

Comparative analysis of two methods of interpreting remote spectrometric data on the state of water ecosystems

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Received September 17, 2001

Peculiarities of two methods of interpreting remote spectrometric data on the state of water ecosystems are analyzed. The first method deals with the optically active components, and the second one with the optical state of a water ecosystem. The accuracy of determination of optically active components in traditional method of interpretation is estimated. The conditions for applicability of each method are given. It is shown that remote spectrometric data are an objective indicator of the ecosystem's state.

Advantages and disadvantages of the use of airborne spectrometers for monitoring water ecosystems are known quite well. The main advantages are the short time needed for obtaining the information, the possibility of real-time survey over vast territories, and contactless (nondestructive) methods of obtaining information. The main disadvantages of remote control methods are low resolution among the components and low accuracy of their determination.

Omitting the discussion of obvious advantages of these methods, let us consider the disadvantages in detail. Let us, first, consider the subject of our study. If the subject is an ecosystem, then the object is its emitting properties in the visible region, i.e., the spectra of upwelling radiation. The task is to find the direct relation between the radiation recorded with a remote sensor and the subject of the study. It is a classic inverse problem.

the spectra of radiation going upward from the water surface mostly have no peculiarities characteristic of emission spectra. From the viewpoint of classic spectroscopy, such a behavior of the spectra is quite understandable. Narrow spectral peaks merge into an unresolved (in the spectral meaning) band, and transitions to internal atomic levels are absent. The exclusion is only the fluorescence of chlorophylls and phycobilins.

The theory of brightness spectra and the spectra of the brightness coefficient (BC) is well developed.^{4,5} A sufficiently good agreement between the model BC spectra and the experimental data has been achieved⁶ (Fig. 1). In the approximation of "anisotropic scattering at a noticeable absorption"^{4,5} with the allowance for fluorescence of chlorophylls and phycobilins, the equation for calculation of the BC spectra has the following form:

$$\rho(\lambda) = \frac{\sum_i \sigma_i^\gamma(\lambda) C_i + \alpha_{\text{water}}(\lambda) + 0.5 \sigma_{\text{water}}(\lambda) + w_{\text{chl}}(\lambda) C_{\text{chl}} + w_{\text{pb}}(\lambda) C_{\text{pb}}}{\sum_i [\alpha_i(\lambda) + (1 - \Phi_i(\lambda)) \sigma_i(\lambda)] C_i},$$

In passive remote methods, the sun is a source of radiation, and the radiation going upward from the water surface is the solar radiation transformed due to scattering and/or absorption by a water ecosystem. The ecosystem components contributing to the re-emission processes and changing the complex refractive index $m = n + in'$ are referred to as optically active components (OACs). The spectral properties of the optically active components are rather thoroughly studied and described in many papers (see Refs. 1–3). Here we would like to note only the following. The absorption and scattering spectra of almost all optically active components are nonselective, except for the absorption spectra of phytoplankton pigments. Therefore,

where $\alpha(\lambda)$, $\sigma(\lambda)$, and $\sigma^\gamma(\lambda)$ are the specific coefficients of absorption, scattering, and scattering at the angle γ by water or the i th OAC with the concentration C_i ; w is the specific yield of fluorescence of chlorophyll or phycobilin; Φ is the integral of the scattering phase function, which represents the fraction of radiation scattered to the rear hemisphere by particles of the i th kind; λ is the wavelength, for which the calculation is performed. Hereinafter, we use the following abbreviations for the optically active components: MSM – mineral suspended matter, phy – phytoplankton, DOM – dissolved organic matter, chl – chlorophyll a , c – carotenoids, pb – phycobilins.

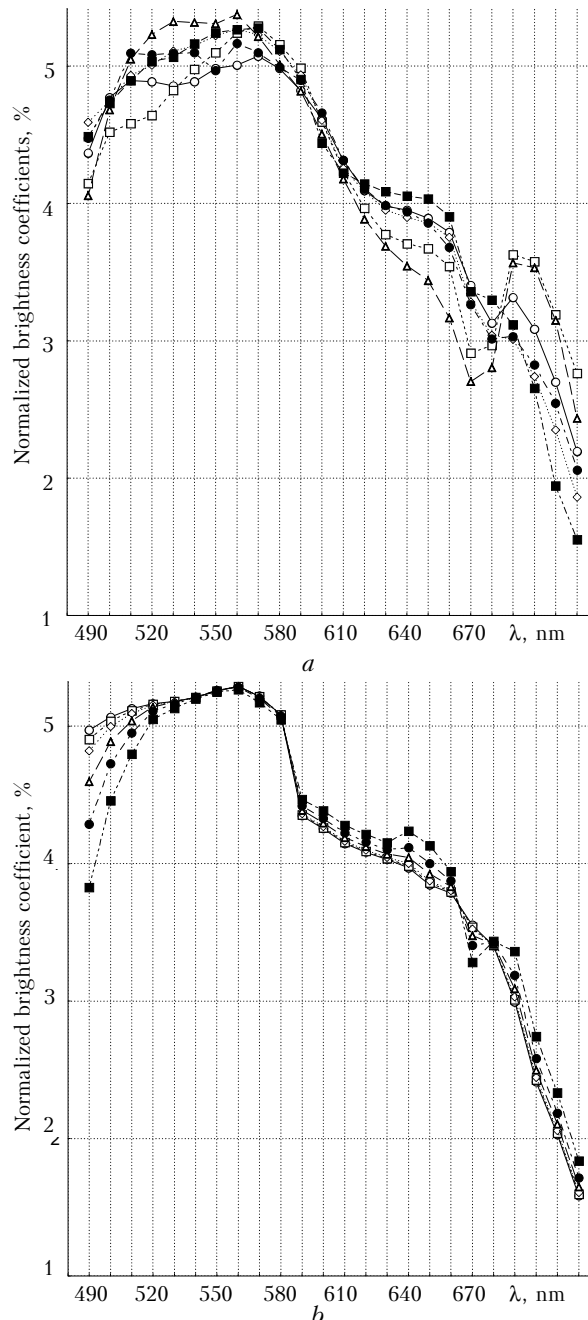


Fig. 1. Normalized spectra of the brightness coefficients of radiation going upward from the water surface: experiment (a) and model (b). The spectra with different concentrations of optically active components are marked by different marks.

It can be seen that in the general case it is impossible to derive a simple analytical equation for an individual optically active component. However, taking into account that the absorption and scattering properties can be partly separated in the visible spectral region, some algorithms are proposed for reconstruction of the OAC concentrations with the use of radiative parameters representing the ratio $\rho(\lambda)$ in the region of λ , where the effect of an OAC is maximum to the wavelength region, where the effect of all OACs, except for that to be determined, is maximum. Thus,

the algorithms were proposed for determination of the concentration of phytoplankton (from the chlorophyll *a* concentration), mineral suspended matter, and dissolved organic matter (see Refs. 1 and 9 and references therein, as well as Refs. 7 and 8). These algorithms are different for clean sea and ocean waters and surface inland waters because of the different composition of optically active components in the water medium. In some papers, it was mentioned that these algorithms can be successfully applied,^{1,8,9} but only as “regional”⁹ or as obtained in the approximation of a “constant matrix.”⁶ The approach, in which the OAC concentration is determined from the spectrometric information, will be referred to as the OAC representation.

Let us consider this representation in a more detail, using the model spectra obtained in this approximation.^{6,10} Figure 2 depicts the points, by which the dependence $C_{\text{phy}} = A(RP)^B_{C_j}$, $j = 1 \dots p$, is drawn for different concentrations of the mineral admixture. Here C_j are the concentrations of OACs changing the complex refractive index of water medium for different values of j , A and B are the coefficients of regression, RP is the radiative parameter, i.e., the brightness ratio (or BC ratio) at two wavelengths. The values of C_{phy} are the set varying from 0 to 110 mg/l, and for every C_{phy} value the value of C_{MSM} varied from 0 to 50 mg/l. All other OACs in this series of spectra kept unchanged, that means that, we can use the “constant matrix” approximation.

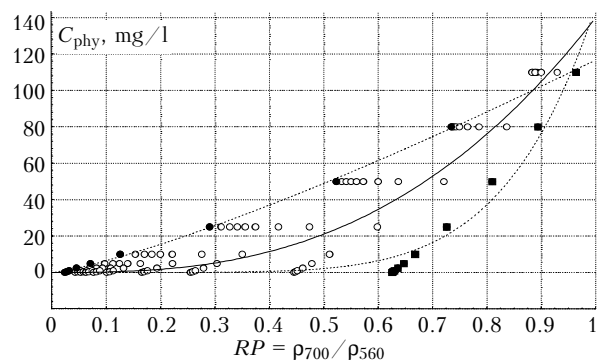


Fig. 2. Regression dependences $C_{\text{phy}} = A(RP)^B_{C_j}$ drawn from the model spectra. Closed circles are for RP values calculated at $C_{\text{MSM}} = 0$ (row 9 of Table 1), closed squares are for $C_{\text{MSM}} = 50$ mg/l (row 11 of Table 1), and open circles are for the intermediate values of C_{MSM} .

If C_{MSM} keeps constant, the points can be described by the regression dependence $A(RP)^B$ with high accuracy. But, as soon as C_{MSM} begins to change, the coefficients A and B of this dependence change as well. This change is marked (cf. rows 9–11 of Table 1 and see Fig. 2). Therefore, in the general case, at a significant change of all OACs except for the one under study it proves although possible though not always correct to determine the coefficients A and B from the BC spectra.

If we draw the regression dependence as a mean for all spectra, where C_{MSM} varies from 0 to 50 mg/l, then we obtain the dependence close to that determined from the experimental data (row 10 of Table 1). The

correlation coefficient $r[C_{\text{phy}}, RP]$ is close to and even higher than that determined from the experimental data. However, it is seen from Fig. 2 that the spread of points about the mean dependence is rather wide. In calculating $r[C_{\text{phy}}, RP]$, this spread is compensated for by an increase in the number of points, therefore the correlation coefficient varies only insignificantly. At variation of the concentrations of other OACs included in the model for BC calculation, we may obtain almost any values of A and B (Ref. 11) coefficients (cf. rows 9 and 13, 11 and 14 and the mean dependences, as well as rows 10 and 13). Thus, the OAC representation can be successfully used if the concentrations of other OACs are constant. The term “constant matrix” follows just from here.

The above condition is often fulfilled in water bodies having roughly the same OAC composition and hydrological conditions varying relatively weakly over the area of the water body. (From the practice of

research missions, it is known that, when constructing regression models, high correlation coefficient $r[C_{\text{phy}}, RP]$ is observed in the case of surveys conducted under fine weather conditions in daytime of one and the same day. If the weather conditions vary or different water objects with different hydrological conditions are surveyed, then the points used to draw the regression dependence are grouped specifically. Formally, single regression dependence can be constructed, but it is clearly seen that this dependence consists of several dependences.)

Another method to interpret remote spectrometric data is to represent them as an optical state of a water ecosystem in the space of optical states (SOS).¹⁰⁻¹⁴

In this representation, every spectrum is represented in the SOS as a point with coordinates $f1$, $f2$, and $f3$. The spectral distribution of factor loads, i.e., SOS axes $F1$, $F2$, and $F3$, is shown in Fig. 3 as obtained from the series of model and experimental spectra.

Table 1. Parameters of regression models (rows 1–8 – from experimental spectra, rows 9–14 – from model spectra)

#	Water object, year	A	B	$r[C_{\text{phy}}, RP]$	C_{phy} mean, mg/l
1	Lake Balaton, Hungary, 1985	125.21	2.32	0.95	48.8
2	Lake Balaton, Hungary, 1986	94.63	2.19	0.95	63.3
3	Lake Balaton, Hungary, 1988	68.03	2.59	0.86	10.2
4	Lake Muggelsee, Germany, 1985	217.2	1.84	0.95	101.4
5	River Don, Russia, 1983	67.36	2.84	0.97	18.5
6	River Don, Russia, 1984	71.52	2.91	0.84	12.9
7	River Severny Donets, Russia, 1983	72.54	2.82	0.92	7.9
8	River Severny Donets, Russia, 1984	58.56	2.25	0.98	24.6
Our calculations					
9	$C_{\text{MSM}} = 0, C_{\text{DOM}} = 2, C_{\text{chl}} = 0.2, C_c = 0.2, C_{\text{pb}} = 0.01$	125.70	1.36	0.99	
10	$C_{\text{MSM}} = 13.9, C_{\text{DOM}} = 2, C_{\text{chl}} = 0.2, C_c = 0.2, C_{\text{pb}} = 0.01$	139.95	2.73	0.92	11
11	$C_{\text{MSM}} = 50, C_{\text{DOM}} = 2, C_{\text{chl}} = 0.2, C_c = 0.2, C_{\text{pb}} = 0.01$	145.69	6.14	0.98	
12	$C_{\text{MSM}} = 0, C_{\text{DOM}} = 50, C_{\text{chl}} = 0.9, C_c = 0.8, C_{\text{pb}} = 0.05$	27.42	1.61	0.99	
13	$C_{\text{MSM}} = 13.9, C_{\text{DOM}} = 50, C_{\text{chl}} = 0.9, C_c = 0.8, C_{\text{pb}} = 0.05$	41.23	1.44	0.92	49.5
14	$C_{\text{MSM}} = 50, C_{\text{DOM}} = 50, C_{\text{chl}} = 0.9, C_c = 0.8, C_{\text{pb}} = 0.05$	35.82	4.44	0.99	

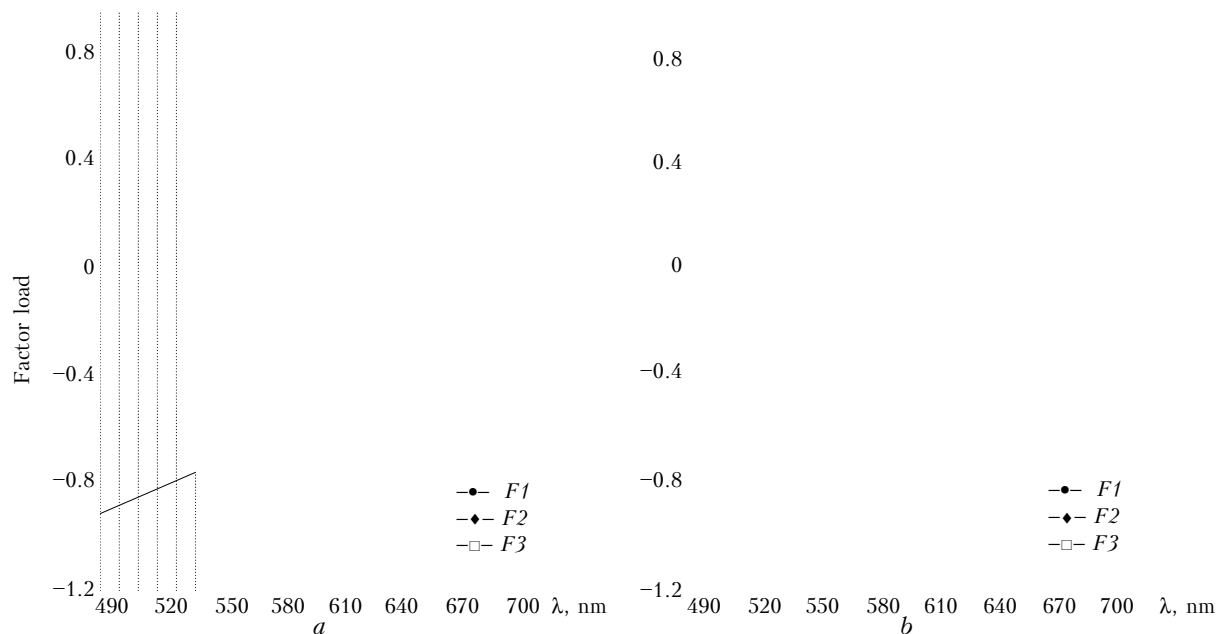


Fig. 3. Factor loads for arrays of experimental (a) and model (b) spectra.

The comparison allows us to check that such arrays have formally identical structure from the mathematical point of view. This indirectly confirms once more the correctness of selecting the model for calculation of the BC spectra. The first eigenvalues obtained from only experimental spectra are 14.33, 5.63, and 2.47, and those obtained from the model spectra are 16.08, 3.87, and 2.09. In Ref. 11 it was shown that it is most informative to represent the

spectrometric information on the SOS state in the planes of the factors 1–3 and 2–3. Figure 4 depicts the same spectra, as those used to draw the regression dependences shown in Fig. 2 (see rows 9–11 of Table 1), in SOS projections onto the planes of the factors 1–3 and 2–3, respectively. The contour of the SOS obtained from 7200 model spectra is plotted as a dashed curve. It is shown that almost all experimental spectra fall within the SOS drawn from the model spectra.¹⁰

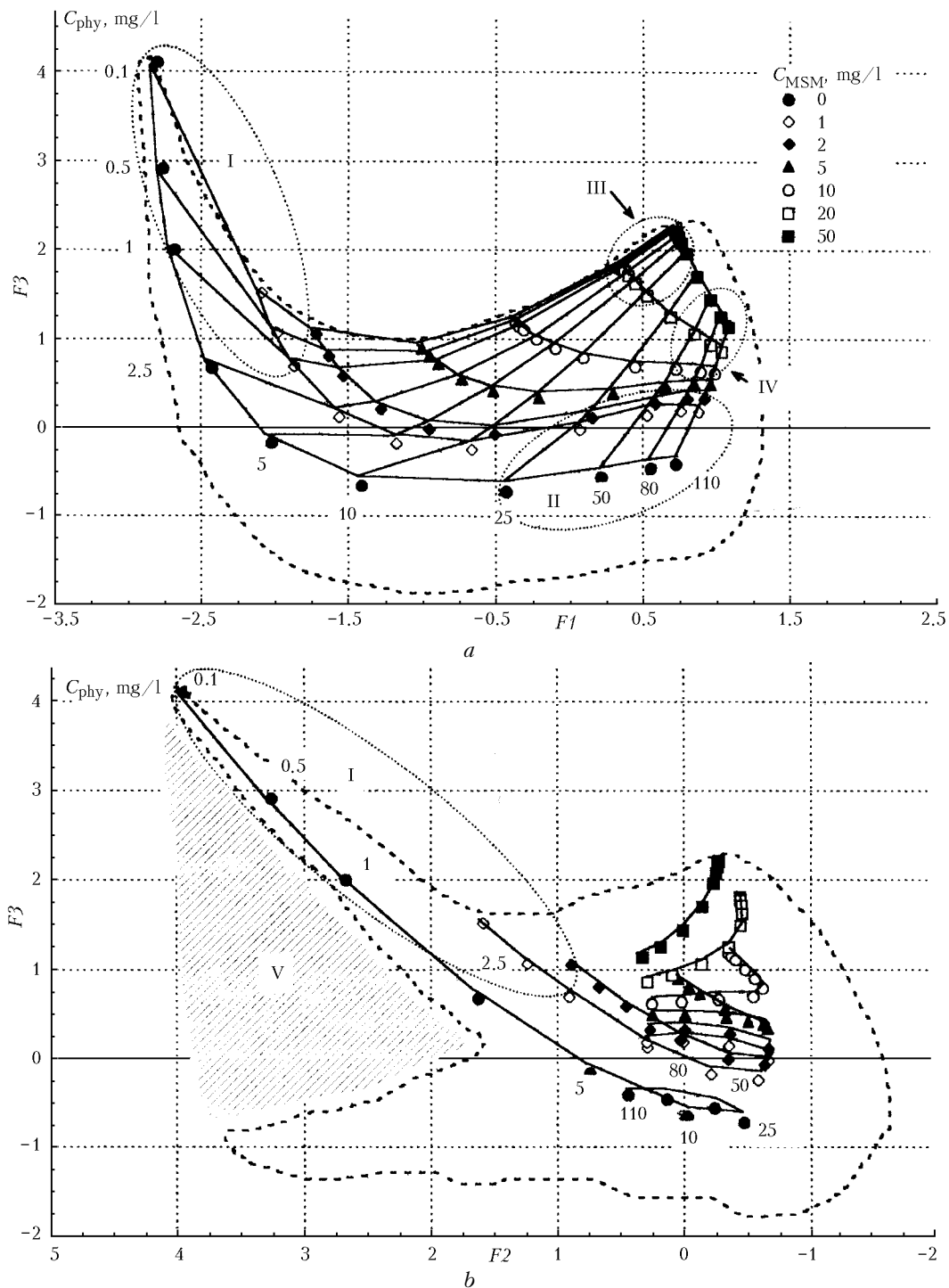


Fig. 4. Model spectra in SOS projections onto the planes of factors 1–3 and 2–3.

Table 2. Coupled coefficients of correlation between the OAC concentrations and regression ratios

	C_{pb}	C_c	C_{chl}	C_{DOM}	C_{MSM}	C_{phy}	$F1$	$F2$	$F3$
$F1$	-0.011	0.022	0.060	0.253	0.437	0.612	1.000	0.000	0.000
$F2$	0.125	-0.056	0.096	-0.289	-0.073	0.597	0.000	1.000	0.000
$F3$	0.112	-0.077	-0.325	-0.041	0.617	-0.292	0.000	0.000	1.000
$RP(700/560)$	0.060	0.000	0.157	0.072	0.213	0.881	0.780	0.581	-0.169
$RP(590/630)$	0.004	0.000	0.069	-0.242	-0.622	-0.253	-0.838	0.285	-0.354
$RP(690/590)$	0.071	0.000	0.203	0.029	-0.099	0.734	0.532	0.629	-0.360
$RP(690/580)$	0.064	0.000	0.195	0.035	-0.058	0.765	0.571	0.635	-0.333
$RP(690/570)$	0.057	0.000	0.194	0.043	-0.041	0.771	0.587	0.631	-0.322
$RP(620/560)$	-0.072	0.000	0.041	0.229	0.610	0.528	0.967	-0.001	0.189
$RP(620/570)$	-0.061	0.000	0.063	0.191	0.563	0.592	0.977	0.064	0.123
$RP(620/550)$	-0.097	0.000	0.064	0.260	0.607	0.506	0.962	-0.025	0.180

This space is open, and the contour envelopes only its part, which is filled with spectra calculated in this work. Table 2 serves as a key to interpretation of the results obtained in this representation; it gives the coefficients of correlation between OACs, factors, and the values of RP used to draw the regression dependences.

The factor 1 has significant and comparable in magnitude coefficients of correlation with many OACs. This can be explained, if we consider its behavior presented in Fig. 3. It is almost nonselective and vanishes near $\lambda \approx 580$ nm. Therefore, the meaning of this factor, or the change in the position of the point along the axis $F1$, can be interpreted as the "total pollution" of water.

The factor 2 has maximum coefficient of correlation with C_{phy} and significant coefficients of correlation with both C_{DOM} and C_{pb} . The correlation coefficient has positive sign, i.e., $F2$ increases with the increase of C_{phy} . This factor can be interpreted as an indicator of the state of ecosystem biota, species diversity of the phytoplankton.

The factor 3 has maximum coefficient of correlation with C_{MSM} and significant, but smaller coefficients of correlation with C_{chl} , C_{DOM} , and C_{phy} . With a certain care, it can be interpreted as pollution of water with substances of biotic origin.

Let us consider the behavior of spectra in the SOS. Separate a series of spectra, in which only C_{phy} and C_{MSM} vary. All other OACs are assumed constant and, in this particular case, minimum of all the values used to draw the SOS. The assumption of constant OACs is equivalent to selecting SOS cross section by a surface, at which C_{phy} and C_{MSM} vary with other OACs kept unchanged, i.e., the transition to approximation of "constant matrix" occurs. Let us join the spectra, in which either C_{phy} or C_{MSM} is constant. Curves in such a family are called double isopleths. The space bounded by extreme isopleths is a bounded area on this surface. In Fig. 4, such a surface area is separated in the SOS and represented in projections of the coordinates $F1-F3$ and $F2-F3$, respectively. In the projection $F1-F2$, this area proves to be turned sideways and, except for the case of low C_{MSM} , it is degenerated.¹¹

The highest variance of C_{phy} and C_{MSM} is observed in the projection on the axis $F1-F3$ (Fig. 4a). We can keep track of the optical state of a water ecosystem in sufficient detail by analyzing the behavior of spectra in this plane. Some regions of the SOS can be interpreted unambiguously, namely, the region of unpolluted water I, in which the variance of the optical state of a water ecosystem is maximum, the region of transparent, but "blooming" water II, the region of much polluted water IV, and the region of polluted water, but without phytoplankton III. The term "polluted" water is used conditionally and has only physical meaning: unpolluted water is water without admixtures, and any admixture is considered as a pollutant. Certainly, this is incorrect from the ecological point of view.

The SOS projection onto the axes $F2-F3$ (Fig. 4b) is remarkable, because here we can find the forbidden region V with no spectra falling in at any variations of OACs.

The 3D space – SOS – results from the shift of the considered surface due to variation of other OACs. However, in this case, the surface is not only shifted but also disturbed, what becomes especially marked at the significant variation of the concentrations of all OACs.

The considered representations can be compared through calculation of the correlation coefficients $r_{i,j} = r[RP_i, F_j]$, where RP_i is the radiative parameter, F_j is the factor score, $j = 1, 2, 3$. These correlation coefficients, along with some other parameters, are given in Table 2. Analysis of this table allows us to draw an analogy between the representations. If the radiative parameters correlating closely with the factors $F1, F2, F3$ are used in place of these factors, then formally we can draw the SOS in the RP representation. However, the radiative parameters in this case have the meaning of indicators of the state of an ecosystem, rather than the indicators of OACs.¹⁰⁻¹⁴

This is the main difference between the considered methods of interpretation of the spectrometric information. The first method can be used in the general case to determine the OAC concentrations. The accuracy of determination depends on the variability of the concentrations and on the qualitative composition

of all OACs except for the one to be determined. In this case, only two wavelengths in the recorded spectrum are used. The second method is used to determine the integral characteristics of an ecosystem, omitting determination of the OAC concentrations and using the entire visible spectrum. In some particular cases, or whenever necessary, one can pass to determination of the OAC concentrations.

Thus, the disadvantage mentioned in the first part of this paper pertains only to the first method of interpretation. To evaluate the ecological state of water ecosystems, one has to deal with concepts formed by generalization of a large number of different physical, chemical, and biological indices. In this case, the indices determined by remote spectrometric methods give an ideal or reference characteristic of the state of an ecosystem. Certainly, the problem of relations between the optical and ecological indices is still open, and its solution should be a subject of further research in this area. Besides, all the above-said applies only to the photic zone and cannot be used to study deep layers of water objects.

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