the corresponding exponent,  $n_r$  is close to that for Rayleigh scattering (-4.09). The departure from this value, which varies according to the sun position, results from the (weak) anisotropy of the Rayleigh phase function. The shape of the phase function is left practically unaltered in the quasi-single scattering regime, which prevail at 865 nm, whereas it is smoothed by the effect of multiple scattering at 445 nm. Indeed (Fig. 9), the proportion of multiply scattered photons in the total signal increases from less than 5% at 865 nm, to 29% at 445 nm.

(2) The Ångstrøm exponent for the maritime aerosol is -0.4, well reproduced by  $n_a$  (Fig. 8(a)). The radiative regime is almost the same at the two wavelengths, to the extent that the contribution of multiple scattering remains similar, 43% and 50% at 865 and 445 nm, respectively (Fig. 9); the  $\theta_0$  dependence is weak in this rather diffuse regime.



**Figure 8.** Exponents depicting the variations of the various partial reflectances between  $\lambda = 445$  and  $\lambda = 865$  nm, plotted as a function of  $\theta_0$ , and for two aerosol types (see text) and  $\tau_a(550) = 0.3$ . Note that the vertical axes are interrupted and the scales different for the upper and lower part of each panel.

Figure 9. Relative importances (expressed as %) in the total signal (integrated over all azimuths and over  $0^{\circ}$ -70° for  $\theta_{,}$ ) of various scattering events, grouped as a function of their order and type of scattering. Computations are carried out for a 50layer atmosphere and an aerosol of the maritime type, with RH = 70%. The sun zenith angle is  $40^{\circ}$ . The upper and lower panels are for  $\lambda = 445$  and 865 nm, respectively. They show the results for the single component atmospheres and the corresponding compound atmosphere, with  $\tau_a = 0.33$  and 0.25 at 445 and 865 nm, respectively, in correspondence with  $\tau_{\rm c}(550) = 0.30$ . Columns and raws are numbered according to the number of scattering events : 0, 1, 2, 3, and 4 or more scattering events, either of molecular or aerosol type, respectively. The parallelepipeds are proportional in height to the percentages of the scattering order and type in question. They are replaced by gray shades for the compound atmosphere.



**Figure 10.** Reflectances as a function of  $\tau_a$ , and when  $\theta_0 = 40^\circ$ ,  $\theta_v = 30^\circ$ ,  $\Delta \phi = \pi/2$ , and  $\tau_r = 0.2$  (*i.e.*,  $\lambda \sim 460$  nm); the phase function is that of the maritime model for RH = 70%. The four panels are as in Fig. 5, and each curve in each of these panels is for one value of  $\varpi_a$ , as indicated.

(3) The Ångstrøm exponent for the rural aerosol is -1.2, whereas  $n_a$  amounts to about -1.0. With multiple scattering events forming 30% (at 865 nm) or 50% (at 445 nm) of the global flux (not shown), the radiative regime is not the same at the two wavelengths, and leads to a departure from the Ångstrøm exponent value.

(4) For compound atmospheres (Figs. 8(a) and 8(b)), the situation is much more complex. The operational exponent related to the aerosol contribution,  $n_{a}^{*}$ , strongly departs from the preceding value,  $n_{a}$  (and thus from the Ångstrøm exponent). Similarly  $n_{r}^{*}$  differs from  $n_{r}$  (and from -4.09) in response to changes in the radiative regime. The exponent  $n_{ra}^{*}$  for the heterogeneous scattering contribution appears to be totally disconnected from the Ångstrøm exponent and akin to the Rayleigh exponent, in spite of wide variations (-3.6 to -4.6). The spectral variations of  $\rho_{ra}^{*}$  are not only due to the specific spectral dependency of both scatterers, but also to their varying proportions along the spectrum (as  $\eta_{a}$  and  $\eta_{r}$  are not constant). Illumination conditions are also involved through the shape of the phase functions, so that  $n_{ra}^{*}$  and  $n_{a}^{*}$  are  $\theta_{0}^{-}$  dependent. Therefore these exponents are apparent, in this

sense that they depend on the varying combinations of  $\tau_a$  and  $\tau_r$ , and are not easily predictable for practical applications.

Influence of aerosol absorption. All the results presented in the preceding sections have been obtained for non-absorbing aerosols, while moderately or even strongly absorbing aerosols may be carried in the atmosphere. The impact of absorption on the three partial reflectances  $\rho_{r}^*$ ,  $\rho_{a}^*$ , and  $\rho_{ra}^*$ , as well as on their integrated values (*i.e.*, the  $\rho_{\chi}$  terms), has thus been examined through some additional simulations. In principle, making the aerosol absorbing (*i.e.*,  $\varpi_a < 1$ ) implies concomitant changes in its phase function. Nonetheless, and for the sake of comparing the results of the present simulations with the previous ones for  $\overline{\omega}_{a} = 1$ , the phase function (that of the maritime model with RH = 70%) was kept unchanged and used with  $\varpi_a = 0.8$  or 0.6 instead of 1. The aerosol vertical distribution was also as in Fig. 1(a). The partial reflectances  $\rho_{\rm r}^*, \rho_{\rm a}^*$ , and  $\rho_{\rm ra}^*$ , and their sum  $\rho_{\rm path}$ , are displayed in Fig. 10 (a-d), as a function of  $\tau_a$  and for  $\overline{\omega}_a = 1$ , 0.8, and 0.6. In this figure,  $\tau_r$  is given the constant value 0.2 (in correspondence with  $\lambda \sim 460$  nm), instead of being set for fixed wavelengths, as done in Fig. 5. As expected, all reflectances are decreasing





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as  $\varpi_a$  decreases, and all the partial reflectances apparently tend toward asymptotic values, even if the  $\tau_a$  domain considered is not wide enough to always reach a plateau. The level of these plateaus are diminished by increasing absorption. The slopes of the  $\rho_{path}(\tau_a)$  curves are lowered by absorption. Adding more and more absorbing particles does not increase the path reflectance as rapidly as do non-absorbing aerosols, and can even lead to a decrease of the path reflectance below its value for a pure molecular atmosphere, *i.e.*,  $\rho_{path}$  becomes lower than  $\rho_r$ . This feature is observed, for instance, when  $\tau_a = 0.1$ , and for  $\varpi_a = 0.6$  (Fig. 10(d)).

The above results seem however contradictory with previous findings. Indeed, Gordon<sup>17</sup> found that there is "an increase in the significance of the Rayleigh-aerosol interaction" as  $\varpi_a$  decreases. In fact, both conclusions are compatible when it is acknowledged that the true heterogeneous scattering,  $\rho^*_{ra}$ , is considered in the present work, while in Gordon's study the Rayleigh-aerosol interaction is depicted by the corrective term  $C_{ra}$ . The latter is well increasing (in absolute value) as  $\varpi_a$  decreases, because the bracketed differences in Eq. 6 result in negative values whose sum is greater than  $\rho^*_{ra}$ . The apparent contradiction between both studies emphasizes the ambiguous meaning of the corrective term  $C_{ra}$ , which is usually and erroneously referred to as the coupling between aerosol and molecule scattering.

As regards the integrated reflectances and their respective contributions to  $\rho_{\text{path}}$  (*i.e.*, the  $\rho_x$  and  $<\rho_x >$  terms, respectively), should the results of the present simulations have been used to redraw Figs. 6 and 7, the patterns in these figures (for instance the arrangement of isolines in Fig. 7) would have been nearly identical to those already displayed for  $\varpi_a = 1$ . The changes in the values of the  $<\rho_x >$  terms, however, cannot be discussed because the  $\rho_{\text{path}}$  value varies when  $\varpi_a$  changes. On the contrary, the mean relative changes in  $\rho_r$ ,  $\rho_a$ , and  $\rho_{\text{ra}}$  can be computed; over 25  $\tau_a$ - $\tau_r$  couples (in correspondence with  $\tau_a = 0.05, 0.1, 0.3, 0.5, 0.7, \text{ and } \tau_r = 0, 0.05, 0.1, 0.2, 0.35$ ), the mean changes are of about -5, -18, and -20%, respectively, when  $\varpi_a = 0.8$  instead of 1, and of about -11, -35, and -40%, respectively, when  $\varpi_a = 0.6$ .

# 4. Application to atmospheric correction of ocean color observations from space

The process which consists in retrieving the radiances emerging from the ocean (the "marine signal") from the TOA total signal recorded by a satellite borne sensor is generally termed atmospheric correction. To achieve this correction, the path reflectance must be estimated with a very high accuracy to preserve an acceptable accuracy in the estimate of the marine signal, as the former represents at least 80%, and often more, of the total signal. For the new generation of ocean color sensors (POLDER<sup>18</sup>, OCTS<sup>19</sup>, SeaWiFS<sup>20</sup>, MERIS<sup>21</sup>), the general scheme for the atmospheric correction over Case 1<sup>22</sup> waters consists of identifying the nature, and quantifying the contribution, of the local aerosol by using the signals recorded at two wavelengths in the near infrared (where oceanic Case 1 waters are black). This information is used to predict  $\rho_{\text{path}}$  in the visible part of the spectrum;  $\rho_{\text{path}}$  is then subtracted from

the total reflectance at the TOA level, and the marine contribution is assessed. The present scheme follows this mandatory pathway.

As shown above, the reflectance due to heterogeneous scattering,  $\rho_{ra}^*$ , is an important contribution to  $\rho_{path}$ , even for reduced aerosol loads (Figs. 5 and 6), and sometimes exceeding the homogeneous scattering by aerosols only,  $\rho_{a}^*$ . These reflectances,  $\rho_{ra}^*$  and  $\rho_{a}^*$ , however, are not derivable in an independent way, as the aerosol type and concentration are unknown when the atmospheric correction process is started. To the extent that  $\rho_r^*$  also differs from  $\rho_r$ , as a result of the presence of aerosols, this term is also unpredictable. In fact the quantities available are the measured reflectance  $\rho_{path}$  and the computed reflectance  $\rho_r$ , for molecules in absence of aerosols. In the *Gordon and Wang's* technique<sup>6</sup>, these quantities are used by forming the difference [ $\rho_{path} - \rho_r$ ], which is related to  $\rho_{as}$ , the reflectance due to aerosols in the single scattering approximation (Eqs. 3 and 6)

$$\rho_{\text{path}} - \rho_{\text{r}} = \rho_{\text{a}}^{*} + \rho_{\text{ra}}^{*} + [\rho_{\text{r}}^{*} - \rho_{\text{r}}] = f(\rho_{\text{as}})$$
(10a)

In this scheme,  $\rho_{as}$ , which has no physical reality, is utilized as a descriptor of the aerosol and as an index to identify its loading and type.

Taking advantage of the results shown in Fig. 5, the same quantities can be used by forming the ratio  $\rho_{\text{path}} / \rho_{\text{r}}$ , with a view to reducing the effect of changes in barometric pressure, so that

$$\rho_{\text{path}} / \rho_{\text{r}} = (\rho_{a}^{*} + \rho_{ra}^{*} + \rho_{r}^{*}) / \rho_{\text{r}} = f(\tau_{a})$$
 (10b)

This ratio represents the relative increase in reflectance when aerosols are progressively added to molecules, and it can be related to  $\tau_a$ . The monotonous relationship  $f(\tau_a)$  again depends on aerosol type and loading, and on geometry. The above Eqs. 10a and 10b have to be written for each wavelength, each geometrical configuration, and each aerosol type.

Examples of the variations in  $\rho_{\text{path}} / \rho_{\text{r}}$  as a function of  $\tau_a(\lambda)$  are displayed in Fig. 11, for the two wavelengths 865 and 775 nm. This figure also serves for describing the proposed scheme. To any measured value of  $[\rho_{\text{path}} / \rho_{\text{r}}]$  at 865 nm, it is possible to associate a set of values of  $\tau_a(865)$ ; each one corresponds to a given aerosol model (steps 1 and 2 in Fig. 11), because multiple scattering effects are different for different aerosols. A corresponding set of  $\tau_a(775)$  values is simply obtained by using the ratio of the aerosol extinction coefficients at the two wavelengths (step 3), according to

$$\tau_{a}(775) = \tau_{a}(865) \left[ c(775) / c(865) \right]$$
(11)

To each  $\tau_a(775)$  value corresponds a fixed value of the ratio  $[\rho_{\text{path}} / \rho_r]$  at 775 nm (step 4, *i.e.*, the converse of step 2). A set of plausible estimates for this ratio is produced, and contains values, which generally differ according to the aerosol type (step 5). The final step (6) consists in comparing these plausible values to the actual ratio  $[\rho_{\text{path}} / \rho_r]$  at 775 nm, in



view of selecting the two aerosol models which enclose the actual  $[\rho_{\text{path}} / \rho_{\text{r}}]$  value. From these two bracketing values of  $[\rho_{\text{path}} / \rho_{\text{r}}]$ , and from the actual one, a "mixing ratio" is computed as in the *Gordon and Wang's* method. By assuming that this ratio is wavelength-independent, it is then possible to

transfer the estimate of  $[\rho_{\text{path}} / \rho_r]$  toward the visible spectrum, provided that the relationships with  $\tau_a$  have been previously established for all wavelengths. The path reflectance, hence the marine signal, are then straightforwardly obtained in the visible.



**Figure 11.** Relative variation of the path reflectance at 865 and 775 nm for the maritime aerosol model, displayed as a function of  $\tau_{a}$ , and expressed as the ratio  $\rho_{\text{path}} / \rho_{r}$ , when  $\theta_0 = 40^\circ$ ,  $\theta_v = 30^\circ$ , and  $\Delta \phi = \pi/2$ . The four curves are for 4 values of the relative humidity, as indicated. Arrows symbolize a possible way for identifying a couple of aerosol models enclosing the actual aerosol. The circled numbers identify the successive steps of this scheme, as discussed in the text.

#### 5. Conclusion

A new and exact decomposition of the atmospheric path radiance has been proposed, and the behavior of its three constitutive terms has been studied in response to changes in optical thicknesses ( $\tau_a$  and  $\tau_r$ ). Between radiances computed for single component atmospheres and those computed for realistic compound atmospheres, notable differences exist which have been quantified. These changes are attributable to rearrangements of the radiative field, which occur when both molecules and aerosols simultaneously scatter (with extremely different phase functions) within all atmospheric layers. The coupling between scattering by aerosols and molecules  $(\rho_{ra}^*)$ always contributes significantly to the path reflectance. Even for aerosol optical thickness as low as  $\tau_a \sim 0.05$ ,  $\rho_{ra}^*$  represents about 7% of  $\rho_{\rm path}$  in the near infrared, and more than 10% in the visible (Fig. 7); this contribution becomes 10% (near infrared) and 25% (visible) when  $\tau_a \sim 0.2$ . The approximate character of splitting the aerosol and molecule contributions has been emphasized, even for small  $\tau_a$  and  $\tau_r$ . The use of such an approximation for future atmospheric correction algorithms is challenged if full benefit is to be taken from the improved radiometric accuracy of the new-generation ocean color sensors.

The atmospheric correction scheme proposed here makes use of the ratio  $[\rho_{path} / \rho_r]$ . This ratio has a clear physical meaning, as it represents the relative increase in  $\rho_{path}$  when a given amount of aerosols is introduced within a molecular atmosphere. Based on the previous analysis it is shown that this ratio can be simply related to the aerosol optical thickness, so that its value is easily transferred from a wavelength to another one, in particular between the two wavelengths in the near infrared, which are used to identify the aerosol type and loading.

The main differences compared to other schemes, in particular that of Gordon and Wang<sup>6</sup>, are as follows. There is no need to rely, and thus to produce, the single scattering reflectance  $\rho_{as}$  (Eq. 2) with a view to identifying the aerosol type. The transfer from one wavelength to another one is directly effected via the changes in aerosol optical thickness,  $\tau_a(\lambda)$ , which depends on the Ångstrøm exponent only and not on the geometrical configuration (in contrast with the  $\varepsilon(\lambda_i, \lambda_j)$  coefficients in Gordon and Wang's method, which are varying with geometry). Relationships like those shown in Fig. 11, however, have to be precomputed for all possible geometrical





configurations, aerosol types, and wavelengths. As a result, the size of the lookup tables is similar for the present algorithm and that of Gordon and Wang<sup>6</sup>. Both methods have the advantage of providing (as a by-product of the atmospheric correction) an estimate of the aerosol content (via  $\tau_a$  and provided that the aerosol type has been properly identified). Deriving a climatology of the aerosol distribution above the ocean is an important application of the ocean color sensors.

## Appendix

The Monte Carlo code used in the present work has been already described<sup>9,10</sup> and validated against other radiative transfer codes<sup>11</sup>. The geometry is that of a plane-parallel atmosphere; as a consequence, the results for slant directions  $(\theta_0 \text{ or } \theta_v > 70^\circ)$  cannot be reliably discussed because the sphericity of the earth is not accounted for<sup>23</sup>. The photons are collected at different levels (and up to the TOA level) within 480 equal solid angles, by dividing the  $0-\pi$  azimuth interval into 24 equal angles, and the  $0-\pi/2$  zenith angle interval into 20 angular intervals, equally spaced with respect to  $sin(\theta_{y})$ . There is no counter directly aimed at nadir. In the simulations, the bottom of the atmosphere is bounded by a perfectly absorbing ocean, which is simply represented by a Fresnel-reflecting flat interface (no wind). Atmosphere and ocean are thus uncoupled, and multiple crossings of the air-sea interface by photons are discarded, as this phenomenon is of second order importance. This uncoupling is totally justified for case 1 waters in the near infrared bands, and is an acceptable approximation for the visible domain. The polarization is not accounted for. The apparent diameter of the sun disk is set to 0.5°. For Rayleigh scattering, the anisotropy of the molecules is ignored and the depolarization factor is zero. The spectral dependency is expressed as  $\lambda^{-4.09}$ . The scattering coefficient is set, for each atmospheric 1-km layer, to the value corresponding to its average altitude14. The resulting total optical thickness is that of a standard atmosphere with a barometric pressure of 1013.25 hPa.

The aerosol phase functions have been calculated via the Mie theory, and the cumulative distribution functions numerically derived from these phase functions. The humiditydependent refractive indices, and the lognormal particle size distributions are those of the oceanic and tropospheric aerosol components described by Shettle and Fenn<sup>15</sup>. Two basic models are constructed, namely the maritime (99% of tropospheric particles, 1% of oceanic) and the rural (100% of tropospheric particles) models; their optical properties are modified when changing the relative humidity (see also in Ref. 6). These aerosols are considered as non-absorbing ( $\overline{\omega}_{a} = 1$ ); their actual single scattering albedos are greater than 0.98 (maritime model) or 0.96 (rural aerosol; except in the near infrared, where  $\omega_a \sim 0.94$ ). The wavelengths considered are those generally selected for ocean color remote sensing. No attempt is made to account for the width and shape of the actual spectral channels of a given sensor. In other words the optical characteristics are those of the nominal wavelengths as indicated.

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The directional counters actually are split into sub-counters where the photons are sorted out and cumulated as a function of the number and type of collisions they have experienced before escaping the medium. Two examples of such photon sorting are provided in Fig. 9 for  $\lambda = 445$  and 865 nm. The two single-component atmospheres (molecules only or aerosols only) are represented with the relative proportions of photons escaping the atmosphere after 1, 2, 3, or 4 and more scattering events. The total number of photons constitutes the terms  $\rho_a$  or  $\rho_{\rm r}$ . The associated compound atmosphere, with the same amount of molecules and particles, is represented by the "chessboard", where percentages of collisions of various kinds are indicated. The reflectance  $\rho_{a}^{*}$  corresponds to all the terms appearing in the first column (no scattering by molecules) and  $\rho_{\ \rm r}^{*}$  corresponds to the first row (no aerosol scattering). The reflectance  $\rho^*_{\ \rm ra}$  corresponds to the 16 other boxes containing photons having interacted several times with molecules and aerosols. The box 1-1, generally dominant in magnitude in the heterogeneous scattering, correspond to two successive scattering events, once on aerosol, once on molecule (or conversely).

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#### Table 1. Symbols and definitions

Symbol	definition	Dimension / units
$ heta_0$	Sun zenith angle	degrees
$ heta_{\mathbf{V}}$	Viewing angle	degrees
$\Delta \phi$	Azimuth difference between the sun-pixel and pixel-sensor half vertical planes	degrees
$F_0(\lambda)$	Extraterrestrial irradiance	W m <sup>-2</sup> nm <sup>-1</sup>
$\eta_{\mathrm{a}}$	Contribution of aerosols to the total optical thickness	dimensionless
$\eta_{ m r}$	$1 - \eta_a$	-
λ	Wavelength	nm
$L(\lambda, \theta_0, \theta_v, \Delta \phi)$	Radiance	W m <sup>-2</sup> nm <sup>-1</sup> sr <sup>-1</sup>
n	Operational exponent	dimensionless
$P_a(\gamma)$	Aerosol phase function	sr <sup>-1</sup>
$P_r(\gamma)$	Rayleigh phase function	sr <sup>-1</sup>
$\gamma \pm  ho(\lambda,  heta_{\Omega},  heta_{J}, \Delta \phi)$	Scattering angle Reflectance defined as $\pi L / F_0 \cos(\theta_0)$	degrees dimensionless
	Subscripts : r: Rayleigh reflectance. rs: Rayleigh reflectance (single scattering only). a: aerosol reflectance. as: aerosol reflectance (single scattering only). ra: heterogeneous aerosol-molecule scattering.	path: path reflectance.
$\overline{ ho}$	Bulk reflectance integrated over a solid angle $\Omega$ of 4.4 sr	dimensionless
$<\overline{ ho}>$	Relative contribution of $\overline{ ho}$ to $\overline{ ho}_{path}$ (indices as above)	%
$ ho_{\mathrm{F}}( heta)$	Fresnel reflection coefficient for angle $\theta$	dimensionless
RH	Relative humidity	%
$ au_{ m a}$	Aerosol optical thickness	dimensionless
$ au_{ m r}$	Rayleigh optical thickness	-
$\overline{w}$	Single scattering albedo	-

Table 2. Parameters defining the 64 cases used for comparison of atmospheres made up of 2 or 50 layers

Rayleigh optical thickness, $\tau_r$	0.23 and 0.015, in correspondence with $\lambda = 445$ and 865 nm
Aerosol models	Maritime model, with RH = 70%; Ångstrøm exponent <sup>†</sup> -0.4 Rural model, with RH = 98%; Ångstrøm exponent <sup>†</sup> -1.2
Aerosol optical thickness, $\tau_a$	0.05, 0.1, 0.3, 0.5 at 550 nm the $\tau_{\rm a}$ values range from 0.03 to 0.6, according to $\lambda$
Sun zenith angle	0, 20, 40, and 60°

<sup>†</sup> the exponent has been computed between  $\lambda = 865$  and 445 nm

# 9. Appendix 2 : Paper presented at the Ocean Optics XIV conference (SPIE), Kailua Kona, Hawaii, 10-13 November 1998.

# AN ALGORITHM FOR DETECTION OF DESERT DUST FROM TOA OCEAN COLOR SPECTRA (MERIS INSTRUMENT) : DEMONSTRATION USING SEAWIFS DATA

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## ABSTRACT

Quantitative assessment of desert dust from satellite observations of ocean color will become routine with the new generation of sensors like SeaWiFS (Hooker *et al.*, 1992), MERIS (Rast and Bézy, 1995) or MODIS (Salomonson *et al.*, 1989), which provide, or will provide soon, spectral observations with high spectral resolution and radiometric accuracy in the adequate spectral bands. A method is proposed here for detecting desert dust when performing atmospheric correction of MERIS observations; it has been successfully applied to SeaWiFS data acquired off Mauritania and within the Mediterranean Sea. The detection threshold for desert dust seems to be at an optical thickness of about 0.1 at 865 nm, which is probably enough to catch most of the dust plumes circulating over the ocean.

## INTRODUCTION

The interest taken in the study of desert dust originates in its potential effect on the radiative budget and climate of the whole planet (*e.g.*, Charlson *et al.*, 1992; Li *et al.*, 1996); Large-scale effects are expected because Saharan or Asian dust indeed concern extended regions far from their sources (*e.g.*, Prospero and Carlson, 1972; Savoie and Prospero, 1977; Li *et al.*, 1996). In a more controversial way, sand particles could either fertilize the upper oceanic layers by releasing substances adsorbed onto their surface (*e.g.*, Donaghay *et al.*, 1991; Duce *et al.*, 1991), or on the contrary deplete surface waters from phosphorus — a possible "feeding" source of phytoplankton — by carrying it away through adsorption and sinking (Krom *et al.*, 1991). Identifying desert dust occurrences over the ocean, and possibly quantifying the associated burden, are therefore important missions for the new-generation ocean color sensors. After a brief synthesis about desert aerosols radiative properties, a method is presented and tested with SeaWiFS data from Mauritania and from the Mediterranean Sea.

## DESERT DUST OPTICAL PROPERTIES

Despite large differences due to their various origins, desert dusts have in common a dominant fraction of quartz and clay (in terms of mass), a non-hygroscopic character, nearly no carbon, and a strong dependence of the coarse mode representation upon wind speed and distance from the source. The mean radius of sand particles is usually larger than 0.5  $\mu$ m, so the scattering coefficient is less in the "blue" (around 440 nm) than

in the near infrared (around 800 nm). The real part of the refractive index is within 1.5-1.6 (Longtin *et al.*, 1988) for the visible wavelengths, where the imaginary part is, however, strongly varying with the respective contribution of quartz and hematite (the latter being a mineral embedded in quartz crystals). Defining a typical model for desert dust is therefore always a compromise, and sensitivity studies are mandatory to assess the response of the remotely sensed dust optical thickness to changing properties of the actual dust. It is also noteworthy that among natural aerosols sand particles are those for which applying the MIE theory is probably the more questionable (Mishchenko *et al.*, 1997).



**Figure 1**. Variation of the path reflectance at 865 and 775 nm as a function of  $\tau_a$ , and shown as the ratio  $[\rho_{\text{path}} / \rho_r]$ . Sun zenith angle is 40°, viewing angle is 30°, and the perpendicular plane is considered. The maritime aerosol model is used for 4 values of the relative humidity, as indicated. Arrows illustrate a possible way for identifying a couple of aerosol models enclosing the actual aerosol.

## OUTLINE OF THE MERIS ATMOSPHERIC CORRECTIONS

The basic principle of the atmospheric correction of MERIS ocean color observations was presented in Antoine and Morel (1998a), and the corresponding algorithm was devised in Antoine and Morel (1997, 1998b), along with various tests and sensitivity studies. Very briefly, the scheme (see Fig. 1) starts with computing the ratio of the near infrared path reflectances,  $\rho_{\text{path}}$  (as measured by the sensor at 775 and 865 nm; no oceanic contribution there) to the reflectances of a hypothetical pure Rayleigh atmosphere at the same wavelengths,  $\rho_{\rm r}$  (note that reflectance is here radiance multiplied by  $\pi / E_{\rm s} \mu_{\rm s}$ , where  $E_{\rm s}$  is the extraterrestrial irradiance and  $\mu_{\rm s}$  is the cosine of the sun zenith angle). These ratios have been shown to be monotonous functions of the aerosol optical thickness,  $\tau_{\rm a}$ , and are unique for a given aerosol and geometry. They allow an aerosol type to be selected among several predefined models, by using Lookup tables (LUT) generated from radiative transfer simulations, and which contain the ratio  $[\rho_{\text{path}} / \rho_{\rm r}]$  for several aerosol models, geometries, and all relevant wavelengths. The selection of a couple of aerosol models, with their known spectral attenuation coefficients, allows the near infrared path reflectance to be propagated towards the visible, where the correction for the aerosol contribution becomes thus possible. The accuracy of such a multiple scattering algorithm is of ±0.002 in reflectance at 443 nm. For several reasons this multiple scattering algorithm is different from, yet similar in spirit to, that developed for the SeaWiFS instrument (Gordon and Wang, 1994; Gordon, 1997). The reader is referred to Antoine and Morel (1997; 1998a,b) for further details about the algorithm, as well as about the method for detection of aerosol absorption presented below.

#### DETECTION OF AEROSOL ABSORPTION

Errors exceeding the  $\pm 0.002$  acceptable limit occur when absorbing aerosols are present within the atmosphere (Gordon, 1997), except if their presence is *a priori* known and a specific LUT has been generated for that peculiar aerosol. Absorption is hardly detectable in the near infrared, because the spectral changes in scattering in this spectral domain are mainly determined by the aerosol size distribution, which can be similar for non-absorbing and strongly absorbing aerosols. In contrast, significant changes in the imaginary part of the refractive index may occur from the near infrared to the visible, the effect of which on the radiative regime is reinforced by multiple scattering. The marine contribution becomes however significant at these wavelengths, and varies with the chlorophyll concentration in waters; therefore it interferes with attempts of detecting aerosol absorption alone. Hypotheses about the oceanic signal are therefore mandatory. In the present work, and on the basis of numerous field values, we assume that the oceanic reflectance at 510 nm, in spite of being noisy, is independent of the chlorophyll concentration of waters, and averages 2% (see Antoine and Morel, 1997, 1998b).

In order to separately identify several kinds of aerosols (in particular absorbing as desert dust), the correction is performed at first with a limited set of five aerosol models, supposedly representative of standard maritime atmospheres (maritime models; Shettle and Fenn, 1979). Using the assumption of a constant oceanic reflectance at 510 nm, the error in atmospheric correction is obtained at this wavelength as the difference between the total reflectance (measured), the path reflectance (estimated with the maritime models), and the ocean reflectance (adopted mean value). If this error is negative and below a predefined threshold, it is an indication that  $\rho_{\text{path}}$  has been overestimated, and it is believed that desert dust is present. The correction is then redone by using specific LUTs, constructed for a given dust model, until the minimum error is found at 510 nm (note that a similar procedure is actually also applied for large positive errors, supposed to indicate the presence of continental aerosols, mainly composed of small and slightly absorbing water-soluble particles with a strong spectral dependence of scattering; see Fig. 2).

This method is different from others previously published (*e.g.*, Jankowiak and Tanré, 1992; Dulac *et al.*, 1996; Moulin *et al.*, 1997), as it is based on a preliminary detection of absorption before trying to infer optical thickness from the path reflectance. Therefore the present algorithm can be applied in a routine and global processing of ocean color, without the *a priori* knowledge of the area that is actually observed. DESERT DUST MODELS

The desert aerosol model of Schütz (1980) has been used here. The particle size distribution follows a lognormal law (mean radius = 0.5  $\mu$ m,  $\sigma/\ln(10) = 0.35$ ), and the wavelength-independent index of refraction is [1.53 – i 0.0055]. The ratio of extinction at



**Figure 2**. Aerosol extinction normalised at 865 nm, as a function of wavelength. The solid curves are for maritime aerosol models) at various relative humidities (Shettle and Fenn, 1979), and for an example of continental aerosol. The two dashed curves are for dust, either from (Schütz, 1980) or from WCRP (1986).

443 nm to extinction at 865 nm, as computed to the MIE theory, is 0.92 (see Fig. 2). The single scattering albedo of this strongly absorbing aerosol varies from 0.79 (443 nm) to 0.87 (865 nm). The LUTs are generated with the dust in the 2-12 km layer (the "free troposphere"), above the maritime aerosol located in the 0-2 km boundary layer. Various sharing of the tropospheric aerosol optical DETECTION LIMIT (THEORETICAL)

thickness among these two layers have been considered.

For sensitivity studies, another model has particle been selected, namely the "dust-like" component described in WCRP (1986),characterized by a modified gamma distribution (A = 5461.33,  $\alpha = 1$ ,  $\gamma = 0.5$ , and b = 16), and an index of refraction varying from [1.53 - i 0.008] at 443 nm to [1.52 - i 0.008] at 865 nm. The single scattering albedo is less than for the model of Schütz, and varies from 0.63 (443 nm) to 0.70 (865 nm). Yet the ratio of extinction at 443 nm to extinction at 865 nm is larger (0.96 instead of 0.92) because of the slightly decreasing real part of the refractive index between these two wavelengths.

At 510 nm,  $\rho_{\text{path}}$  is 0.06-0.07 for  $\tau_a \sim 0.1$ . The diffuse reflectance of the ocean, R, is about 0.02 at the same wavelength, and the corresponding value of the "normalised water leaving reflectance",  $[\rho_w]_N$ , which is about half R, is therefore 0.01. The scatter of field data around this mean value is of ±0.01 in R, so of ± 0.005 in  $[\rho_w]_N$ . Therefore, when subtracting from the total reflectance (measured) the sum [estimated  $\rho_{\text{path}} + \text{supposed mean value of } [\rho_w]_N$ ], the remaining quantity is the sum of the error in atmospheric correction (*i.e.*, the error in  $\rho_{\text{path}}$ ), plus the error in the guessed value for  $[\rho_w]_N$ . The error in  $\rho_{\text{path}}$  is therefore obtained at ±0.005, *i.e.*, something like 10%. If this uncertainty is above the error caused by wrongly using a maritime aerosol model while the actual aerosol is dust, the shortcoming cannot be detected. The errors in  $\rho_{\text{path}}$  due to the selection of an irrelevant aerosol model become, however, greatly larger than the ±0.005 uncertainty as far as  $\tau_a$  become greater than 0.1-0.2, which is usually the case when absorbing aerosols are blown above the ocean. In summary, the detection limit of the present method should be at  $\tau_a \sim 0.1$  at 865 nm.

# RESULTS

SeaWiFS images acquired above the Mediterranean Sea (7<sup>th</sup>, 8<sup>th</sup>, and 9<sup>th</sup> of May, 1998, plates 1, 2, and 3) and off Mauritania (3<sup>rd</sup> of October, 1997, plate 4) have been acquired at NASA/GSFC through the DAAC web interface, and processed by using the technique described above (with the necessary adaptation to the spectral characteristics of SeaWiFS, not detailed here). Any pixel for which the radiance at 865 nm is lower than 23 mW cm<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup> has been processed (this crude test allows most of clouds and lands to be rejected from the analysis). The results are displayed here as 3 plates for each image, showing the radiances at 865 nm (SeaWiFS level 1a data), the type of aerosols identified by the present technique, and their optical thickness at 865 nm.

On May 7 (plate 1), an intense dust plume originating from Libya extends over the Ionian Sea, leaving the coast around 33°N, 14°E. The aerosol load is so large that part of the plume has been classified as clouds by the simple single-threshold test cited above. The rest of the image is mainly covered by maritime aerosols,

except near the coasts of the Adriatic Sea and the south of France, where continental influences may prevail. The dust plume, whose optical thickness is between 0.2 and 0.5, is still there the day after and partly masked by clouds (May 7, Plate 2, SeaWiFS aims now at the easternmost part of the plume), while it has probably collapsed on May 8 (Plate 3, the large white area centered on Sicily is sun glint), giving way to aerosols classified here as continental ones (*i.e.*, aerosols with a strong spectral dependence of scattering). Dust plumes have been often observed at the same location (*e.g.*, Moulin *et al.*, 1997; they used Meteosat data). This succession is quite coherent with the progressive sink of the largest sand particles during transport above the ocean (these large particles being mainly responsible for ratios c(443)/c(865) < 1), leading to a progressive increase of the spectral dependence of aerosol scattering.

The dust outbreak off Mauritania, obvious when looking at the level 1a radiances, is well detected (Plate 4), with optical thicknesses often above 0.5 (values up to 2 have been retrieved).

Should the dust model of WCRP (1986) had been used instead of that proposed by Schütz (1980), the results would not have been significantly altered neither qualitatively (aerosol identification) nor quantitatively (optical thickness).

#### CONCLUSION

It is demonstrated here that detecting desert dust — even at relatively low concentration — is possible with SeaWiFS, and will be possible with MERIS (detection limit at  $\tau_a \sim 0.1$ ), owing to a relatively simple algorithm. The systematic use of such an algorithm when processing satellite observations of ocean color should allow a more thorough detection and quantification of atmospheric dust transport than in the past and with other sensors. Sun photometer measurements would be extremely valuable, however, in order to validate the retrieved optical thicknesses.

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(numerical counts in the range 0-1024).

Plate 1b : aerosol types identified in the image of May Plate 1a : SeaWiFS Level 1a image of May 7, 1998. 7, 1998 (plate 1a). Light gray, gray, and black are for The radiance at 865 nm is shown as raw data maritime aerosols, continental aerosols, and desert dust respectively. White areas are for lands, as well as for clouds and possibly sun glint (indicated by the letter G).



Plate 1c : aerosol optical thickness at 865 nm, for the image of May 7, 1998 (see plates 1(a) and 1(b)).



Plate 2a : SeaWiFS Level 1a image of May 8, 1998.Plate 2b : aerosol types identified in the image of MayThe radiance at 865 nm is shown as raw data8, 1998 (plate 2a). Gray scale as in Plate 1a.(numerical counts in the range 0-1024).



Plate 2c : aerosol optical thickness at 865 nm, for the image of May 8, 1998 (see plates 2(a) and 2(b)).



Plate 3a : SeaWiFS Level 1a image of May 9, 1998.The radiance at 865 nm is shown as raw data(numerical counts in the range 0-1024).Plate 3b : aerosol types identified in the image of May 9, 1998 (plate 3a). Gray scale as in Plate 1a.



Plate 3c : aerosol optical thickness at 865 nm, for the image of May 9, 1998 (see plates 3(a) and 3(b)).



**Plate 4a** : SeaWiFS Level 1a image of October 3, 1997. The radiance at 865 nm is shown as raw data (numerical counts in the range 0-1024).

**Plate 4b** : aerosol types identified in the image of October 3, 1997 (plate 4a). Gray scale as in Plate 1a.



Plate 4c : aerosol optical thickness at 865 nm, for the image of October 3, 1997 (see plates 4(a) and 4(b))

# 10. Appendix 3 : colour plates for selected SeaWiFS images



**Plate 1.** Map of the chlorophyll concentration, as derived from a SeaWiFS image (May 7, 1998). Left panel corresponds to the use of the MERIS algorithms, while the right panel shows the data produced through SeaDAS v3.2. Colour coding corresponds to increasing chlorophyll concentrations, in mg m<sup>-3</sup>. The "trace" of the dust plume is seen on the left panel, north of Lybia (see text, section 5.3 and Appendix 2).





**Plate 2.** Map of the chlorophyll concentration, as derived from a SeaWiFS image (March 5, 1998). Left panel corresponds to the use of the MERIS algorithms, while the right panel shows the data produced through SeaDAS v3.2. Colour coding corresponds to increasing chlorophyll concentrations, in mg m<sup>-3</sup>. The "trace" of the dust plume is seen on the left panel, off Africa (see text, section 5.3 and Appendix 2).

# ATBD 2.7 — MERIS data product summary sheet (water-leaving reflectances)

Product Name:	Water-leaving reflectance
Product Code:	MERIS-LW
Product Level:	2
Description of the product:	Normalised Water-leaving reflectance

 $\rho'_{w}(\lambda,\theta_{s},\theta_{v},\Delta\phi) = \pi \cdot \frac{L_{w}(\lambda,\theta_{s},\theta_{v},\Delta\phi)}{E_{d}(0+)(\lambda,\theta_{s})}$ 

where  $L_w(\lambda, \theta, \theta_s, \Delta\phi)$  is the Water-leaving radiance, i.e. the radiance exiting the ocean at a given wavelength, for given geometrical conditions,  $E_d(0+)(\lambda, \theta_s)$  the down-welling irradiance above the water surface

# **Product Parameters:**

Coverage:	global
Packaging:	Half-orbit (RR), image (FR)
Units:	dimensionless
Range:	00.2
Sampling:	pixel-by-pixel
Resolution:	
Accuracy:	0.002
Geo-location Requirements:	latitude, longitude, Sun and view zenith angle, azimuth difference
Format:	2 bytes per band, linearly scaled
Appended Data:	geo-location, flags.
Frequency of generation:	every orbit
Size of the Product:	

# **Additional Information:**

Identification of bands used in algorithm: Assumptions on MERIS input data: 510, 705, 775, 865 nm used to correct bands 1 to 8 TOA reflectance, corrected for stratospheric aerosol (if present) and gaseous absorption

Identification of ancillary and auxiliary data: ancillary data: wind speed, ozone, pressure Assumptions on ancillary and auxiliary data:

# ATBD 2.7 — MERIS data product summary sheet (aerosol optical thickness at 865 nm)

<b>Product Name:</b> Product Code: Product Level: Description of the product:	Aerosol optical thickness at 865 nm MERIS-TAUA 2 Aerosol optical thickness at 865 nm.
<b>Product Parameters:</b>	
Coverage:	global
Packaging:	Half-orbit (RR), image (FR)
Units:	dimensionless
Range:	0.01-2
Sampling:	pixel-by-pixel
Resolution:	
Accuracy:	about 15%, or 0.02 for moderate values ( <i>i.e.</i> , around 0.1-0.2)
Geo-location Requirements:	latitude, longitude, Sun and view zenith angle, azimuth difference
Format:	1 byte, linearly scaled
Appended Data:	geo-location, flags.
Frequency of generation:	every orbit
Size of the Product:	

# **Additional Information:**

Identification of bands used in algorithm: Assumptions on MERIS input data: 775 and 865 nm TOA reflectance, corrected for stratospheric aerosol (if present) and gaseous absorption

Identification of ancillary and auxiliary data: ancillary data: wind speed, ozone, pressure Assumptions on ancillary and auxiliary data:

# ATBD 2.7 — MERIS data product summary sheet (aerosol type)

Product Name:	Aerosol Epsilon
Product Code:	MERIS-AER
Product Level:	2
Description of the product:	ratio between aerosol reflectance at 775 and 865 nm
	$\varepsilon(775,865) = \frac{\rho_a(775)}{\rho_a(775)} = \frac{\rho_{path}(775) - \rho_R(775)}{\rho_R(775)}$

$$(7/5,865) = \frac{\rho_a}{\rho_a(865)} = \frac{\rho_{path}}{\rho_{path}(865) - \rho_R(865)}$$

where  $\rho_{path}$  is the atmosphere reflectance,  $\rho_R$  the reflectance due to Rayleigh scattering,  $\rho_a$  the aerosol reflectance

# **Product Parameters:**

Coverage:	global
Packaging:	Half-orbit
Units:	Dimensionless
Range:	0.92
Sampling:	pixel-by-pixel
Resolution:	
Accuracy:	
Geo-location Requirements:	latitude, longitude, Sun and view zenith angle, azimuth difference
Format:	1 byte /pixel, linearly scaled
Appended Data:	geo-location, flags.
Frequency of generation:	every orbit
Size of the Product:	

# **Additional Information:**

Identification of bands used in algorithm: Assumptions on MERIS input data:

Identification of ancillary an auxiliary data: Assumptions on ancillary and auxiliary data: 775, 865 nm TOA reflectance, corrected for stratospheric aerosol (if present) and gaseous absorption

# ATBD 2.7 — MERIS data product summary sheet (aerosol flags)

Product Name:	Absorbing Aerosol Flags
Product Code:	
Product Level:	2
Description of the product:	Boolean flags indicating
	the presence of continental aerosol
	the presence of desert dust aerosols
Product Parameters:	
Coverage:	global
Packaging:	Half-orbit, with pixel annotation flags
Units:	Boolean
Range:	{False, True}
Sampling:	pixel-by-pixel
Resolution:	
Accuracy:	
Geo-location Requirements:	latitude, longitude, Sun and view zenith angle, azimuth difference
Format:	2 bits/pixel, linearly scaled
Appended Data:	geo-location, flags.
Frequency of generation:	every orbit
Size of the Product:	

# **Additional Information:**

Identification of bands used in algorithm: Assumptions on MERIS input data:

Identification of ancillary an auxiliary data: Assumptions on ancillary and auxiliary data: 510, 705, 775, 865 nm TOA reflectance, corrected for stratospheric aerosol (if present) and gaseous absorption