

Modelling of bio-optical parameters of open ocean waters*

OCEANOLOGIA, 43 (4), 2001.

pp. 469–477.

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KEYWORDS

Light absorption
Bio-optical modelling
Chlorophyll pigments
Yellow substance
Suspended matter

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Manuscript received 16 November 2001, reviewed 20 November 2001, accepted 25 November 2001.

Abstract

An original method for estimating the concentration of chlorophyll pigments, absorption of yellow substance and absorption of suspended matter without pigments and yellow substance in detritus using spectral diffuse attenuation coefficient for downwelling irradiance and irradiance reflectance data has been applied to sea waters of different types in the open ocean (case 1). Using the effective numerical single parameter classification with the water type optical index m as a parameter over the whole range of the open ocean waters, the calculations have been carried out and the light absorption spectra of sea waters tabulated. These spectra are used to optimize the absorption models and thus to estimate the concentrations of the main admixtures in sea water.

The value of m can be determined from direct measurements of the downward irradiance attenuation coefficient at 500 nm or calculated from remote sensing

* This paper was presented at the 'Third Workshop on Luminescence and Photosynthesis of Marine Phytoplankton', Sopot–Sulęcyno, 8–12 October 2001.

data using the regressions given in the article. The sea water composition can then be readily estimated from the tables given for any open ocean area if that one parameter m characterizing the basin is known.

1. Introduction

The optical properties of sea water in the open ocean are determined entirely by the optical properties of pure water and natural admixtures, namely those of phytoplankton pigments, yellow substance and suspended matter. On the other hand, if some optical characteristics of sea water have been obtained, the concentrations of the natural admixtures can be estimated. In this paper the optical spectra of light absorption in sea waters of different types, including the spectrum of pure sea water, have been determined from a large number of contact measurement data of the spectral diffuse attenuation coefficient for downwelling irradiance and the irradiance reflectance. Using these spectra the absorption models have been optimized and the main sea water admixture concentrations estimated.

2. The pure sea water absorption spectrum

Modelling light fields in sea water or above the sea surface requires a basic characteristic, namely, the spectral absorption coefficient of pure sea water $a_{W,\lambda}$. In order to estimate this characteristic, measurements were carried out after the water samples had been purified in various ways, but the results were quite different (Tyler et al. 1972, Kopelevich 1976, Pope & Fry 1997), mostly because of the poor accuracy of light absorption measurements in small volumes or owing to the difficulties of removing dust from the samples. We suggested estimating $a_{W,\lambda}$ from measurements carried out in the sea itself (*in situ* measurements) through layers a few metres thick. We used the measurements of the spectral downward irradiance attenuation coefficient $K_{d,\lambda}$ and the irradiance reflectance R_λ in the visible light spectrum. The absorption coefficient in water is calculated from these measurements using the divergence of the vector of irradiance \mathbf{E} according to the method given by Pelevin (1985).

The divergence of the vector of irradiance \mathbf{E} is equal to the spatial density of light energy absorption in an elementary volume (Gershun 1958). Taking into account non-linear effects in the water medium (fluorescence and Raman-effect), we obtain

$$\operatorname{div} \mathbf{E} = -a E^o + \int_{320}^{780} a_{\lambda_1} E_{\lambda_1}^o K_{\lambda_1 \rightarrow \lambda} d\lambda_1, \quad (1)$$

where a is the absorption coefficient in the medium, E^o is the spectral scalar irradiance of the given volume, the second term on the right-hand side

takes into account the non-linear effects in the medium (fluorescence and Raman-effect), $K_{\lambda_1 \rightarrow \lambda}$ is the coefficient of absorbed light transmission from λ_1 to λ by luminescence and Raman radiation. Since the horizontal gradients of the optical properties of sea water are much smaller than the vertical ones (a vertically stratified medium) and the dimension of non-uniformity in surface irradiance by daylight far exceeds the dimension of vertical variability of the light field in the water, the horizontal gradients of \mathbf{E} can be neglected. The vertical component of this vector H_z is equal to $E_{\downarrow} - E_{\uparrow}$, where E_{\downarrow} is the downward and E_{\uparrow} is the upward irradiance at depth z . In the upper layers of the sea the second term on the right-hand side of eq. (1) describing fluorescence and Raman-scattering is small in comparison to the first one and can be neglected. Thus, eq. (1) takes the form $d/dz(E_{\downarrow} - E_{\uparrow}) = -a E^o$ (Pelevin 1965). Dividing eq. (1) by $(E_{\downarrow} - E_{\uparrow}) = E_{\downarrow}(1 - R)$, where R is the irradiance reflectance by the sea ($R = E_{\uparrow}/E_{\downarrow}$), and taking into account $K_d = -1/E_{\downarrow}(dE_{\downarrow}/dz)$, we derive the formula

$$K_d \{1 + (dR/dz)/K_d/(1 - R)\} \cong a E^o / (E_{\downarrow} - E_{\uparrow}). \quad (2)$$

The irradiance reflectance R varies only slightly with depth. It was shown by the processing of numerous experimental data that the second term in brackets is no more than 0.04 and can therefore be ignored (Pelevin 1965). The right-hand side of eq. (2) contains the expression for the mean cosine of the angle of radiation incidence $\mu = (E_{\downarrow} - E_{\uparrow})/E^o$. Eq. (2) then takes the form

$$a \cong K_d \mu. \quad (3)$$

Special model experiments in artificial media and series of measurements carried out in the Indian Ocean (Pelevin & Prokudina 1979) showed that the mean cosine of the angle of light incidence is highly correlated with the irradiance reflectance according to the regression

$$\mu \cong 1 - 0.185 \sqrt{R}. \quad (4)$$

The error in determining μ from this formula is rather small ($-0.03 < \Delta\mu < 0.04$). Thus, using measured values of K_d and R , the water absorption coefficient can be estimated with an error of no more than 8%:

$$a \cong K_d (1 - 0.185 \sqrt{R}). \quad (5)$$

Since the solar light field parameters K_d and R can be obtained in any body of water, a can be determined by this method both in open-sea and shelf waters.

To obtain the pure sea water absorption we used our measurements of K_d and R in the central Pacific Ocean south-east of the Cook Islands (Otchakovskii et al. 1978). It was in this area during the 5th voyage of r/v 'Dmitrii Mendeleev' that V. M. Pavlov measured the maximum Secchi disc visibility depth in the World Ocean (67 metres) (Pavlov 1978). The optical properties of such water can be regarded as the properties of pure sea water. The values of the absorption coefficient calculated from experimental data obtained in the surface water layers from 2 (for the red spectral band) to 20 metres (for the blue spectral band) are given in Table 1.

Table 1. Absorption coefficient spectrum for pure sea water in $[\text{m}^{-1}]$

λ [nm]	$a_{W,\lambda}$	λ	$a_{W,\lambda}$	λ	$a_{W,\lambda}$	λ	$a_{W,\lambda}$
380	0.013	440	0.011	500	0.019	560	0.061
390	0.012	450	0.012	510	0.026	570	0.075
400	0.012	460	0.012	520	0.035	580	0.088
410	0.011	470	0.012	530	0.038	590	0.121
420	0.011	480	0.013	540	0.043	600	0.162
430	0.011	490	0.017	550	0.052		

3. Absorption spectra of sea waters in the open ocean.

The optical classification of open sea waters

There are several different water type classifications, which make it possible to characterize sea water using simple indices of water type (see, for example, Jerlov 1976, Morel & Prieur 1977, Prieur & Sathindranath 1981) or surface chlorophyll concentrations (Baker & Smith 1982, Morel 1988). But we selected a classification that enables the characteristics of the solar light field in sea water to be determined using only one parameter, defined as the water type optical index m (Pelevin & Rutkovskaya 1977). This parameter is proportional to the downward irradiance attenuation coefficient at 500 nm

$$m = 100 \lg e / K_{d,500} / \cong 43.43 / K_{d,500} / . \quad (6)$$

$/K_{d,500}/$ is a non-dimensional value equal to $K_{d,500}$ measured by a Solar angle of more than 35 circular degrees or by an overcast sky and given in $[\text{m}^{-1}]$.

The smallest value of m (1.15) was measured in the central Pacific south-east of the Cook Islands (Otchakovskii et al. 1978). The values of m from 1.15 to 2 correspond to oligotrophic waters, the values from 2 to 5 correspond to mesotrophic ones, and larger values characterize eutrophic waters. The distribution of m in the Pacific, Indian and Atlantic

Table 2. Absorption coefficient spectra for ocean waters of different types in [m⁻¹]

m λ [nm]	1.2	1.5	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0	11.0
380	0.014	0.023	0.036	0.074	0.105	0.142	0.183	0.220	0.254	0.290	0.330	0.369
390	0.014	0.022	0.035	0.071	0.100	0.136	0.175	0.210	0.243	0.277	0.318	0.356
400	0.013	0.021	0.034	0.068	0.097	0.131	0.169	0.203	0.235	0.269	0.309	0.347
410	0.012	0.020	0.033	0.066	0.093	0.126	0.163	0.197	0.228	0.262	0.302	0.340
420	0.012	0.019	0.032	0.064	0.091	0.123	0.159	0.192	0.222	0.256	0.296	0.334
430	0.012	0.020	0.032	0.063	0.089	0.120	0.155	0.187	0.216	0.250	0.290	0.327
440	0.013	0.020	0.032	0.061	0.086	0.117	0.150	0.181	0.210	0.242	0.281	0.318
450	0.013	0.020	0.032	0.059	0.083	0.112	0.144	0.174	0.201	0.232	0.269	0.305
460	0.013	0.020	0.031	0.057	0.079	0.107	0.137	0.165	0.190	0.219	0.254	0.288
470	0.013	0.020	0.030	0.054	0.075	0.100	0.128	0.154	0.177	0.205	0.237	0.268
480	0.014	0.019	0.028	0.050	0.070	0.093	0.119	0.142	0.164	0.189	0.218	0.246
490	0.018	0.023	0.031	0.051	0.069	0.091	0.114	0.135	0.155	0.177	0.203	0.228
500	0.020	0.024	0.032	0.050	0.066	0.086	0.106	0.126	0.144	0.164	0.187	0.209
510	0.027	0.031	0.038	0.054	0.070	0.087	0.106	0.123	0.140	0.158	0.178	0.198
520	0.036	0.040	0.046	0.061	0.076	0.092	0.108	0.124	0.140	0.156	0.174	0.192
530	0.039	0.042	0.047	0.061	0.075	0.090	0.106	0.120	0.135	0.150	0.166	0.182
540	0.044	0.047	0.052	0.065	0.078	0.092	0.107	0.121	0.135	0.149	0.164	0.179
550	0.053	0.056	0.061	0.073	0.086	0.100	0.114	0.127	0.141	0.154	0.169	0.183
560	0.062	0.065	0.069	0.081	0.094	0.107	0.121	0.135	0.148	0.161	0.176	0.190
570	0.075	0.079	0.083	0.094	0.107	0.121	0.134	0.148	0.161	0.175	0.189	0.203
580	0.088	0.092	0.096	0.107	0.120	0.134	0.148	0.161	0.174	0.188	0.203	0.217
590	0.122	0.125	0.129	0.141	0.154	0.167	0.181	0.195	0.208	0.222	0.237	0.252
600	0.163	0.166	0.170	0.181	0.194	0.208	0.222	0.236	0.249	0.263	0.278	0.293

Oceans obtained by numerous contact measurements are given by Pelevin & Rutkovskaya (1978, 1979) and Pelevin et al. (1982). These papers also give the tables and nomograms for the determination of the spectra of the downward irradiance attenuation coefficient and irradiance reflectance for given values of m . We calculated these spectra for the whole range of m in the open ocean and obtained the spectra of absorption coefficients (Table 2).

Using a method analogous to the one for estimating the water absorption index, we obtained the backscattering radiation spectra for sea waters of different types. It was shown that when the concentration of natural admixtures in sea water rose, the light backscattering spectrum of the suspended matter became 'anomalous': the shorter the wavelength, the smaller the backscattering index. We thus suggest that the yellow substance contained in detritus and absorbed on the surface of particles significantly influences backscattering: the particle albedo for short waves decreases, and it is this which leads to the above-mentioned spectral anomaly. The effect can be seen in basins with an optical sea water index $m > 3$, that is by a pigment concentration of $> 0.5 \text{ mg m}^{-3}$.

4. The concentration of the principal admixtures for the whole range of sea water types in open ocean

To determine the concentration of the principal natural admixtures in sea water from the obtained absorption coefficient we assumed that the absorption coefficient depends mainly upon four factors:

$$a_{\lambda}^{\text{mod}} = a_{W,\lambda} + C_p a_{p,\lambda}(C_p) + a_{ys} \exp(-g(\lambda - \lambda_0)) + a_{sm}, \quad (7)$$

where $a_{W,\lambda}$ is the absorption coefficient for pure sea water, C_p is the concentration of phytoplankton pigments, mg m^{-3} , $a_{p,\lambda}(C_p)$ is the coefficient of specific absorption by phytoplankton pigments depending on the pigment concentration (Wozniak & Ostrowska 1990), a_{ys} is the absorption coefficient for yellow substance contained both in solution and in detritus at wavelength λ_0 , and a_{sm} is the absorption coefficient for suspended particles, excluding the absorption of phytoplankton pigments and the absorption of yellow substance in particles.

Now, by using the method proposed by Pelevin & Rostovtseva (1995) we calculate the optimal values of these three parameters for absorption spectra of different types of waters and thereby estimate the concentrations of the main natural admixtures. The results are given in Table 3.

The numerous data obtained by ship-board measurement of chlorophyll concentration from the research vessel 'Vityaz' in the Atlantic Ocean in 1991 and averaged for every value of m fall within the above error in estimating the chlorophyll concentration (Fig. 1). As far as the yellow substance

Table 3. Concentration of chlorophyll pigment C_P , ‘yellow substance’ absorption at 500 nm a_{ys} and suspended matter absorption a_{sm} versus the water type optical index m in the open ocean

m	C_p [mg m^{-3}]	a_{ys} [m^{-1}]	a_{sm} [m^{-1}]
1.5	0.02	0.0007	0.0032
2.0	0.16	0.0014	0.0057
3.0	0.52	0.0045	0.0135
4.0	0.81	0.0067	0.023
5.0	1.16	0.0093	0.033
6.0	1.6	0.0122	0.042
7.0	2.0	0.0145	0.052
8.0	2.3	0.017	0.061
9.0	2.9	0.019	0.070
10.0	3.6	0.021	0.079
11.0	4.3	0.022	0.087

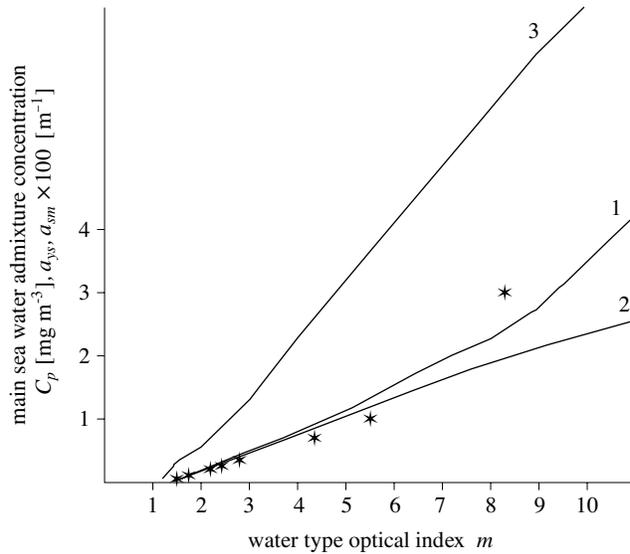


Fig. 1. Chlorophyll concentration C_p in [mg m^{-3}] (1), yellow substance absorption coefficient $a_{ys} \times 100$ in [m^{-1}] (2) and suspended matter absorption coefficient $a_{sm} \times 100$ in [m^{-1}] (3) as a function of the optical index of water type m ; dots – direct measurements of chlorophyll concentration in sea water

concentration is concerned, the numerous relevant data in the open ocean give the light absorption range referred to 500 nm from 0.0002 m^{-1} to 0.02 m^{-1} (Monin 1983, pp. 159–160). These values are in good agreement with the results obtained by our method.

Now to estimate the water composition one needs to obtain just one parameter in any sea basin, namely the ‘water type optical index m ’ that is proportional to the downward irradiance attenuation coefficient at 500 nm. It can be measured directly or calculated from the remote sensing reflectance R_{rs} . For example, the empirical dependence can be used (Pelevin 1979):

$$m = 1.3 + 3.5 R_{rs, 560} / R_{rs, 430}, \quad (8)$$

with standard deviations of 20%. Then the light absorption spectrum and the concentration of chlorophyll and other natural admixtures in sea water in this area can be estimated with ease from the tables given earlier.

5. Conclusions

All types of open ocean waters are characterized by the water type optical index m . Their spectra of light absorption and backscattering have been determined. On the basis of these spectra the concentrations of the main sea water admixtures have been calculated and tabulated for every water type. One need obtain only the single parameter m to assess the water composition in any open sea area using the given table. It should be stressed, however, that the data in this table are valid only for such areas where no substances of continental origin are present, and so the chlorophyll, detritus and dissolved organic matter concentrations are determined only by the phytoplankton life cycle, i.e. the balance between living and dead organic matter.

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