Reconstruction of integral ecological characteristics of the marine environment from results of multispectral optical sounding

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Various aspects of solving direct and inverse problems of optical sounding of the ocean are considered. It is simulated how the vertical distribution of optically active admixtures affects the variability of the sea color index. Practical procedures for fast reconstruction of ecological characteristics of the marine environment from the results of contact measurements of its spectral transmittance are presented.

Remote optical techniques are now widely used to study natural and anthropogenic processes in the ocean. In this respect, approaches to solution of direct and inverse problems of multispectral optical sounding of the ocean and the ocean–atmosphere interface are of great interest. Some aspects of this problem are considered here.

1. Influence of dynamics of vertical distribution of optically active admixtures in the marine environment on variability of sea color index

It is well-known that maximally reliable results can be obtained at simultaneous optical sounding of the marine environment from different observation levels using not only remote but also contact hydrooptical equipment. Thus, for example, the same change of the sea color index detected at remote sounding of the ocean with an illumination photometer from a spaceborne platform can be caused both by the corresponding change of the total (integral) concentration of phytoplankton pigments throughout the sounded sea surface layer and by the vertical redistribution of pigments with the unchanged total concentration. To remove this ambiguity of sounding results, additional synchronous investigations are needed (e.g., use of airborne lidar systems with gating of backscattering signals or application of contact optical sounding of the surface layer from shipborne hydrooptical equipment).[1,2]

Here we discuss in detail the results of shipborne measurements during a complex experiment on synchronous remote and contact sounding of the sea surface layer near the northern seacoasts of the Black Sea. This experiment was aimed at studying the influence of the dynamics of the vertical distribution of chlorophyll A concentration measured by *in-situ* fluorimeter on variability of the sea color index monitored by a shipborne illumination photometer. It should be noted that the sea color index I_{12} is

$$I_{12} = B_1/B_2, \qquad (1)$$

where B_1 and B_2 are the brightness of the upward flux of natural light from the sky and the Sun upon diffusive reflection by the sea depth at the wavelengths $\lambda_1 = 443$ nm and $\lambda_2 = 550$ nm.

Figure 1 shows the typical vertical profiles of temperature and the intensity of chlorophyll A fluorescence in the sea surface layer before and after natural hydrodynamic disturbance (presumably, collapse of internal waves). As follows from this figure, such sea disturbance resulted in "compression" of the chlorophyll surface layer: its upper boundary went down, whereas the lower boundary (in the region of the seasonal layer where hydrophysical characteristics change sharply) went up as compared with the background position. Since the visibility of the Secchi disk (z_S) in this water area did not exceed 8–10 m and the depth of the seasonal layer was 25 m, the main contribution to the observed variation of the color index was evidently due to the shift of just the upper boundary of the chlorophyll A layer (initially located at the depth of 1–1.5 m). Deepening of this boundary in this case can be associated not only with the efficient decrease of the chlorophyll concentration near the sea surface but also with the partial destruction of this pigment under the hydrodynamic action.

Now let us consider the technique for solving the direct problem of optical sounding for actual values of hydrooptical characteristics of the marine environment.

We use a standard set of average values of hydrooptical characteristics for surface water in coastal zones of the northern part of the Black Sea at a wavelength of 443 nm (in the chlorophyll absorption band)[3]:

– survival probability of photon $\Lambda(443) =$ $= b/c = 0.86$;

– extinction coefficient $c(443) = a + b = 0.42$ m^{-1};

– scattering coefficient $b(443) = 0.36$ m^{-1};

– absorption coefficient $a(443) = 0.06$ m^{-1};
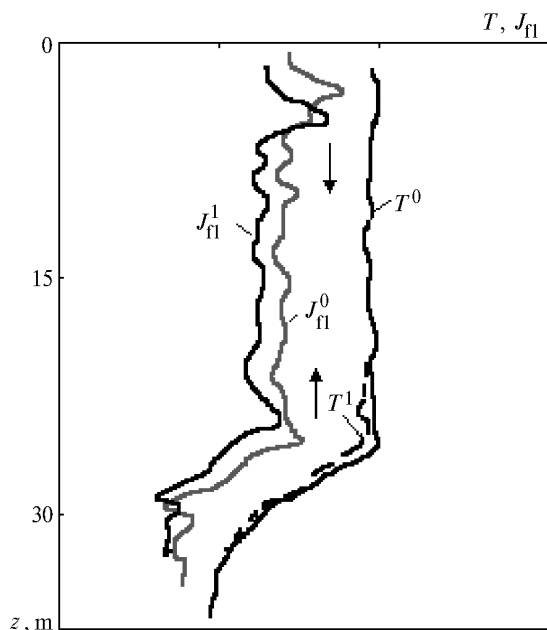
– light penetration depth $z_{0.95} = 17$ m.

Fig. 1. Variability of vertical distribution of hydrophysical characteristics: J_{fl} and T are the vertical profiles of intensity of chlorophyll A fluorescence and temperature before (J_{fl}^0 and T^0) and after (J_{fl}^1 and T^1) natural hydrodynamic disturbance, z is the depth.

Taking into account the above comments, we select a two-layer stratification model of hydrooptical characteristics (Fig. 2) using the experimentally measured values of vertical attenuation of underwater irradiance k_d and backscattering coefficient b_b for each of the layers. Now we assume that the sea color index $I_{443/550}$ can be presented as

$$I_{443/550} \sim R(443)/R(550), \qquad (2)$$

where $R(443)$ and $R(550)$ are the coefficients of diffuse reflection of the sea depth at the wavelengths of 443 and 550 nm, respectively.

Since light absorption by chlorophyll is minimum at the wavelength of 550 nm (that is why spectral analysis has been chosen as a reference one), the variability of the sea color index ($I_{443/550}$) due to the dynamics of the vertical distribution of this pigment is determined almost completely by the corresponding variability of the coefficient of diffuse reflection

$R(443)$ of the sea in the 443-nm chlorophyll absorption band (working spectral channel).

In accordance with Ref. 4, in a multilayer ocean model the coefficient of diffuse reflection $R(\lambda)$ of N sea water layers with different hydrooptical characteristics can be presented in the form:

$$R(\lambda) = \sum_{n=1}^{N} R_n(\lambda) \prod_{i=2}^{n} T_i^2(\lambda), \qquad (3)$$

where λ is the radiation wavelength, $R_n(\lambda)$ is reflection of the nth layer

$$R_n(\lambda) = \frac{b_b(\lambda)}{2k_{dn}(\lambda)} \left\{ 1 - \exp\left[- 2k_{dn}(\lambda)\, \Delta z_n \right] \right\};$$

T_i is the transmittance of the ith layer, $T_i(\lambda) =$ $= \exp[- k_{di}(\lambda)\, \Delta z_i]$; b_b is the coefficient of light backscattering by the marine environment; $k_{dn}(\lambda)$ is the coefficient of vertical light extinction by the nth layer; Δz_n is the thickness of nth layer (within which k_{dn} and b_b are considered to be constant); n and i are the numbers of layers in the marine environment.
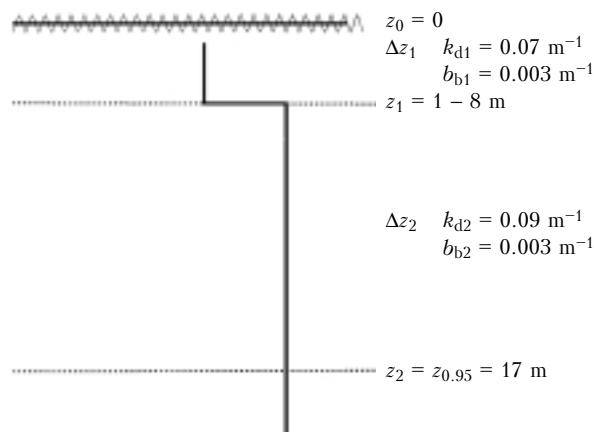

Fig. 2. Two-layer stratification model of hydrooptical characteristics: Δz_1 is the thickness of surface layer with low chlorophyll content; Δz_2 is the thickness of surface layer with maximum chlorophyll content; k_{d1} and k_{d2} are the indices of vertical attenuation of underwater irradiance for the first and second layers, respectively; b_b is the backscattering coefficient of the marine environment (determined by the content of mineral suspended matter in it), this coefficient is roughly the same for both layers; the layer of sharp change is at a depth of 23–27 m.

Now let us calculate the relative variability $\Delta R(443)/R(443)$ as a function of the depth of the upper boundary of the surface chlorophyll layer for the practical case shown in Fig. 2. For simplicity, we neglect the contribution of chlorophyll scattering (i.e., we believe that light is backscattered in the surface layer at a mineral suspended matter distributed evenly up to the layer of sharp change $b_b = b_{b1} \approx b_{b2}$). Then Eq. (3) takes the form

$$R(443) = \frac{b_b}{2k_{d1}} \left[1 - \exp(-2k_{d1}\,\Delta z_1) \right] +$$

$$+ \frac{b_b}{2k_{d2}} \left[1 - \exp(-2k_{d2}\,\Delta z_2) \right] \exp(-2k_{d1}\,\Delta z_1) \ . \ (4)$$

As an example, let us calculate the variation of the diffuse reflection coefficient $R(443)$ in the 443-nm chlorophyll absorption band as the upper boundary of the surface chlorophyll layer goes down from the sea–atmosphere interface to a depth of 8 m. If the upper boundary z_1 coincides with the sea–atmosphere interface (i.e., $z_1 = 0$), then from Eq. (4) it follows that $R(443) = 0.015$. The calculated dependence $\Delta R(z_1)/R_1$ (where R_1 is the coefficient of diffuse reflection with the upper boundary of the surface chlorophyll layer being at a depth of 1 m) is shown in Table 1.

It is seen from Table 1 that as the upper boundary of the surface chlorophyll layer shifts by 1 m, the sea color index changes by 1–2%, what can be measured experimentally.

Table 1. Relative variability of the diffuse reflection coefficient $R(443)$ for a two-layer model as the upper boundary z_1 of the layer of maximal chlorophyll A content goes in depth of the marine environment

z_1, m	1	2	3	4	5	6	7	8
$R\cdot10^2$	1.71	1.72	1.74	1.78	1.81	1.84	1.86	1.88
$\Delta R/R_1$, %	0	0.6	1.8	4.1	5.9	7.6	8.7	9.9

Now let us consider the practical procedure of fast reconstruction of ecological characteristics of the marine environment from the results of contact measurements of its spectral transmittance *in situ*.

2. Fast estimation of ecological characteristics of the marine environment from results of contact multispectral sounding

Recall that extinction of a parallel monochromatic light beam in the natural marine environment due to its absorption and scattering by water and optically active admixtures (OAA's) is described by the Bouguer law[5,6]:

$$P(\lambda) = P_0(\lambda) \exp[-c(\lambda)L], \ \ c(\lambda) = a(\lambda) + b(\lambda), \ (5)$$

where λ is the wavelength of the sounding light beam; $c(\lambda)$, $a(\lambda)$, and $b(\lambda)$ are the extinction, absorption, and scattering coefficients; $P_0(\lambda)$ and $P(\lambda)$ are the power of the light flux at the entry to the water layer of thickness L and at the exit from it.

In the first (linear) approximation,[1,4] the absorption coefficient $a(\lambda)$ and the scattering coefficient $b(\lambda)$ are related with the volume concentrations C of the corresponding OAA's as

$$a(\lambda) = a_0(\lambda)C; \qquad (6)$$

$$b(\lambda) = b_0(\lambda)C, \qquad (7)$$

where $a_0(\lambda)$ and $b_0(\lambda)$ are the specific absorption and scattering coefficients.

Light extinction by the natural marine environment (with a "standard" set of OAA's of natural origin) can be described by the following equation[1,4]:

$$c(\lambda) = a_w(\lambda) + b_w(\lambda) + a_{ph}(\lambda) + b_{ph}(\lambda) + a_y(\lambda) + a_s(\lambda) + b_s(\lambda) \approx$$

$$\approx c_w(\lambda) + a_{ph}(\lambda) + a_y(\lambda) + b_s(\lambda) \qquad (8)$$

or

$$c(\lambda) - c_w(\lambda) \approx a_{0ph}(\lambda)C_{chl} + a_{0y}(\lambda)C_y + b_{0s}(\lambda)C_s, \ (9)$$

where $c_w(\lambda)$ is light extinction by pure water (tabulated value) due to absorption $a_w(\lambda)$ by water molecules and scattering $b_w(\lambda)$ at them; $a_{ph}(\lambda)$, $a_y(\lambda)$, and $a_s(\lambda)$ are the coefficients of absorption by phytoplankton pigments, yellow substance, and suspended particles ($a_s(\lambda)$ is usually neglected); $b_s(\lambda)$ and $b_{ph}(\lambda)$ are the coefficients of overall scattering at suspended particles and phytoplankton ($b_{ph}(\lambda)$ is usually neglected as well); $a_{0ph}(\lambda)$ and $a_{0y}(\lambda)$ are the specific coefficients of absorption by phytoplankton pigments and yellow substance; $b_{0s}(\lambda)$ is the specific coefficient of light scattering at suspended particles; C_{chl}, C_y, and C_s are the volume concentrations of chlorophyll A, yellow substance, and suspension.

Let us assume that in the general case the natural marine environment containing n types of OAA's is sounded in p spectral channels chosen so to correspond to the spectral peculiarities of the OAA's. Then at the depth z the net light extinction coefficient can be presented as[1]:

$$c(\lambda_j, z) - c_w(\lambda_j) = \sum_{i=1}^{n} \alpha_{0i}(\lambda_j)\, C_i(z), \qquad (10)$$

where $j = 1, 2. \ldots, p$.

Here λ_j is the sounding wavelength corresponding to the jth spectral channel; $\alpha_{0i}(\lambda_j)$ is the generalized specific absorption or scattering coefficient of the ith OAA (a known value); $C_i(z)$ is the concentration of the ith OAA at the depth z.

As an example, let us consider the experiment on studying the spatial distribution of the spectral transmittance of water in the Nevskii Bay of the Gulf of Finland of the Baltic Sea in order to evaluate ecological conditions at places of intense anthropogenic effect.[3] In this experiment, transmittance was measured from aboard a fast motorboat simultaneously in four spectral channels of the visible and UV spectral regions. The spectral channels (360, 443, 550, 650 nm) were selected so to correspond to spectral peculiarities of the most widespread natural OAA's (yellow substance, phytoplankton pigments, suspended matter).

Table 2. Spectral extinction coefficients measured experimentally in contact photometric measurements and ecological characteristics reconstructed from them

Experimentally measured spectral coefficients of light extinction by sea water				Reconstructed hydrooptical and ecological characteristics of sea water			
$c(360)$, m^{-1}	$c(443)$, m^{-1}	$c(550)$, m^{-1}	$c(650)$, m^{-1}	$a_y(360)$, m^{-1}	$b_s(650)$, m^{-1}	C_y, mg/l	C_s, mg/l
9.4	5.5	2.8	2.4	5.4	2.1	23.8	4.2
8.8	4.9	2.4	2.1	5.5	1.8	24.2	3.6
7.6	4.1	1.8	1.7	5.2	1.4	22.9	2.8

The measured extinction coefficients for one of the monitored areas are given in Table 2. Taking into account the spectral peculiarities of the selected OAA's and pure water, the set of equations (10) can be simplified:

$$c(360) - c_w(360) \approx a_y(360) + b_s(360);$$

$$c(443) \approx a_{ph}(443) + a_y(443) + b_s(443); \qquad (11)$$

$$c(550) \approx a_y(550) + b_s(550);$$

$$c(650) - c_w(650) \approx b_s(443).$$

In Eq. (11) it is assumed that:

− In the UV spectral region, light extinction is determined by absorption due to yellow substance, as well as by scattering at the suspended matter;

− In the blue-violet spectral region, light extinction is determined by absorption due to pure water, yellow substance, and phytoplankton pigments, as well as by scattering at the suspended matter;

− In the green spectral region, extinction is determined by absorption due to yellow substance and scattering at the suspended matter;

− In the red spectral region, extinction is determined mainly by scattering at the suspended matter;

− In the blue and green spectral regions, extinction by pure water can be neglected.

For fast estimates such rough assumptions are quite justified.[3]

Now let us use the relations verified for the water of the Baltic Sea[3,6,7]:

$$b_s(\lambda) \sim 1/\lambda; \qquad (12)$$

$$a_y(\lambda) = a_y(360) \exp[-0.017(\lambda - 360)] \qquad (13)$$

in the wavelength region from 360 to 490 nm;

$$a_y(\lambda) = 0.154 \, a_y(360) \exp[-0.011(\lambda - 500)] \quad (14)$$

in the wavelength region from 500 to 680 nm.

Then from Eqs. (11) and (12) it is easy to determine $b_s(650)$, $b_s(360)$, and $a_y(360)$. Further, from Eqs. (12) and (13) we can estimate $a_y(443)$, $b_s(443)$, and $a_{ph}(443)$ using the values of $a_y(360)$ and $b_s(650)$. Then, in the same way, from Eqs. (12) and (14) we can determine $a_y(550)$ and $b_s(550)$ using $a_y(360)$ and $b_s(650)$, and so on. Table 2 gives thus reconstructed values of the absorption coefficient of the yellow substance (at the wavelength of 360 nm) and the

coefficient of scattering at the suspended matter (at the wavelength of 650 nm). Using the corresponding values (known from the literature) of the specific absorption coefficients of the yellow substance and the specific coefficients of scattering at the suspension for inland water bodies and coastal sea waters,[6] we can reconstruct the concentrations of these OAA's (given in Table 2).

Unfortunately, it is impossible to reconstruct the absorption coefficient of phytoplankton in a similar way and to estimate its content in the seawater from the results of *in situ* contact measurements of water transmittance. The fact is that very high concentrations phytoplankton pigment (12−30 mg/m^3 and higher) are typical of the studied water areas in the Gulf of Finland.[8] This causes the strong dependence of the specific absorption coefficient $a_{0ph}(\lambda)$ on the content of these pigments in the seawater, and Eq. (6) ceases to be valid. In this case, to solve the formulated problem, it is worth using contact measurements of chlorophyll A fluorescence in the seawater.[7]

Analysis of the reconstructed hydrooptical and ecological characteristics of the marine environment given in Table 2 shows that the observed marked variability of the experimentally measured coefficients of light extinction by the seawater is mostly caused by the space and time variability of the content of suspended particles. The absorption coefficient and the concentration of the yellow substance are much less variable. The relatively high values of the absorption coefficient of the yellow substance and the coefficient of scattering at the suspension, as well as their concentrations are indicative of the high level of anthropogenic load on the monitored water areas of the Gulf of Finland. The error of reconstruction of the ecological characteristics of natural waters from the results of hydrooptical studies does not exceed 20−30%. This value is quite acceptable for real-time ecological monitoring. Arbitration estimates of these characteristics should be made by analytical methods with specially prepared samples of sea water.[7,8]

Conclusion

Thus, the simplified algorithms for reconstructing ecological characteristics of the marine environment from the results of multispectral optical sounding make possible real-time estimation of the ecological state of a

monitored water area. This is especially important in ecological monitoring of areas subject to strong technogenic impact (including places of underwater disposal of chemical and radioactive wastes, underwater mining operation, areas of intense navigation, and so on).

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