In-water remote sensing algorithms for the detection of chlorophyll and yellow substances in the Pomeranian Bay^{*}

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> > **KEYWORDS**

Marine optics Remote sensing Local algorithms

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Abstract

In-water remote sensing algorithms for estimating chlorophyll concentration and the absorption of light (400 nm) by yellow substances valid for the surface layer of the Pomeranian Bay are described. The accuracy of the algorithms has been estimated at 20–60%. The statistical analysis of data collected during a two-year experiment in 1996–1997 enable algorithms to be constructed which use a linear combination of spectral reflectances at selected wavelengths, all of them in the log-log form. The wavelengths in nm are 510, 550, 589 or 510, 625 in the 'chlorophyll' case, and 589, 665 or 490, 665 in the 'yellow substances' case. The correlation coefficient between the log-transformed reflectance ratios and the chlorophyll concentration is around 0.9. The correlation coefficient between the log-transformed reflectance ratios and the yellow substance absorption coefficient at $\lambda = 400$ nm is around 0.6.

1. Introduction

The remote sensing reflectance (Lee *et al.* 1997, Mueller *et al.* 1997) was one of the physical parameters investigated in Pomeranian Bay waters during a series of research cruises in 1996–1997 (Kowalczuk *et al.* 1999).

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This parameter was measured in the surface layer, together with the chlorophyll concentration and absorption of light by yellow substances. The principal aim of the experiment was to determine the correlative relationships between the above parameters, in the form of an in-water remote sensing algorithm. Such an algorithm is a very important tool for remote sensing the organic matter content in the Bay. This is highly productive, fertile and turbid Case 2 (WC2) water (Kaczmarek & Woźniak 1995) where no standard oceanic remote sensing algorithms can be applied; finding local formulas thus becomes necessary. These relationships have a distinctly local character, because of the specific features of the basin, which is a semi-enclosed coastal region of the Baltic strongly influenced by the river Odra (Oder).

2. Methods and materials

The experimental part of this work is based on underwater measurements of the remote sensing reflectance $R_{rs}(\lambda, z^{-})$ (Olszewski & Darecki 1999), chlorophyll *a* concentration C_a and absorption coefficient of light by yellow substances $a_y(\lambda = 400 \text{ nm})$. The measurements were made in the surface layer of the Pomeranian Bay from on board r/v 'Oceania' from March 1996 to September 1997, excluding winter and mid-summer. The measurement points were distributed all over the Bay and yielded a number of data sets specified in Figs. 2 and 3. The grid of these points is shown in Kowalczuk *et al.* (1999), where the methodological procedures involving chlorophyll and yellow substances are also described.

The reflectance $R_{rs}(\lambda, z^{-})$ was measured using a MER2040 spectrophotometer (Biospherical Instruments USA) at ten spectral channels with central wavelengths as follows: 412, 443, 490, 510, 550, 589, 625, 665, 683, 710 nm. The spectrophotometer was immersed from a 6 m-long boom on the sunny side of the ship's stern. The values obtained were extrapolated up to the surface as $R_{rs}(\lambda, 0^{-})$.

A licensed SigmaPlot program was used to process the data, and all the statistical parameters are in accordance with this program (SigmaPlot 4.0 for Windows, 1997).

3. Results

The remote sensing signature of a marine region is the spectrum of its remote sensing reflectance $R_{rs}(\lambda)$. The averaged spectrum of spectral reflectance, obtained after almost two years of measurements in the Pomeranian Bay is shown in Fig. 1 (solid line). Values between the discrete results are linearly interpolated in order to demonstrate the probable shape of the spectra (a straight line fit was chosen instead of a smoothed one to



Fig. 1. Average spectrum and standard errors of remote sensing reflectance in the surface layer of the Pomeranian Bay (1996–1997, sample size n = 140) compared to the average spectrum in open waters of the central and southern Baltic (1993–1997, sample size $n_0 = 363$; after Darecki 1999); solid line – Pomeranian Bay, dashed line – Baltic

avoid unexplained displacements of extremes). As an identification of the investigated basin the spectrum is highly satisfactory. This is confirmed by comparison with the spectrum for the open Baltic (dashed line), also shown in the figure. The features differentiating the 'Bay' spectrum from the 'open water' spectrum are its much higher absolute values, a sharper but not shifted (!) principal maximum at $\lambda = 550 \text{ nm}$ and the absence of a principal minimum at $\lambda = 665 \text{ nm}$. It is worth noting, though, that the reflectance spectrum is a characteristic integral type, *i.e.* each of its points results from the overall effect of the light field's interaction with all seawater components. Thus, inspection of the separate reflectance values does not permit any specific proportions of these components to be inferred. Conclusions are possible only after the relations between the reflectance values at different spectral ranges have been examined. Such relations are merely the foundation of all the algorithms for the remote detection of seawater components.

During the two years of the Pomeranian Bay experiment the measurements of the reflectance R_{rs} were performed simultaneously with those of the chlorophyll concentration and of the 400 nm light absorption in yellow substances a_y . Sets of points connecting the reflectance with the chlorophyll concentration and the yellow substance absorption are presented in



Fig. 2. Remote sensing reflectance at different wavelengths vs. chlorophyll concentration in the surface layer of the Pomeranian Bay (1996–1997, sample size n = 122)



Fig. 3. Remote sensing reflectance at different wavelengths vs. yellow substance absorption (400 nm), in the surface layer of the Pomeranian Bay (1996–1997, sample size n = 86)

Table 1. Correlation coefficients r and standard errors of estimation (SEE) calculated for the linear regression between the logarithm of the chlorophyll concentration $C_a \, [\text{mg m}^{-3}]$ and the logarithm of the ratios of the remote sensing reflectances $R_{rs}(\lambda_i)/R_{rs}(\lambda_0)$ at various wavelengths λ_i and λ_0 ; surface layer of the Pomeranian Bay 1996–1997, sample size 122

λ_i [nm]	412	443	490	510	550	589	625	λ_0 [nm]
r (SEE)	$\begin{array}{c} 0.528 \\ (0.347) \end{array}$	$0.649 \\ (0.311)$	$\begin{array}{c} 0.675 \\ (0.301) \end{array}$	$0.706 \\ (0.289)$	_	_	_	550
	$\begin{array}{c} 0.753 \\ (0.269) \end{array}$	$\begin{array}{c} 0.830 \\ (0.228) \end{array}$	$0.859 \\ (0.209)$	$0.883 \\ (0.191)$	$\begin{array}{c} 0.900\\(0.178)\end{array}$	_	_	589
	$\begin{array}{c} 0.790 \\ (0.251) \end{array}$	$0.852 \\ (0.214)$	$0.872 \\ (0.200)$	$0.880 \\ (0.194)$	$0.859 \\ (0.209)$	$\begin{array}{c} 0.746 \\ (0.272) \end{array}$	_	625
	$0.794 \\ (0.248)$	$0.840 \\ (0.221)$	$0.849 \\ (0.216)$	0.855 (0.212)	$0.816 \\ (0.236)$	$\begin{array}{c} 0.654 \\ (0.309) \end{array}$	$\begin{array}{c} 0.131 \\ (0.405) \end{array}$	665

Figs. 2 and 3 respectively. On this experimental basis correlations were sought which could enable the proper algorithm to be constructed in the most simple and common form of the linear log-log function (O'Reilly *et al.* 1998). The variables of this algorithm are the dependent logarithm of the concentration C_a or absorption a_y , and the independent logarithm of the reflectance ratio $R_{rs}(\lambda_i)/R_{rs}(\lambda_0)$ at various pairs of the wavelengths λ_i and λ_0 . All the significant correlations obtained for the chlorophyll are gathered in Table 1, the best of them being marked in bold. As one can see, the best correlation coefficients and error estimates appear at wavelengths 510, 550, 589 and 625 nm. Taking this into account, we suggest two algorithms with the above wavelengths. The first of them is slightly better but uses the wavelength 589 nm, which is not of the SeaWiFS satellite system standard. This consists of the ratio of the geometrical average of the reflectances at 510 and 550 nm to the reflectance at 589 nm and yields the chlorophyll concentration $C_a [\text{mg m}^{-3}]$ as

$$\log(C_a(R_{rs})) = 0.5876 \pm 0.0180 - (3.5446 \pm 0.1545) \times \log\{(R_{rs}(550) \times R_{rs}(510))^{0.5} / R_{rs}(589)\}.$$
(1)

Fig. 4 presents the experimental set of points linking the variables of algorithm (1): $Y = \log(C_a)$ and $X = \log\{(R_{rs}(550) \times R_{rs}(510))^{0.5}/R_{rs}(589)\}$, as well as the straight line of regression, representing the above algorithm. The correlation coefficient r between the measured values of Y_n and X_n is 0.902. The standard error of the estimate (SEE) is 0.1760, which after re-calculation into physical values gives a relative standard error of



Fig. 4. Log-log dependence of chlorophyll concentration $C_a \, [\text{mg m}^{-3}]$ on the optimal combination of remote sensing reflectances $R_{rs}(0^-, \lambda_i) \, [\text{sr}^{-1}]$ in the surface layer of the Pomeranian Bay (1996–1997, sample size n = 122, correlation coefficient r = 0.902)



Fig. 5. Comparison of chlorophyll concentrations measured and those calculated by remote sensing algorithm (1) in the surface layer of the Pomeranian Bay (1996–1997, sample size n = 122; the solid line denotes equality $C_a = C_a(R_{rs})$)

 $\Delta C_a/C_a = +50\% - 27\%$. Fig. 5 illustrates the final result of using algorithm (1), *i.e.* a comparison of the values of the chlorophyll concentration obtained in the laboratory and those calculated from the remote sensing reflectance with the aid of this algorithm. This comparison will be commented on in the next section.

The next algorithm proposed is not quite as good, but it still satisfies the SeaWiFS standard. This comprises the ratio of the reflectance at 510 nm to that at 625 nm and reads:

$$\log(C_a(R_{rs})) = 0.9391 \pm 0.0321 - (1.9388 \pm 0.0955) \times \log(R_{rs}(510)/R_{rs}(625)).$$
(2)

The correlation coefficient r between the measured values of $Y_n = \log(C_a)_n$ and $X_n = \log(R_{rs}(510)/R_{rs}(625))_n$ is equal to 0.900. The standard error of the estimate (SEE) is 0.1940, which after re-calculation into physical values gives $\Delta C_a/C_a = +56\% - 36\%$.

Table 2. Correlation coefficients r and standard errors of estimation (SEE) calculated for the linear regression between the logarithm of the yellow substance absorption coefficient a_y (400 nm) [m⁻¹] and the logarithm of the ratios of the remote sensing reflectances $R_{rs}(\lambda_i)/R_{rs}(\lambda_0)$ at various wavelengths λ_i and λ_0 ; surface layer of the Pomeranian Bay 1996–1997, sample size 86

$\begin{array}{c} \lambda_i \\ [\mathrm{nm}] \end{array}$	412	443	490	510	550	589	625	λ_0 [nm]
r(SEE)	$\begin{array}{c} 0.393 \ (0.147) \end{array}$	$\begin{array}{c} 0.532 \\ (0.135) \end{array}$	$\begin{array}{c} 0.562 \\ (0.132) \end{array}$	$\begin{array}{c} 0.526 \\ (0.136) \end{array}$	_		_	550
	0.427 (0.145)	$\begin{array}{c} 0.507 \\ (0.138) \end{array}$	$0.517 \\ (0.137)$	$0.485 \\ (0.140)$	$\begin{array}{c} 0.4.3 \\ (0.146) \end{array}$	_	_	589
	0.451 (0.143)	$\begin{array}{c} 0.517 \\ (0.137) \end{array}$	$0.529 \\ (0.136)$	$0.506 \\ (0.138)$	0.455 (0.142)	$0.479 \\ (0.140)$	_	625
	$\begin{array}{c} 0.512 \\ (0.137) \end{array}$	$\begin{array}{c} 0.573 \ (0.131) \end{array}$	$0.587 \ (0.130)$	$\begin{array}{c} 0.573 \ (0.131) \end{array}$	$\begin{array}{c} 0.549 \\ (0.134) \end{array}$	$\begin{array}{c} 0.615 \\ (0.126) \end{array}$	$\begin{array}{c} 0.396 \\ (0.147) \end{array}$	665

The correlations obtained in the case of yellow substances were significantly worse (Table 2); again, the best ones are marked in bold. Here, the highest correlation coefficients and smallest errors of the estimate appear at wavelengths 490, 589 and 665 nm. Bearing this in mind, the two algorithms are put forward for computing the 400 nm light absorption coefficient in yellow substances a_y [m⁻¹]. The better of the two uses the ratio of the reflectance at the non-standard 589 nm wavelength to that at 665 nm and reads as follows:

$$\log(a_y(R_{rs})) = 0.4518 \pm 0.0897 - (1.4547 \pm 0.2034) \times \log(R_{rs}(589)/R_{rs}(665)).$$
(3)

Figure 6 presents the experimental set of points and the regression line connecting the variables of algorithm (3): $Y = \log(a_y)$ and $X = \log(R_{rs}(589)/R_{rs}(665))$. The correlation coefficient r between the measured values of Y_n and X_n is equal to 0.615. The standard error of the estimate (SEE) is equal to 0.1261, which after re-calculation into physical values gives the relative standard error as $\Delta a_y/a_y = +34\% - 25\%$. Fig. 7 illustrates the final result of using algorithm (3), a comparison of the absorption coefficients of the yellow substances obtained in the laboratory and those calculated from the remote sensing reflectance with the aid of the algorithm (see next section for comments).



Fig. 6. Log-log dependence of yellow substance absorption a_y (400 nm) [m⁻¹] on the optimal combination of remote sensing reflectances $R_{rs}(0^-, \lambda_i)$ [sr⁻¹] in the surface layer of the Pomeranian Bay (1996–1997, sample size n = 86, correlation coefficient r = 0.615)

The second algorithm is not as good as the first one but still fits the SeaWiFS spectral channels. This is the ratio of the reflectance at 590 nm to that at 665 nm and reads:

$$\log(a_y(R_{rs})) = -0.0184 \pm 0.0284 - (0.4705 \pm 0.0708) \times \log(R_{rs}(490)/R_{rs}(665)).$$
(4)



Fig. 7. Comparison of yellow substance absorption coefficients measured and those calculated by remote sensing algorithm (3) in the surface layer of the Pomeranian Bay (1996–1997, sample size n = 86, solid line denotes equality $a_y = a_y(R_{rs})$)

The correlation coefficient r between the measured values of $Y_n = \log(a_y)_n$ and $X_n = \log(R_{rs}(490)/R_{rs}(665))_n$ is now equal to 0.587. The standard error of the estimate (SEE) is 0.1295, which after re-calculation into physical values becomes $\Delta a_y/a_y = +35\% - 26\%$.

4. Discussion and conclusions

The comparison between the calculated (X) and measured (Y) physical values (Figs. 5 and 7) is simply a linearisation of the results obtained from the log-log algorithms (1) and (3). This has been done merely to visualise the results, not for a detailed discussion of their quality on the linear scale. Generally, such a comparison for the logarithms of physical values would yield:

- equality of the mean values: $\bar{\log Y} = \bar{\log X}$;
- regression lines $\log Y = \log X$;
- correlation coefficients and standard errors of the estimate exactly the same as in the algorithms, with constant relative errors for physical values.

In the linear-linear scale, as in Figs. 5 and 7, we have instead:

- non-equality of the mean values: $\bar{Y} \ll \bar{X} \ (\bar{Y} > \bar{X});$
- regression lines $Y \ll X$ (Y > X);
- worse correlation coefficients and relative errors of the estimate dependent on X, giving very high errors for small X.

Though not very great, the quantitative differences are sufficiently pronounced to show up the advantage of the log-log form of algorithms.

The reflectance spectrum shown in Fig. 1 as well as its spectral bands, optimal for the chlorophyll or yellow substance detection, reveal differences between the investigated basin and its open sea neighbourhood. The search for the proper local remote sensing algorithms is thus well grounded. The reflectance spectrum of the Bay is elevated in relation to that of the open Baltic over all the visible range from *ca* 25% in the short wavelength part to more than 55% in the long wavelengths. This is illustrated by the spectral distribution of the ratio of the two reflectances shown in Fig. 8. Here the linear interpolation between the discrete values is done for exactly the same reasons as in Fig. 1. If, for the sake of simplicity, we make the approximation that the reflectance is proportional to the backscattering and inversely proportional to the absorption of light (Olszewski & Darecki 1999), the suspensions are responsible for the increase in all reflectance values. Since suspended matter scatters light strongly but with weak selectivity, selective molecular scattering and absorption in seawater components are



Fig. 8. Spectrum of the ratio of the remote sensing reflectance in the Pomeranian Bay to the remote sensing reflectance in the open Baltic

masked. This inference is supported by the position of the maximum of the reflectance ratio, seen in Fig. 8 at 550 nm. The principal minimum of total absorption for this type of water occurs at this point (Kowalczuk & Darecki 1998), and so long as no other selective processes are prevailing, it is this that causes the maximum mentioned. On the other hand, the disappearance of the reflectance minimum at the 665 nm chlorophyll absorption band, confirmed by the strong maximum of the reflectance ratio in Fig. 8, is evidence for the relative decrease in the proportion of chlorophyll in the suspended matter. So we can expect that the dominant constituent of the Bay water is inorganic suspended matter. As a result of weak selective scattering by this suspended matter, the shape of the reflectance spectrum remains almost unchanged even though its values rise distinctly. This is also confirmed by the spectral bands regarded as the best for detecting chlorophyll. With the same form of remote sensing algorithms these bands are also the same as for the open Baltic (Darecki 1998), the corresponding correlation coefficients being similar or even a little better (0.86-0.88 for the Baltic, 0.90 for the Bay).

The question of yellow substances seems much more complicated. The insensitivity of short wave reflectance to a_y has been noted even in the open Baltic, which is somewhat surprising in view of the strong absorption of light by the yellow substances in that spectral region. In the Baltic the best correlation of a_y with the reflectance has been obtained for the ratios of the reflectance at 490-510 nm, the most sensitive, to that at 589-625 nm, the reference (Darecki 1998). However, to obtain any sensible results at all in the Bay, the spectral range for the most effective detection should be shifted even further towards the long wave end of the spectrum, to 589 nm as the most sensitive and to 665 nm as the reference. The only logical explanation for such an effect seems to be the existence of certain seawater components that strongly mask the short-wave absorption of light by yellow substances, regardless of the high concentration of this latter constituent. Still, the results obtained are not all that good either. With the remote sensing algorithms in similar form, the corresponding correlation coefficients for the Baltic are at the 0.69-0.70 level, so they are distinctly better than those for the Bay. One of the possible causes of this is the very weak correlation that has been noticed between the chlorophyll concentration and the yellow substance index (a_y) (Fig. 9). This could be evidence of the great complexity of the origins of yellow substances.

The cautious formulation of the above environmental conclusions is connected with the subject of the paper, because they were deduced somewhat incidentally, without proper experimental backing (*e.g.* by measuring the suspended matter concentration or determining the pigment components).



Fig. 9. Correlation between yellow substance absorption coefficients at 400 nm and the chlorophyll concentration in the surface layer of the Pomeranian Bay (1996–1997, sample size n = 82, correlation coefficient r = 0.417)

The main conclusion here is of a methodological nature, namely, that a quantitative evaluation of the concentration indices for chlorophyll and yellow substances is possible in the Pomeranian Bay if the underwater upward light field is measured in two or three spectral bands using the algorithms proposed in the paper. Thus, it should also be possible with the use of remote above-water measurements, including satellite techniques. When the algorithms are applied to subsurface measurements, an accuracy of 20–60% is obtained. The standard spectral bands of the SeaWiFS satellite system can be used in the algorithms, although adding the extra yellow band yields slightly better results.

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