

# Vicarious adjustment of MERIS reflectances using an inverse technique.

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## ABSTRACT

The method used for the vicarious adjustment of the SeaWiFS & MERIS ocean colour data relies on the assumptions that the water-leaving radiance is negligible in the Near Infra-Red (NIR) in oligotrophic waters, and the NIR band is perfectly calibrated. Here, a novel approach to vicarious adjustment is proposed that does not need these assumptions: a least-squares inverse technique is used to adjust the most uncertain parameters in the atmosphere model: the aerosol scattering ( $\rho_a$ ) and the error in the ozone optical depth ( $d\tau_{oz}$ ) within their error bars to obtain a best fit between the satellite and buoy water reflectance. Examples are presented using match-ups of satellite and in situ observations from MERMAID (the MERIS Match-up In-situ Database) for the MOBY, Gustav Dalen, BOUSSOLE and AAOT platforms. The new method predicts the lowest  $d\tau_{oz}$  for MOBY, the lowest  $\rho_a$  for the Gustav Dalen site, and the largest values of both at AAOT. The method is simple to code, potentially more flexible than the present gain method, can weight observations for reliability and predicts poorly-known atmospheric properties. However, it requires accurate physics, a good initial guess, enough data for convergence and cannot correct biases. The method could be tested by running it in parallel with the existing method.

## 1. INTRODUCTION

The total top of atmosphere reflectance (symbol:  $\rho_{gc}$ ) seen by the MERIS (Medium Resolution Imaging Spectrometer) instrument onboard ESA's ENVISAT satellite is given by the formula

$$\rho_{gc}(\lambda) = [\rho_R(\lambda) + \rho_a(\lambda) + \rho_w(\lambda)t_d(\lambda)]\tau_{oz} \quad (1)$$

Where  $\rho_R(\lambda)$  is the Rayleigh scattering from the atmosphere,  $\rho_a(\lambda)$  is the aerosol scattering plus coupling with the Rayleigh scattering,  $\rho_w(\lambda)$  is the water reflectance; the required parameter which enables the prediction of ocean colour and

chlorophyll concentration,  $\tau_{oz}$  is the ozone optical depth which can be written in terms of an error  $d\tau_{oz}$

$$\tau_{oz} = e^{-d\tau_{oz}m} \quad (2)$$

and  $t_d$  is the diffuse transmittance, the fraction of the water-leaving radiation that can penetrate upwards through the atmosphere, and is given by

$$t_d = e^{-\frac{\tau m}{2}(1-f_w)\tau_{aer}m} \quad (3)$$

where  $\tau$  is the Rayleigh scattering optical depth, typically 0.1 m, and  $m=1/\cos\theta_s+1/\cos\theta_v$ . Where  $\theta_s$  is the satellite Solar zenith angle and  $\theta_v$  is the satellite viewing angle. If we neglect the aerosol part of the total transmission (the term with  $\tau_{aer}$ ) then

$$t_d = e^{-\frac{\tau m}{2}} \quad (4)$$

Rearranging (1) for  $\rho_w$  and substituting we have

$$\rho_w(\lambda) = [\rho_{gc}(\lambda)e^{d\tau_{oz}m} - \rho_R(\lambda) - \rho_a(\lambda)]e^{\frac{\tau m}{2}} \quad (5)$$

The current method for adjusting SeaWiFS and MERIS data (simplified here for brevity) takes in-situ measurements of  $\rho_w$  co-located with satellite observations. An atmosphere model is then used to predict the top of the atmosphere signal. A gain for each observed wavelength is then defined by dividing this predicted signal by the satellite TOA observation. The gain is averaged to obtain a mission gain, and this is then applied to correct the satellite data. For further details, see [1] and [2].

This gain method is a crude way to correct the data, for uncertainties may exist in many components of the atmospheric model (on the right hand side of Eq. 5) and the single gain parameter has to cover the errors in all of them.

Therefore a new method is tried here: the two most uncertain parameters in the atmosphere model, the aerosol scattering  $\rho_a$  and the error in the ozone optical depth:  $d\tau_{oz}$  are adjusted to achieve the best

least squares fit between the satellite and in-situ observations (more parameters, or different ones, could be adjusted instead). A least squares inverse technique based on [3] was used. They used this method to adjust air-sea heat flux coefficients to minimise differences in the ocean northward heat transport observed from ship transects and calculated by integrating the air-sea fluxes. In this case the method determines the values of  $\rho_a$  and  $d\tau_{oz}$  that best fit the  $\rho_w$  derived from the satellite data to the in-situ values. The advantages of this technique are

1. The adjustments will be nonlinear (see Eq. 5) and potentially more flexible than the gain method (see the discussion).
2. The predicted  $\rho_a$  and  $d\tau_{oz}$  are measurable values and so can be checked against observations to see if they are sensible. The gain cannot be so easily checked.
3. The weighting matrix (see below) allows us to weight our reliance on each buoy observation or each buoy in accordance with our knowledge of its reliability. For example, high wind events could be included in the analysis in a natural way.
4. The method has been easily coded in IDL.
5. Only a few iterations are needed to achieve all the adjustments.
6. Any of the parameters in Eq. 5 can be adjusted (given enough data).
7. The method can predict the values of poorly-known atmospheric properties, which is of scientific value.

Disadvantages of this technique are that

1. A large number of varied observations are required for an accurate convergence.
2. The method needs a good initial guess.
3. Systematic errors (biases) in the in-situ or satellite data would not be corrected.
4. It relies on correct physics (Eq. 5).
5. The method is novel (in its application to satellites) so would need rigorous testing.

## 2. METHOD

The first step of the least squares inverse procedure is to differentiate the water reflectance  $\rho_w$  given by Eq. 5 with respect to the adjustable parameters  $\rho_a$  and  $d\tau_{oz}$ , neglecting changes in the other parameters. The differential of  $\rho_w$  with respect to the aerosol scattering  $\rho_a$  is

$$\frac{\partial \rho_w(\lambda)}{\partial \rho_a(\lambda)} = -e^{\tau m/2} \quad (6)$$

and the differential of  $\rho_w$  with respect to the error in the ozone optical depth  $d\tau_{oz}$  is

$$\frac{\partial \rho_w(\lambda)}{\partial d\tau_{oz}(\lambda)} = \rho_{gc}(\lambda) e^{\tau m/2} e^{d\tau_{oz} m} m \quad (7)$$

The optimum values of  $\rho_a$  and  $d\tau_{oz}$  can now be found for each wavelength  $\lambda$  by least squares adjustment. Following [3] we can write the problem in matrix form as

$$\mathbf{x} = \mathbf{W}_e^{-1} \mathbf{A}^T [\mathbf{A} \mathbf{W}_e^{-1} \mathbf{A}^T + \mathbf{W}_b]^{-1} \mathbf{h} \quad (8)$$

The matrix  $\mathbf{x}$  contains the amount by which each uncertain parameter ( $d\tau_{oz}$ ,  $\rho_a$ ) should be varied,  $\mathbf{W}_e$  is the weighting matrix containing the uncertainties in the in-situ observations on its diagonal,  $\mathbf{W}_b$  is a weighting matrix containing the uncertainties in the adjustable parameters.  $\mathbf{A}$  is the matrix containing the differentials of  $\rho_w$  with respect to the parameters to be varied ( $d\tau_{oz}$  and  $\rho_a$ ) and  $\mathbf{h}$  is a matrix containing the difference between the observed and predicted water reflectances.

If we only had 3 observations, matrix  $\mathbf{A}$  would be:

$$\begin{bmatrix} \frac{\partial \rho_w}{\partial d\tau_{oz}}(1) & \frac{\partial \rho_w}{\partial \rho_a}(1) \\ \frac{\partial \rho_w}{\partial d\tau_{oz}}(2) & \frac{\partial \rho_w}{\partial \rho_a}(2) \\ \frac{\partial \rho_w}{\partial d\tau_{oz}}(3) & \frac{\partial \rho_w}{\partial \rho_a}(3) \end{bmatrix}$$

In the examples discussed below we have 25 values so there would be 25 rows. Substituting the derivatives, matrix  $\mathbf{A}$  becomes:

$$\begin{bmatrix} \rho_{gc}(1) e^{\tau m/2} e^{d\tau_{oz} m} m & -e^{\tau m/2} \\ \rho_{gc}(1) e^{\tau m/2} e^{d\tau_{oz} m} m & -e^{\tau m/2} \\ \rho_{gc}(1) e^{\tau m/2} e^{d\tau_{oz} m} m & -e^{\tau m/2} \end{bmatrix}$$

IDL code was written to calculate the adjustments needed to  $\rho_a$  and  $d\tau_{oz}$  to make a best fit. The initial guesses for  $\rho_a$  and  $d\tau_{oz}$  were 0.05 (rather high) and 0.0 m (the assumption that the error in  $\tau_{oz}$  is zero). The Rayleigh optical depth  $\tau$  was assumed to be 0.145. The code read in all the match-ups for a given day from the named buoy, from a csv file output from the MERMAID (MERis Match-up In-situ Database, for details of MERMAID see [4]), containing the 25 values in a 5x5 grid box around the in-situ point. The differences between the in-

situ observed and the satellite-predicted water reflectance were put into matrix **h**. Values for  $\rho_{gc}$ ,  $\rho_w$ , and  $\theta$  were also taken from the MERMAID match-up file for matrix **A**. The observations weighting matrix  $W_e$  was set up with errors of 0.02 on its diagonal and the parameter weighting matrix  $W_b$  had errors of 0.1 on its diagonal. One advantage of this method is that these errors could vary to reflect our confidence in each observation. A correction vector **x** for  $\rho_a$  and  $d\tau_{oz}$  was derived by iteration, recalculating the satellite water reflectance at each step, and the predicted values of  $\rho_a$  and  $d\tau_{oz}$  were output.

### 3.1 RESULTS FOR MOBY

One example of the convergence of the algorithm is shown in Fig. 1 for the MOBY buoy near Hawaii for the 24<sup>th</sup> October 2003, using 25 satellite match-ups to one in-situ value. The x axis is the iteration number, and the vertical axes show the parameters as they were adjusted. In the upper plot the prediction for  $\rho_a$  converged within 3 steps from the initial guess of 0.05 to the predicted best value of 0.02. For comparison [5] found that the aerosol scattering coefficient ( $m^{-1}$ ) at the MOBY site was about  $3 \times 10^{-6} m^{-1}$  up to 3 km height. From this we can estimate a total aerosol scattering of  $0.5 \times 3 \times 10^{-6} \times 3000 = 0.0045$  (with perhaps a 50% error). This is one quarter of the value predicted in Fig.1.

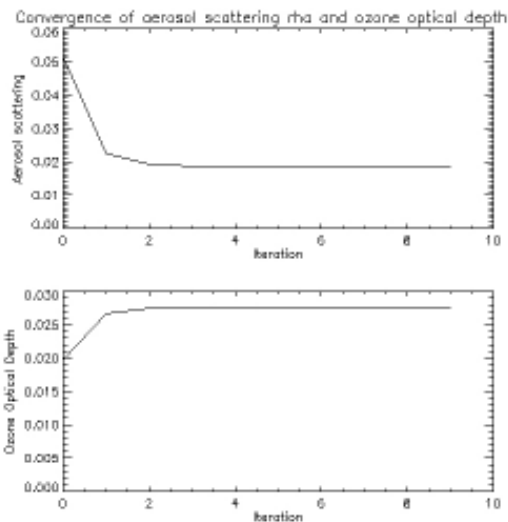


Figure 1. The convergence of the algorithm in aerosol scattering at 490 nm (the upper box, dimensionless) and the error in the ozone optical depth lower box (m) for the MOBY matchup data for the 24<sup>th</sup> October 2003.

The predicted value for the error in the assumed ozone optical depth  $d\tau_{oz}$  converged on 0.027 m.

Figure 2 shows the least squares best fit values for  $\rho_a$  and  $d\tau_{oz}$  for MOBY for August through to November 2003. This plot shows that the method does not always converge on a realistic value – for one day the predicted  $\rho_a$  was negative (at the end of August). The average  $\rho_a$  was  $0.021 \pm 0.021$  (not significantly different from zero). The average  $d\tau_{oz}$  was  $0.024 \pm 0.01$  m. It should be noted that on many days the algorithm did not converge and these results are not shown (see the discussion).

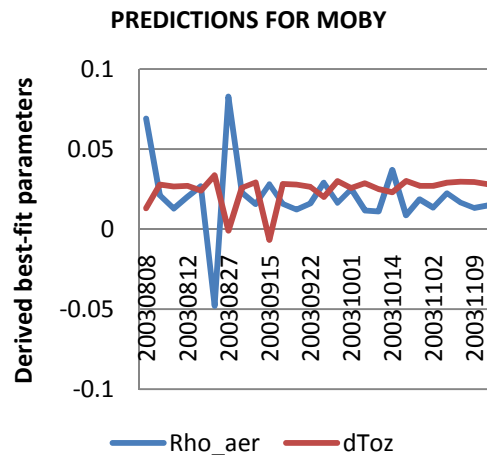


Figure 2. The predicted daily aerosol scattering (blue line, dimensionless) & error in the ozone optical depth (red line, m) at 490 nm for the MOBY buoy August – November, 2003.

The MOBY buoy is located in the central Pacific so the aerosol scattering should be relatively low. The (positive) peaks in August coincide with a volcanic eruption that occurred at that time, but these may be erroneous values – note the large unphysical negative value also derived using this method.

### 3.2 RESULTS FOR GUSTAV DALEN

The Gustav Dalen Lighthouse Tower is on one of the Åland islands off the coast of Finland. The results in Fig. 3 show the predicted temporal variation of  $\rho_a$  and  $d\tau_{oz}$  for this site. The averages over the time period were  $\rho_a = 0.018 \pm 0.003$  and  $d\tau_{oz} = 0.027 \pm 0.001$  m (results from days on which the algorithm failed to converge were omitted).

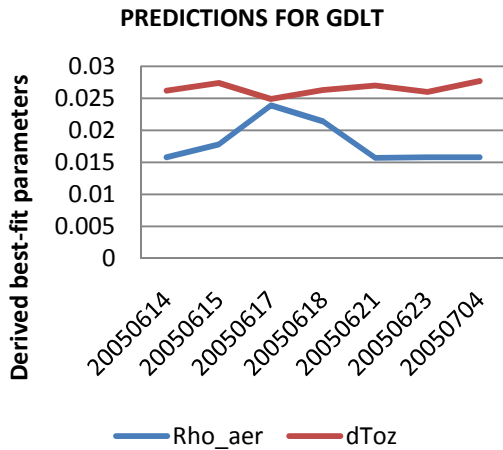


Figure 3. The predicted daily aerosol scattering (blue line, dimensionless) & error in the ozone optical depth (red line, m) at 490 nm for the Gustav Dalen Tower, June-July, 2005.

### 3.3 RESULTS FOR BOUSSOLE

The BOUSSOLE buoy is located between the French coast and Corsica.

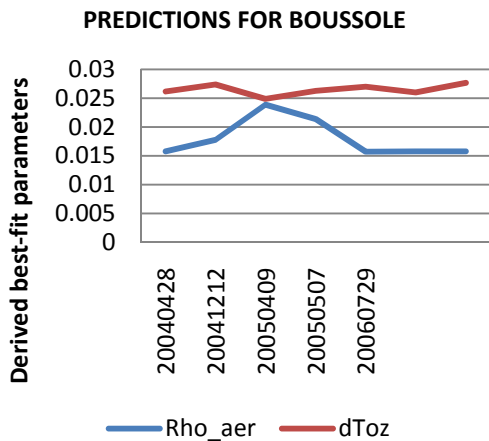


Figure 4. The predicted daily aerosol scattering at 490 nm (blue line, dimensionless) & error in the ozone optical depth (m) for BOUSSOLE from April, 2004 to July, 2006.

The average aerosol scattering at 490nm was predicted to be  $0.021 \pm 0.007$  and the error in the ozone optical depth was  $0.027 \pm 0.002$  m.

### 3.4 AAOT

The AAOT (Acqua Alta Oceanographic Tower) buoy is in the northern Adriatic Sea. The results in Fig. 5 show that the aerosol scattering was more variable than at the GDLT and the average predicted values for aerosol scattering and the error

in the ozone optical depth were  $\rho_a = 0.025 \pm 0.007$  and  $d\tau_{oz} = 0.028 \pm 0.001$  m. These values were higher than at the other buoys, suggesting that aerosol and ozone content were larger in this area.

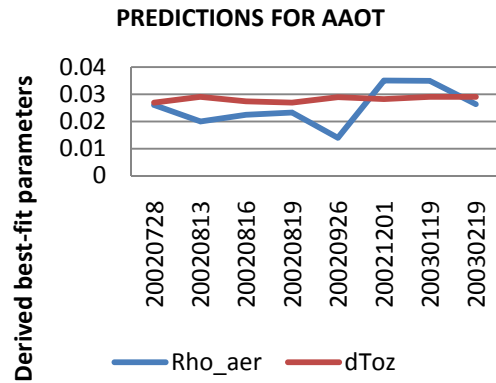


Figure 5. The predicted daily aerosol scattering at 490 nm (dimensionless) & the error in the ozone optical depth (m) for the AAOT, February 2002 – February 2003.

## 4.0 DISCUSSION

The results are summarised in Table 1. The sites names are shown in column 1, and columns 2 and 3 show the average predicted values for  $\rho_a$  and  $d\tau_{oz}$  and the standard deviation. The Gustav Dalen tower had the lowest predicted aerosol scattering and the MOBY site had the lowest error in the ozone optical depth,  $d\tau_{oz}$ . AAOT had the highest aerosol scattering and  $d\tau_{oz}$ .

Table 1. The predicted  $\rho_a$  (dl) and  $d\tau_{oz}$  (m) for the sites, at 490 nm, over the periods specified above.

In situ site	Aerosol scattering (dl, average)	Error in ozone optical depth, $d\tau_{oz}$ (m, average)
MOBY	$0.021 \pm 0.021$	$0.024 \pm 0.01$
GDLT	$0.018 \pm 0.003$	$0.027 \pm 0.001$
BOUSSOLE	$0.021 \pm 0.007$	$0.027 \pm 0.002$
AAOT	$0.025 \pm 0.007$	$0.028 \pm 0.001$

The method failed to converge in about a third of the cases considered. These failures may have been caused by the high initial guess for  $\rho_a$  (0.05) and the low number of observations available for each day (25). These problems could be solved by using the previous day's predicted  $\rho_a$  or  $d\tau_{oz}$  as the new guess, and averaging the data over longer times.

The method also produced a few unphysical values as seen in one (possibly 3 cases) out of 25 in the

MOBY results (Fig. 1). The results from the GDLT and AAOT were far more stable.

One criticism of this method is that it derives atmospheric variables that are only valid for the in-situ sites, whereas the standard gain method produces a mission-average gain applicable worldwide. However, the new method has several advantages. For example, if the aerosol scattering is derived at one site, this is a physical parameter that follows a predictable pattern, so a model could be used to extrapolate it to other regions for use in satellite correction there. This cannot be done with the gain. For other advantages and disadvantages, see the lists in the introduction.

## 5.0 CONCLUSION

A novel approach to vicarious adjustment is proposed: a least-squares inverse technique is used to adjust the aerosol scattering and the error in the ozone optical depth within their error bars to obtain a best fit between satellite and buoy reflectances.

The method was demonstrated by using satellite-in-situ matchups from MERMAID to predict the aerosol scattering and error in the ozone optical depth at several observing platforms. The Gustav Dalen tower was predicted to have the lowest aerosol scattering, and MOBY had the lowest  $d\tau_{oz}$ . AAOT had the highest aerosol scattering and  $d\tau_{oz}$ . These results seem physically reasonable.

The new method is simple to code, and is a more flexible way to vicariously adjust satellite data since, instead of relying on a single gain factor, uncertain components of the atmosphere model itself can be adjusted for a best fit. The method can also weight observations for reliability, and predict atmospheric characteristics and their temporal variations. This is of scientific interest, but it also means that atmospheric models could be used to extrapolate these parameters globally and thereby correct global satellite data in a more accurate way.

However, the method relies on correct physics (Eq. 5 must be right), it cannot correct systematic errors,

and it requires a good initial guess and enough data to ensure convergence.

The method needs testing. This could be done by 1) running the algorithm in parallel with the present gain method, perhaps using the ODESA software, 2) comparing predicted timeseries of  $\rho_a$  and  $d\tau_{oz}$  with known atmospheric events (such as volcanic eruptions, or wind-blown dust) and 3) considering cases for which  $\rho_a$  and  $d\tau_{oz}$  are well known.

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