DETERMINATION OF THE SEA WATER ADMIXTURES CONCENTRATION FROM UPWELLING OPTICAL RADIATION SPECTRUM

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We present here the optimization method developed for solving inverse problems on estimation of the chlorophyll concentration in [mg/m^3], *the dissolved organic "yellow" substance and the suspension in units of light absorption* [m^{-1}], *using the spectrum of the radiation upwelling from the water surface. The method will work both in the open ocean and in coastal zones, because no assumptions on the correlation between the sea water components concentration is done when developing it. The efficiency of the proposed method has been demonstrated by processing the experimental data on the sea spectral brightness obtained from a research vessel in the open sea and coastal waters.*

The multichannel optical instrumentation capable of estimating the spectrum of the radiation upwelling from the "ocean-atmosphere" system is developed now for use onboard satellites, for example, SeaWiFS (USA)[1] and MOZ–OBZOR (Germany and Russia). The spectrum of upwelling radiation from the sea surface is reconstructed from these data after correction for the atmosphere. In this connection, solving the inverse problem on determining the ecological state of the sea water from the light scattered by near-surface water layer becomes an urgent problem. The known techniques for determining the chlorophyll concentration from the color index[2,3] do not provide high accuracy, and, moreover, are applicable only for the open ocean. As a rule, it is impossible to use the techniques for estimating the admixtures concentration developed for the open sea. In shallow waters, where the balance between the main light absorbing and light scattering components of the sea water is violated. No such techniques exist.

We have developed a technique for determining concentration of the light scattering and light absorbing admixtures in the sea water from the upwelling radiation spectrum, which can be applied both to the open ocean and shallow water. To solve this inverse problem we propose optimization of the models of light scattering and absorption by the principal admixture components. The optimization is performed so that the deviation of calculated spectrum from the experimentally obtained values is minimum. The estimates of the chlorophyll concentration, absorption coefficients of the dissolved organic matter and the suspension were obtained using such an optimization. The efficiency of the method developed has been demonstrated by processing the data of remote sensing the sea surface from onboard a research vessel in the open sea and coastal zones with different composition of the sea water.

The method proposed can be effectively applied to processing the data obtained from satellites as well as the data of ground support measurements from onboard a ship or an airplane.

1. OPTIMIZATION OF THE MODELS OF SCATTERING AND ABSORPTION OF LIGHT BY THE SEA WATER FOR DETERMINING THE ADMIXTURES CONCENTRATION FROM MULTISPECTRAL MEASUREMENTS OF UPWELLING RADIATION

Let the spectral brightness coefficient (SBC) of the surface be obtained in N spectral ranges in the visible wavelength range (400–600 nm) from remote sensing the ocean surface. The value of SBC is determined by both the absorption coefficient of the sea water ($\varkappa$) and the backscattering coefficient[4] (β):

$$\rho_\lambda = k\, \beta_\lambda / (\varkappa_\lambda + \beta_\lambda)\ , \tag{1}$$

where k is the spectrally nonselective coefficient, determined empirically($k \cong 0.11$).

The absorption coefficient of the sea surface is the sum of the absorption by clear water ($\varkappa_{w\lambda}$), phytoplankton pigments ($\varkappa_{p\lambda}$) dissolved organic matter ($\varkappa_{y\lambda}$) and a suspension ($\varkappa_{sm}$)

$$\varkappa_\lambda = \varkappa_{w\lambda} + \varkappa_{p\lambda} + \varkappa_{y\lambda} + \varkappa_{sm}\ . \tag{2}$$

Spectral dependences of the absorption coefficient of each of the above components are selected as follows. Let us take the values $\varkappa_{w\lambda}$ from the Tables.[4] Let us also consider the light absorption of suspended particles without taking into account the phytoplankton particles $\varkappa_{sm}$ to be nonselective. Spectral dependences of other components are described by the following expressions:

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$$\varkappa_{p\lambda} = C_p \varkappa^*_{p\lambda}\,(C_p)\ , \tag{3}$$

where C_p is the chlorophyll concentration in [mg/m^3], $\varkappa^*_{p\lambda}$ is the specific absorption of light by phytoplankton pigments depending on the chlorophyll concentration[4]

$$\varkappa_{y\lambda} = \varkappa_y \exp[-g(\lambda - \lambda_0)]\ ; \tag{4}$$

$\varkappa_y$ is the absorption coefficient of the dissolved organic ("yellow") substance[5] at the wavelength $\lambda_0 = 500$ nm, $g = 0.015$ nm^{-1}.

The light scattering properties of the sea water are determined by the molecular scattering and scattering by the suspended matter. The following expression is used as a physical model of the light backscattering:

$$\beta_\lambda = \beta_{w500}\,(500/\lambda)^{4.3} + \beta_z\,(590/\lambda)^q\ , \tag{5}$$

where $\beta_{w500} = 9.8{\cdot}10^{-4}$ m^{-1} is the backscattering coefficient of clear water,[4] and β_z is the backscattering coefficient of a suspension at $\lambda = 590$ nm. The values β_z and q depend on the concentration of suspended matter and particle size distribution ($q \to 4.3$ for very small suspended particles, q takes the less values for coarse suspended particles).

By substituting Eqs. (2)–(5) into Eq. (1), we obtain the physical model of SBC depending on five parameters: chlorophyll concentration, absorption coefficients of dissolved organic and suspended substances, scattering coefficients of the suspension at a wavelength of 590 nm, and on the power index q. Their values vary as the sea water composition changes.

To determine the most probable values of these parameters for water where measurements were carried out, the problem was solved on minimization of the sum of squares of deviations of the model spectrum from the measured one.

It should be noted that small experimental errors in SBC can bias the estimates at the minimization over five parameters. To avoid catching local minimum for the main one, we used the existence of correlation between SBC at 590 nm, determined mainly by the scattering coefficient of the suspension (absorption in this range is determined by clear water), and the absorption of the suspension $\varkappa_{sm}$. Indeed, as it was shown earlier,[6] the value of SBC at 590 nm linearly depends on the suspension concentration (in mg/m^3) in quite a wide range. It is natural to suppose that the light absorption by the suspension is also proportional to its concentration. From the generalized experimental data,[7] we have obtained the expression for the dependence of $\tilde{\varkappa}_{sm}$ on ρ_{590}

$$\tilde{\varkappa}_{sm} = 9.5\ \rho_{590} - 0.009\ . \tag{6}$$

Let us assume, however, that some concrete values of $\varkappa_{sm}$ and ρ_{590} are not strictly related, but only correlate with the variance $(\tilde{\varkappa}_{sm}/3)^2$.

Let us now minimize the purpose function:

$$F = \sum_i\,(\rho_{\lambda i}\,(C_p,\ \varkappa_y,\ \varkappa_{sm},\ \beta_z,\ q) - \rho_i)^2 \times$$

$$\times \exp\{[(\varkappa_{sm} - \tilde{\varkappa}_{sm})/(\tilde{\varkappa}_{sm}/3)]^2\}\ , \tag{7}$$

where $\rho_{\lambda i}(C_p, \varkappa_y, \varkappa_{sm}, \beta_z, q)$ are the model values of SBC; ρ_i are the measurement data. One should note that the dependence (6) is physically meaningful at $\rho_{590} > 0.001$, and there are no additional conditions formulated for the value $\varkappa_{sm}$ for processing most transparent water, where the suspended matter concentration is small (the second factor in Eq. (7) is ignored).

Minimization of Eq. (7) was performed in two stages. By selecting the values β_z and q from a preliminary set of possible values of these parameters ($0 \le \beta_z \le 0.05$, and $0 \le q \le 4.3$), we determine the absorption coefficient value for every measured value of SBC corresponding to such a model. At the second stage we look for the most characteristic values of the absorption coefficients of different components of the sea water,[8] for the absorption spectrum obtained, in three-dimensional space of the parameters with coordinates $x = C_p$; $y = \varkappa_y$; $z = \varkappa_{sm}$.

By equalizing the derivatives with respect to y and z to zero, we obtain the system of two equations, linear on y and z. Solving this system relative to y and z, one can obtain the values that provide minimum to the purpose function on the set x. After substituting the obtained expressions, the purpose function is transformed to the function of one variable, x. Since it is not a function of squared x, the "gold section" method[9] is used to determine its minimum. Then the values y and z are calculated by the obtained x.

When applying the "gold section" method, the multiple calculations of the function $\varkappa_{p\lambda}$ are needed. To do this, it is necessary to know the dependence of the specific absorption coefficient of phytoplankton pigments $\varkappa^*_{p\lambda}$ on the chlorophyll concentration. By statistically processing the experimental data, it was obtained in Ref. 10 an expression for the dependence of the specific absorption coefficient of phytoplankton pigments on the color pigment index $C_{\rm In} = \varkappa^*_{p443}/\varkappa^*_{p661}$, and the ranges of the most probable values of $C_{\rm In}$ were established for a wide range of C_p values. The spline approximation of the dependence obtained is performed in the algorithm developed.

The values of unknown parameters (q, β_z, $C_p = x$, $\varkappa_y = y$, $\varkappa_{sm} = z$) obtained from the calculations, are then substituted into Eq. (7) for obtaining the zero approximation of the minimum value of the function $F^{(0)}$. Then we select new values β_z and q and repeat the procedure to obtain the next value $F^{(1)}$, thus performing search for minimum of this function by the coordinate-by-coordinate slope method over two variables.

2. RESULTS OF CALCULATION OF THE SEA WATER COMPOSITION BASED ON THE SPECTRAL BRIGHTNESS COEFFICIENT OF THE SURFACE MEASURED IN THE OPEN OCEAN AND COASTAL ZONE

Let us first apply the algorithm we have developed for estimation of the concentration of ecologically important components of the sea water in the areas off of the coastal zone. The typical dependences of SBC for water of different types were obtained in Ref. 11 based on generalizing numerous measurement data. For calculations we selected the waters characterized by the water type indices of 1.5–1.6 (oligotrophic) and 2.0–2.5, 2.7–3.7 (mesotrophic water). 21 SBC values for each dependence selected in the range 400–600 nm in a 10 nm step (they are marked by asterisks in Fig. 1), were used as reference values when performing the optimization.

The optimum models of the absorption (curves *1*) and backscattering (curves *2*) spectra of the sea water and the corresponding models of SBC (curves *3*) were obtained using a computer program created according to the aforementioned method.

The values of chlorophyll concentration, absorption coefficients of the dissolved organic matter and suspension, scattering coefficient of the suspended particles at 590 nm and the power q obtained from the optimization are given in the Table. It is seen that the values of these parameters determined by concentrations of the sea water components increase in some proportion in the open ocean at transition from transparent water to a more turbid, and biologically more productive water. Thus, the chlorophyll concentration and absorption by the "yellow" substance increase by one and the same factor. The value q varies from 4.3 to 2.0 that is indicative of the increase of contribution from the coarse fraction, the particles of organic origin, into the scattering.

The method proposed was also applied to processing the remote measurements of SBC carried out from onboard a research vessel both in the open sea and the coastal zone. Measurements were carried out by means of a special spectrophotometer constructed by V.A. Matyushenko.[12]

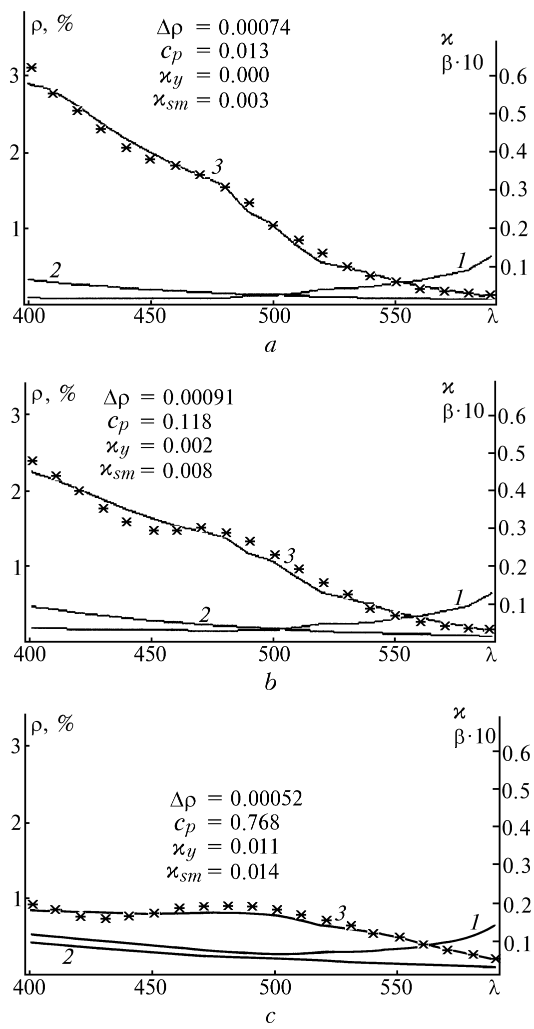

FIG. 1. Determination of the sea water composition from the SBC values characteristic of the open sea: a) oligotrophic water with water type index m = 1.5–1.6; *b) mesotrophic water with* m = 2.0–2.5; *c) mesotrophic water with* m = 2.7–3.7; *(points are values of SBC obtained by averaging the experimental data, 1) model absorption curves; 2) model scattering curves; 3) model dependence of SBC obtained by means of optimization).*

TABLE. Chlorophyll concentration C_p, *absorption coefficients of organic matter* $\varkappa_y$ *and suspension* $\varkappa_{sm}$, *scattering coefficient of suspension at* λ = 590 nm β_z *and the exponent of power dependence, obtained from solving the inverse problem by means of the optimization method, in comparison with the data of direct measurements of* C_p.

Type of water	q	β_z, m^{-1}	C_p, mg/m^3	$\varkappa_y$, m^{-1}	$\varkappa_{sm}$, m^{-1}	Direct measurements C_p, mg/m^3
1.5–1.6	4.3	$7.6\cdot10^{-4}$	0.013	$0.2\cdot10^{-3}$	$0.3\cdot10^{-2}$	0.017±0.05
2.0–2.5	4.3	$1.3\cdot10^{-3}$	0.12	$0.2\cdot10^{-2}$	$0.8\cdot10^{-2}$	0.21±0.10
2.7–3.7	2.0	$2.9\cdot10^{-3}$	0.75	$1.1\cdot10^{-2}$	$1.5\cdot10^{-2}$	0.43±0.27
Ionic sea	4.3	$7.0\cdot10^{-4}$	0.01	$0.1\cdot10^{-2}$	$0.2\cdot10^{-2}$	< 0.02 0.04 (different samples)
Bosporus channel	1.5	$1.5\cdot10^{-2}$	0.82	$7.8\cdot10^{-2}$	$5.4\cdot10^{-2}$	from 0.35 to 2.9 (different samples)

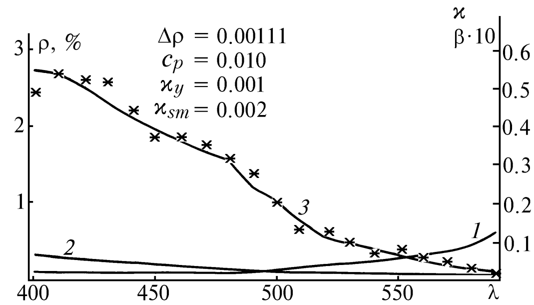

FIG. 2. Determination of the sea water composition from remote measurements of SBC from onboard a research vessel in Ionian Sea.

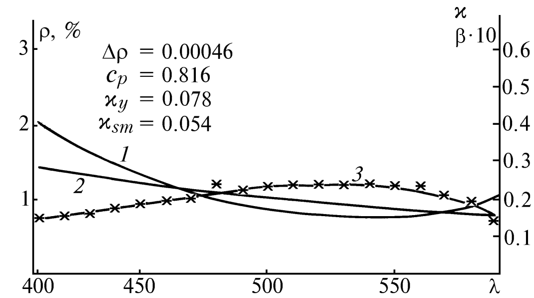

FIG. 3. Determination of the sea water composition from measurements of SBC in the Sea of Marmora, near the entrance to Bosporus.

Figures 2 and 3 show some results of measurements and the curves approximating them in two most characteristic water areas – in Ionian Sea, the water of which is characterized by a very high transparency, and in the Sea of Marmora near the city of Istanbul. It is seen that in both cases the method makes it possible to obtain good approximation of the measured spectral dependences ρ_λ. The values of the chlorophyll concentration in sea water obtained using the optimization are close to those in samples measured.

Thus, the method we have developed for processing the data of remote measurements of the spectrum of radiation upwelling from the sea surface makes it possible to estimate the sea water composition. The method can be applied both to the open ocean and coastal zones, because no assumptions on the correlation between the concentration of sea water components were done when developing it.

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