STUDY OF THE MERIS AEROSOL OPTICAL THICKNESS RETRIEVAL AND SENSITIVITY TO NEAR INFRARED REFLECTANCES

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ABSTRACT

This work is a part of a global revision effort of the MERIS Atmospheric Correction, aiming at reducing recently observed errors in the reflectances of water-leaving radiances. It focuses mainly on the aerosol optical thickness computation, which is one step of the correction. Error estimates at three sites characterized by case 1 waters are first presented, to illustrate the discrepancies between the reflectances measured in situ and those retrieved by the MERIS ground segment algorithm. The algorithm is summarized, emphasizing the role and the weaknesses of the look-up tables involved in the optical thickness retrieval and in the water-leaving reflectances computation. The link between both quantities is made explicit through the generation of look-up tables.

1. INTRODUCTION

Since the first MERIS processing in 2002, a large amount of data is now available for comparing the results of the algorithmic chain with in situ measurements. In this context, the most recent validation activities [1-4] have pointed out some systematic errors in the water branch processing, either directly in the water reflectances, or in the aerosol optical thickness (AOT) retrieval. For instance, and to keep figures in mind, [2] states a significant overestimation of water-leaving reflectances in the Mediterranean sea (few tens of percent in the blue), while [1] notes an averaged overestimation of 70% in AOT at 865nm for the coastal northern Adriatic Sea. This has led us to undertake a step-by-step check of the whole atmospheric correction (AC), from the input top-of-atmosphere (TOA) radiances up to the final marine reflectances.

In this paper, the choice is made to focus on AOT retrieval, although this quantity is generally considered as only a by-product of MERIS. At least three reasons motivate this study:

- Firstly, the computation of the path reflectance (i.e. aerosol and Rayleigh reflectance) and the selection of the aerosol model are directly linked to the near infrared (NIR) AOT, albeit in a rather complex way.
- Secondly, AOT is one of the few quantities that can be easily measured from the ground, in particular with the Aerosol Robotic Network (AERONET), hence constituting a valuable checkpoint of the atmospheric correction.
- Lastly, the Algorithm Theoretical Basis Document of MERIS [4] sets a goal in the AOT retrieval: accuracy of 15% or 0.02 for moderate values, a value that it would be advisable to check.

The first point underlines the difficulty of the analysis. The relationships between AOT and path reflectance is established through the use of Look-up tables, first in the NIR to select the aerosol model, then at other wavelengths to compute path reflectance on the whole spectrum of MERIS. This is why we believe that studying both quantities altogether may be instructive in the understanding of the whole retrieval, even if errors might arise from other sources, like transmittance computation.

The purpose of this study is on the one hand to quantify AOT errors over ideal clear water cases, and on the other hand to identify through a detailed review of the algorithm the source of these errors.

The outline of the paper is as follows: In the next section we introduce the procedure for processing the largest number of matchups as possible under ideal conditions, and determine the observed accuracy of the algorithm in terms of AOT. In the third section a brief summary of the AC algorithm is given, focusing on the link between AOT and path reflectance, as well as error propagation from one quantity to the other. The last section presents a sensitivity study to aerosol LUTs and NIR reflectances, giving some clues as to what can be expected and what could be improved in the current methodology.

2. AOT ERROR ESTIMATES OVER CASE 1 WATERS

2.1 Procedure for data processing

In a first attempt, we want to check the AC independently from other processing branches, under ideal conditions rather than for the whole range of applications of MERIS. Hence case I water sites have been searched for scenes with convenient meteorological conditions to be processed. In addition, the need for reliable and abundant in situ measurements has led us to choose the three following island AERONET sites surrounded by clear water:
- Ascension Islands (7°58’S, 14°24’W) in the South Atlantic,
- Lampedusa (35°31’N,12°37’E) in the Mediterranean sea,
- Lanai (20°44’N, 156°5’W) in the North Pacific.

These sites are giving continuous AOT measurements throughout the year. In order to analyze the largest amount of data, we have processed all orbits passing over the sites from 2002 to 2005, limited of course by the AERONET availability [table 1].

<table>
<thead>
<tr>
<th>Site</th>
<th>2003</th>
<th>2004</th>
<th>2005</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lampedusa</td>
<td>May to Dec.</td>
<td>Jan. to Jun.</td>
<td>None</td>
</tr>
</tbody>
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Table 1. Months of available AERONET measurements

The rule for data screening consists in choosing a window around the island, large enough to include water and small enough to avoid dispersion of the AOT around the sun photometer. Typically, a square of 21x21 Reduced Resolution pixels fulfills these conditions. Then the water pixels are kept only if none of the following MERIS Level 2 flags is raised: PCD_1_13, PCD_19, LOW_SUN, MEDIUM_GLINT, ICE_HAZE, CASE2_ANOM. Let us remind that PCD_19 is precisely a confidence flag for the computation of aerosol Angström coefficient and AOT. Eventually, the match-up is considered correct and a spatially averaged AOT is computed if more than half of the water pixels in the window are valid.

These somehow restrictive criteria filter about ninety percents of the scenes, leaving at the end 17 match-ups for Ascension Island, 26 for Lampedusa and 23 for Lanai, what makes a total of 66 ideal match-ups.

2.1. Observed error estimates

We begin this section by first commenting few individual cases, representative of the AOT retrieval. Fig. 1 shows a typical situation, where the retrieval in the blue lies within the acceptable error bar (-5% of relative error with respect to the in situ data), whereas the error in the NIR reaches more than 30%. This kind of discrepancy makes us doubt both about the initial discrepancy at 865 nm and the aerosol model selection.

By comparison, the spectral dependence in Fig. 2 seems much better retrieved, despite a gap of 43% in the NIR and 27% in the blue.

On the other hand, we have also observed a few very good situations, like the one in Fig. 3: the agreement between MERIS and AERONET is almost perfect along the whole spectrum (error of respectively 13% and 4% in the NIR and blue).

Our worry is then that extremely large errors of doubtful origin may occur even for very clear scene. For instance Fig. 4 displays error of 190% in the NIR and 120% in the blue, despite a very clear and cloud-free area, for which all conditions have been carefully inspected (wind modulus lower than 4.5m.s⁻¹).

The first simple conclusion is the difficulty for MERIS to retrieve low optical thickness in the blue.
The numbers for all matchups are summarized on Fig. 5, where it can be seen that largest errors occur for low optical thicknesses, typically below 0.1. A lot of cases show a relative error around 50%. As for low values the relative error is somehow meaningless, we also display in Fig. 6 the signed error (difference between MERIS and AERONET data), where it is noteworthy that most of the cases lie outside the quality goal of 0.02 (which is also the uncertainty of the CIMEL measurements, see [2]).

The spectral dependence retrieval also fails very often, making MERIS and in situ AOT curves crossing each other around 500 nm, like in Fig. 1.

Consequently the relative error is less pronounced in the blue than in the NIR, though again of several tens of percents.

In the next sections we will try to connect this discrepancy to another observed trend of MERIS, the overestimation of water leaving reflectance by tens of percents. Unfortunately, as there is no ground-based marine reflectance measurement around the three considered islands, we shall study this point more theoretically, looking into more details at the AC algorithm.

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To conclude this section, let us stress that the range of in situ AOT presented in Fig. 5 exposes the limitations of our study and underlines the difficulty of finding appropriate matchups. However the question of such a systematical overestimation in AOT remains open, and we shall investigate carefully the processing algorithm.
3. MERIS ATMOSPHERIC CORRECTION AND AOT RETRIEVAL

3.1. Review of the methodology

In this section we briefly recall the MERIS atmospheric correction, focusing on the aerosol model retrieval and path reflectance computation through AOT estimates. Details and theoretical justifications of the methodology, out of the scope of this proceeding, are fully described in [5-6]. For better legibility, geometrical and wind dependence of LUTs will always be omitted in the following.

The principle of the AC is to start from NIR signal, which is not contaminated by the water reflectance for case 1 waters, due to its strong absorption at such wavelengths. A so-called bright pixel atmospheric correction (BPAC) step is however always activated in the current processor, to remove the possible contribution of water constituent. The input data of the AC consists thus in two TOA reflectances, at 865 and 779 nm, corrected for gaseous absorption, sun glint effect (globally noted \( \rho_{gc} \)) and for BPAC. We shall note in the following these entries of the AC as \( \rho_{AC}(\lambda), \lambda = 865 \) or 779 nm.

Hence these reflectances are supposed to consist only of the path reflectance \( \rho_{path} \), which is the combination of Rayleigh and aerosol reflectance:

\[
\rho_{path}(\lambda) = \rho_{AC}(\lambda) \quad \text{for} \quad \lambda = 865 \text{ and } 779 \text{ nm.} \tag{1}
\]

For other wavelengths, the water-leaving reflectance is not any longer negligible and the TOA reflectance \( \rho_{AC}(\lambda) \) writes

\[
\rho_{AC}(\lambda) = \rho_{path}(\lambda) + t_{d}(\lambda) \rho_{u}(\lambda) + t_{w}(\lambda) \rho_{w}(\lambda), \tag{2}
\]

where \( \rho_{w} \) stands for the water-leaving reflectance at surface level, and \( t_{d} \) and \( t_{w} \) for the total downward and upward transmittances.

The aim of the AC is thus to compute \( \rho_{path} \) and the transmittances at all wavelengths from the two NIR reflectances \( \rho_{AC} \). Because the Rayleigh reflectance \( \rho_{R} \) is known accurately, the atmospheric boils down to the correction to the retrieval of the aerosol reflectance.

The way the current processor computes \( \rho_{path} \) is however not directly based on the signal decomposition into the sum of Rayleigh and aerosol contributions, but on the ratio \( \rho_{path}/\rho_{R} \), noted as \( \zeta \):

\[
\zeta(\lambda) = \rho_{path}(\lambda)/\rho_{R}(\lambda). \tag{3}
\]

This ratio is the core of the AC. Of course determining \( \zeta \) leads directly to \( \rho_{path} \) and reciprocally: hence \( \zeta(865) \) and \( \zeta(779) \) becomes the new inputs of the AC, while they are the new unknowns at other wavelengths. The crucial assumption upon which the whole AC lies is the link, for a given aerosol model, between the ratio \( \zeta \) and the AOT \( \tau \) through a tabulated relationship of the general form

\[
\zeta(\lambda) = P(\lambda, \tau(\lambda), i), \tag{4}
\]

where \( i \) the index of the aerosol model. The exact relation between \( \zeta \) and \( \tau \) will be detailed in the next section. Physically, the ratio is nearly linearly increasing with \( \tau \).

On the other hand, the values of \( \tau \) can be determined at all wavelengths, for a given model, starting from 865 nm through known tabulated spectral dependence:

\[
\tau(\lambda) = f(\tau_{865}, \lambda). \tag{5}
\]

Schematically, the AC formulation is thus composed of two unknowns, the value of \( \tau_{865} \) and the model \( i \), and two equations by the evaluation of Eq. 4 at 865 and 779 nm:

\[
\zeta(865) = P(865, \tau_{865}, i), \tag{6}
\]

\[
\zeta(779) = P(779, f(\tau_{865},779,i),i),
\]

what makes the problem \textit{a priori} well-posed.

In practice, as the unknown \( i \) is constrained to an integer value in a fixed set of models, this system is solved twice, to get an aerosol couple \( \{i_1, i_2\} \) that best fits Eq. 6. Then an averaged AOT \( \tau \) is computed for a mixing model. Finally the correction can be achieved, from \( \tau_{865} \) and \( i \) to \( \tau(\lambda) \) through Eq. 5, then to \( \zeta(\lambda) \) through Eq. 4 and eventually to \( \rho_{path}(\lambda) \) through Eq. 3.

The main relationship Eq. 4 reveals that any error in AOT is strongly coupled to error in the model retrieval and the path reflectance. The aim of the next section is to quantify this coupling.

3.2 Link between path reflectance and AOT

The resolution of Eq. 6 needs an easy evaluation and inversion of the function \( P \). In the current version of the processor, it is approximated by a polynomial of second order in \( \tau \), whose coefficients depend on the wavelengths \( \lambda \) and the aerosol model \( i \). In other words, for each current 34 aerosol models of MERIS and 15 bands, there is a polynomial linking \( \tau \) to the ratio \( \rho_{path}/\rho_{R} \) - we recall here that the geometrical and wind
dependence is omitted in this paper. These polynomials have been constructed by a mean-square fit over outputs of a radiative transfer code (RTC), computing path and Rayleigh reflectances for different aerosol loads, for all aerosol models. The fit has used five points $(\tau, \zeta_i)$ plus the point $(0,1)$ that corresponds physically to an aerosol-free atmosphere. We display on Fig. 5 the plot of such polynomials, for all models.

Several remarks must be made here:
- Firstly a series of aerosols (from 13 to 29) seems to be totally out of range near the origin, missing out the point $(0,1)$. In practice, all of them are not any longer used in the AC – they correspond to absorbing aerosols – and thus can be ignored. This is however not the case for model number 12, which is rather worrying.
- Secondly, looking in details at the other models (from 0 to 11 and 31 to 33) shows again a discrepancy near the origin, although to a lesser extent. In particular curves are crossing each other.
- Thirdly in some situations (other geometries for instance), the polynomials may prove to be not monotonous, decreasing for high AOT (figure not shown here). This problem should not block the inversion of polynomials on the physical range of AOT (low in the NIR), but certainly brings questions about the quality of the least-square fit.

We wonder if some errors in these tabulated functions $\zeta$ could explain error on AOT, as well as on the path reflectance. It is obvious that for a given NIR path reflectance, different slopes of the curves would produce different AOTs, but the combination of two NIR bands may compensate the errors, what does not allow to draw a straightforward conclusion. We will make this point clearer in the next section, and would like here to only link the observed discrepancies in AOTs to errors in path reflectances, whatever the accuracy of the $\zeta$ functions. A very simple rough estimate can be made, as follows.

Assume the link between $\tau$ and $\zeta$ to be linear, which is nearly the case for low AOT (see Fig. 5 and also [5-6]):

$$\zeta(\tau) = a_i \tau + b_i$$

for $\tau << 1$, (6)

where the index $i$ stands again for the aerosol model, supposed to be known or fixed. Then any relative error $\Delta \tau / \tau$ in AOT is equivalent to a relative error in $\zeta$ of

$$\Delta \zeta / \zeta = \frac{d \tau}{d \tau} \Delta \tau / \tau .$$

(7)

For a common case, $\tau < 0.1$, $b_i$ should be unity whatever the model is, and $a_i$ is of the order of 10; note however that this latter coefficient is really dependent on the model, and could be twice as large as shown on Fig. 7. This leads roughly to $\Delta \zeta / \zeta \approx 0.5 \Delta \tau / \tau$, which is consequently also the relative error on $\rho_{\text{path}}$ as soon as the Rayleigh reflectance is correct. Let us take as an example 50% of relative error in $\tau$ at 865 nm, which is a very typical value according to previous analyses (cf. section 1 and [2] for instance); then we conclude that the computed AOT should be the one of a 25% corrupted NIR reflectance! Practically, as in actual fact the algorithm starts from the TOA reflectances, this rough estimate reveals the discrepancy in the aerosol model retrieval, linked to the observed error in NIR AOT.

4. SENSITIVITY OF THE ATMOSPHERIC CORRECTION

To begin this section, since the AC is based on a two bands approach, we would like to summarize it on at two-dimensional graph. This will remove the problem of error compensation between both bands, and make our explanations clearer. For each model and a given AOT at 865 nm, we are indeed able to compute on the one hand $\zeta(865)$, and on the other hand $\zeta(779)$, then $\zeta(779)$. This is done through two LUTs symbolized by Eq. 4 and Eq. 5. Thus each model can be characterized in the NIR by a parameterized curves {[$\zeta(865)$, $\zeta(779)$], see Fig. 8, the parameter being $\tau(865)$}. From this point of view, the AC amounts to start from the actual point ($\zeta(865), \zeta(779)$), and search in this NIR plane the two bracketing curves. This is a resolution of Eq. 6 totally equivalent to the one done in the current processor.

4.1 Sensitivity to NIR reflectance’s

At first sight Fig. 8 makes us strongly wonder about the sensitivity of the algorithm, the curves being really close to each other - even sometimes crossing, which implies the non-unicity of the aerosol retrieval. This is
particularly true in the realistic range of small AOT, hence small $\zeta$.

The simplified point of view of Fig. 8 allows us to study the sensitivity of the AC to NIR reflectance’s, as well as to errors in tabulated $\zeta$ functions: indeed, a few percent error in the polynomial coefficients is strictly equivalent to a few percent error in the NIR bands, by a computation similar to Eq. 7.

We can make a straightforward experiment consisting in corrupting both NIR reflectances by at most 0.5%, and then feeding the processor with them:

$$\rho_{\mathrm{ac}}^j (865) = \rho_{\mathrm{ac}} (865) \times (1 + \varepsilon_j),$$

$$\rho_{\mathrm{ac}}^k (779) = \rho_{\mathrm{ac}} (779) \times (1 + \varepsilon_k),$$

where $\varepsilon_j$ and $\varepsilon_k$ range from –0.005 to +0.005, by a step of 0.0025 (thus taking 5 values). Note that both bands are corrupted independently and simultaneously, to make 25 configurations on total.

The test is made on a different site than the ones used previously, the *Boussole* buoy in Mediterranean sea, because we also would like to draw conclusions on water-leaving reflectances available there and known to be rather poorly retrieved in the blue, see [3] and [4]. In that aim sixteen matchups, chosen for their optimal meteorological conditions, have been processed.

The results in AOT are presented on Fig. 9, where we display the relative change at 865nm with respect to the original AOT; each vertical line corresponds to a single matchup and is composed of the resulting 25 configurations. The relative change ranges from -25% to 50% for low AOT, but on average remains between ±10%. What is noteworthy is the apparently very easy way of reducing the AOT by 10% with only a relative change of 0.5% in NIR reflectance’s, or, equivalently, in AC LUT.

Another interesting feature is the distribution of these relative changes with respect to the configurations in NIR reflectance’s perturbations (see Fig. 10). It appears that largest change occur for transversal perturbations. On the example of Fig.10, only +0.2% at 865nm and -0.25% at 775nm are sufficient to change AOT by around 10%.

Let us now present the resulting changes in water-leaving reflectances, due to the same perturbation in NIR bands. As diffuse transmission should be rather robust to AOT, it is also a way to analyze the path reflectance in the visible spectrum, (cf Eq. 2). On Fig. 11 we can see that the resulting relative changes in water-leaving reflectances range from round –15% to 15%. The mean is around 5%, which is still rather large; furthermore we should not forget that here again a major effect is produced easily by weak NIR perturbations (around 0.2%), if done in a transversal manner. Contours of relative changes in water-leaving reflectances are similar to Fig.10, and are not shown here.
Figure 10. Contours of relative change in AOT at 865nm, in the NIR plane. X-axis: relative perturbation of reflectance at 865nm. Y-axis: relative perturbation at 779nm. Distance between two adjacent curves corresponds to 1% of relative change.

Figure 11. Relative change in water leaving reflectance at 443 nm due to corrupted NIR reflectance’s, versus original value.

4.1 Sensitivity to $\rho_{\text{path}}/\rho_{\text{R}}$ LUTs

Another way to directly emphasize the sensitivity of the AC to the LUTs consists simply in testing different $\rho_{\text{path}}/\rho_{\text{R}}$ tables commonly used by different teams. We today have easily access to at least two set of tables: the one’s of the current processor MEGS 7.4, and the one’s from the Laboratoire d’Océanographie de Villefranche (LOV), provided to us by David Antoine. Although they should contain the same physics, they differ from the RTC that generated them, and also in the polynomial fit (LOV polynomials are sometimes of order one).

The same experiment of section 2.1 has been realized with the LOV tables, and results are presented in Fig. 12, to be compared to Fig. 6. We observed that more points lie in the quality goal of 0.02, despite a larger disparity around $r=0.1$. It is also clear that a bit more points have slipped above the X-axis, i.e. reducing the overestimation trend, particularly for Ascension Island. Our aim is not to advocate for one table or another, but to illustrate the influence of LUTs: here it appears that the quality goal of 0.02 in AOT cannot be met, due to high sensitivity to LUTs.

5. CONCLUSION

Although it is generally admitted that a good AOT retrieval is not sufficient and even not always necessary for a successful atmospheric correction, we have observed that MERIS errors in AOT and water leaving reflectance evolve in the same direction and remain perfectly coherent: for a given NIR reflectance, computing a too high AOT means choosing a too flat model, which result in decreasing the path reflectance at other wavelengths, hence underestimating the atmospheric correction. The other possible source of error, not studied here, could be related to the diffuse downward and upward transmittances (cf. Eq. 2) that could explain on their own, if underestimated, the discrepancy in marine reflectance.

The sensitivity of the algorithm to NIR reflectance’s (or equivalently to AC LUTs) has been quantified over ideal matchups in the following manner: a perturbation of less than 0.5% in NIR reflectance’s produces roughly a 10% change in AOTs at 865 nm, and 5% in water leaving reflectance at 443 nm. But these numbers might double or even triple according to the distribution of the perturbed signal at 779 and 865 nm (transversal perturbation). This sensitivity study shows also that the overestimation both in AOT and water-leaving reflectance could be softened.

This sensitivity puts accuracy constraints on all pre-corrections of the TOA signal (straylight, gas, etc.) as well as BPAC.
Moreover, a general revision of the LUTs seems mandatory, in order to answer the questions: why are the polynomial fits so dubious in some cases and why do they differ so greatly between different RTC versions? Other aspects of LUT generation, for instance the sampling of the $\rho_{pol}/\rho_R$ tables, could also improve the quality of the AC, in particular for low AOTs.

All these points are currently under investigation.

6. ACKNOWLEDGEMENTS

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7. REFERENCES


7. AERONET site: http://aeronet.gsfc.nasa.gov