REGIONAL OCEAN COLOR ALGORITHM: ADAPTATION FOR THE INLAND WATERS STUDY

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1. INTRODUCTION

One of the most informative hydrooptical characteristics is the spectral reflectance coefficient, which is the ratio between irradiance upwelling from the sea and radiance of diffusely reflecting white screen. Upwelling radiation spectrum depends on concentrations of suspended and dissolved matters in the water, such as mineral particles of various origin, phytoplankton cells containing chlorophyll-a and other pigments, nonliving organic particles (detritus) and dissolved organic matter (yellow substance). Commonly the number of unknown seawater characteristics exceeds the number of measured parameters. Evaluation of water mass characteristics based on reflectance data is the classical inverse problem. However, algorithms for solving these problems and retrieving admixture concentrations from the upwelling radiance are insufficiently accurate. Because of the regional seawater specificity, chlorophyll-a concentration evaluations based on the optical data, particularly the satellite ones, can differ significantly from real values, especially in the coastal zones and inland waters.

Regional algorithms for remote assessment of impurities content in natural water bodies are mostly created for different regions of the sea-shelf, coastal and near-shore zones, for example (Vazyulya et al., 2014). For freshwater this problem is more complicated due to the fact that special biooptical regime is created in each inland body as an effect of the inflow of different mineral suspensions and organic substances, in particular, fertilizers, industrial and domestic wastewaters (Kutser, 2009, Mishra et al., 2017, Odermatt et al., 2012). At the same time, satellite monitoring as a method of regular coverage of large water areas is experiencing serious difficulties in assessing the bioproductivity of inland freshwater reservoirs characterized by a weak channel flow and a large number of shallow heated parts (Lavrova et al., 2014). In this work, we propose an approach to solving the inverse problem of hydrooptics for inland water bodies, and to create a regional biooptical algorithm for determining the concentrations of optically active impurities in water by the example of the Gorky reservoir on the Volga river.

2. BACKGROUND

It was shown (Mishra et al., 2014, Randolf et al., 2008) that the best way to create bio-optical algorithms for turbid waters today is to perform hyperspectral measurements of the upwelling radiance, which makes it possible to determine spectral features specific for certain pigments. But, despite the presence of hyperspectral devices, researchers use algorithms to calculate the concentration of chlorophyll a by from regression with spectral ratios (Gitelson et al., 2010, Yakobi et al., 2011) with the intention of applying similar algorithms to satellite data, as well as for the simplicity of calculations.

In this work a regional semi-analytical algorithm developed for the Black Sea coastal waters (Lee et al., 2016) was adapted to calculate the concentrations of phytoplankton pigments, the absorption of dissolved and nonliving suspended organic matter, and backscattering by mineral suspension. The algorithm was successfully applied to processing of satellite and contact data in the study of the Black Sea waters near Crimean South coast. When applying to the satellite upwelling radiance data, the bio-optical algorithm allows to obtain chlorophyll concentration values that are in better agreement with the direct measurements data than the standard satellite products.

This work is concerned with investigation of the spectral features of the water reflectance spectrum of the Gorky reservoir located on the Volga river. At the preliminary stage, the adaptation of the algorithm consisted in selecting spectral regions suitable for determining each unknown parameter, as well as input parameters corresponding to the biooptical properties of the investigated reservoir.

3. APPROACH

The data discussed in this paper were obtained during two field measurements in 2016 (August 1 – 8) and 2017 (June 24 – 30) in the southern part of the Gorky reservoir (56.6 – 57 N, 43.2 – 43.4 E) on the Volga river. The reservoir is subjected to intensive blooms (Fig. 1) of blue-green algae leading to a seasonal change in their concentration by three orders of magnitude, which provides the conditions for observing the optical characteristics of water in a wide range of variation (Molkov et al., 2018). The geometric dimensions of the reservoir (approximately 100*10 km) allow it to be investigated both by remote sensing and by contact methods. It should also be noted that contact measurements of water spectral reflectance have never been carried out on the Gorky reservoir so far.

Hyperspectral measurements of reflectance were performed using the spectrophotometer designed in Marine Optics and Biophysics Department of Marine Hydrophysical Institute (Fig. 2). The spectrophotometer can measure the spectral distribution of the upwelling water radiance normalized at the water surface spectral irradiance in range 390 – 750 nm with spectral resolution 2.5 nm, measurement error is 3%. Calibration of the instrument was carried out using diffusely reflecting screen with known reflectance coefficient. The spectrophotometer was installed approximately 1 m above the water surface on board of research vessel, in such a way that its field of view was not shadowed, the line of view was at 30-45° angle to the water surface. Each measurement consisted of sequential measurements of total reflectance of water mass ρ_{tot} and reflectance of 5cm water layer in a cuvette with dark absorbing walls, representing the water surface ρ_{surf}. Water reflectance was calculated as difference $\rho_w = \rho_{tot} - \rho_{\mathrm{surf}}$. This method allows to accurately take into account the reflection from the surface without skylight radiance measurements and modeling of Fresnel coefficients. The difference in the surface roughness in the sea and in the cuvette appears as a wider scatter of the measured ρ_{tot}, and can be neutralized by averaging of the several successive measurements.

During two research expeditions, about 150 spectra of reflectance were obtained. Averaged spectra for both expeditions are shown in Figure 3. June 2017 is the period before the bloom, and low values and smooth spectral shape of reflectance show that IOPs of water are dominated by CDOM. August 2016 is the peak of the bloom, when the main absorbing and scattering agent is phytoplankton, so maxima and minima produced by chlorophyll *a* absorption are visible, and reflectance values are significantly higher. In each expedition, 10 water samples for chlorophyll *a* concentration and phytoplankton species composition were also taken. At the same time, the accompanying hydrometeorological and hydrophysical measurements were performed, such as water and air temperature, current velocity and direction, and water transparency.

In order to solve inverse problem of bio-optics the reflectance spectrum is usually related to the ratio $b_b(\lambda)/a(\lambda)$, where $b_b(\lambda)$ is the water spectral backscattering, $a(\lambda)$ is the water spectral absorption, that, in turn, are represented as the sum of the respective components. The reflectance spectrum can be described as follows:

$$\rho(\lambda) = k \frac{b_{bw}(\lambda) + b_{bp}(550)(550/\lambda)^{\nu}}{a_w(\lambda) + A(\lambda)C_{Chl}{}^{1-B(\lambda)} + C_{dom}(440)e^{-\alpha(\lambda-440)}}. \tag{1}$$

where $k = 0{,}15$ according to approximation of radiative transfer equation solution (Shybanov, 2001); $b_{bw}(\lambda)$ is pure water backscattering coefficient; ν is backscattering spectral slope , depending on the size of the particles; $a_w(\lambda)$ is pure water absorption coefficient (Pope, Fry, 1997); $A(\lambda)$ and $B(\lambda)$ are spectral functions in pigment specific absorption parameterization, for example (Bricaud et al., 1995), α is nonliving organic matter absorption spectral slope. Model parameters: backscattering coefficient of the suspended particles $b_{bp}(550)$, concentration of the phytoplankton pigments C_{Chl}, nonliving organic matter absorption $C_{dom}(440)$ are usually found using multiparametric optimization.

To stabilize the solution of the inverse problem and to simplify the calculations the modified optimization procedure was proposed (Lee et al., 2016). A numerical experiment was conducted in order to divide the spectral range 390 – 750 nm into sites with a certain substance dominating the optical properties (Korchemkina, Shybanov, 2009). Synthetic dataset of reflectance spectra calculated using equation (1) was created with unknown parameters varying in ranges usually observed in Black Sea. Random normally distributed noise with SD of 10% was added to each unknown. Then multiple rounds of optimization in various spectral sites were performed in order to choose sites with the best retrieval of the initial unknown parameters.

According to the results, the spectral site 390 – 410 nm was used for nonliving organic matter absorption, 420 – 460 nm for the chlorophyll-*a* concentration and 460 – 650 nm for particles backscattering. Unknown model parameters were calculated using least-squares optimization, one parameter at a time, in iterative procedure. The algorithm was shown to perform well for Black Sea coastal waters, including the cases of coccolythophore bloom.

The algorithm has the ability to adapt to the hydro-optical characteristics of a particular water body by choosing the appropriate input parameters and sites for calculating each unknown parameter. In this work the adaptation to inland water conditions was made by choosing pigment absorption parameterization (Staehr, Markager, 2004, Paavel et al., 2016) for eutrophic lake waters, as well as changing the number of unknown parameters and border wavelengths for the spectral sites.

The spectral slope of nonliving organic matter absorption α has a significant effect on the calculated pigment concentrations, and it is very important for the operability of the model to choose the value correctly. To determine it, it is necessary to measure the absorption spectra in samples of nonliving organics. Due to the lack of data of such measurements for eutrophic fresh waters, spectral slope was included in the number of unknown model parameters.

4. RESULTS AND DISCUSSION

Numerical experiment similar to one described above was made in order to take into account spectral shape of reflectance of pigment and CDOM dominated eutrophic waters. Figure 4 presents an example of the distribution of the residual $(C_{Chl} - C_{Chl0})^2$ in coordinates (λ_1, λ_2), where λ_1 and λ_2 are the lower and upper boundaries of the spectral site for calculating the concentration of pigments. The minimum of the residual (shown as red spot) corresponds to λ_1 = 670 nm, λ_2 = 740 nm. The red maximum of chlorophyll absorption with a peak at 680 nm falls into this range; therefore, the obtained result seems to be reasonable. Similarly, sites for non-living organics (390 – 550 nm) and suspended matter (550 – 670 nm) were determined.

The use of the main absorption maximum of chlorophyll *a* at 440 nm for calculating pigments concentration is difficult in this case due to strong variations in the absorption of dissolved organics and detritus in this spectral range. At the same time, variations in the concentration of pigments also have a negative effect on the possibility of retrieving the absorption of non-living organic matter. Therefore, as a result of an additional experiment the 420 – 460 nm range was excluded from the site for nonliving organic matter.

Finally, each stage of the iterative procedure used in the algorithm consists in follows. First, the pigments concentration C_{chl} is calculated by one-dimensional optimization in spectral site 670 – 740 nm, while other unknown parameters have non-zero initial values. Second, $b_{bp}(550)$ is calculated in 550 – 670 nm site, taking into account the known C_{chl}. Third, C_{dom} and α are calculated in spectral sites 390 – 420 and 460 – 550 nm using two-dimensional optimization. Each step uses values obtained in previous steps. It takes about 10 iteration to reach stop condition $\left|C_{chl}^{i} - C_{chl}^{i-1}\right| < 0{,}001$.

Concentrations of phytoplankton pigments were calculated using the iterative method mentioned above and compared with the data of the chlorophyll *a* concentration in samples taken simultaneously with the optical measurements. This comparison is shown in Fig. 5. High pigment concentrations were found to be underestimated by the algorithm. The solution to this problem may be taking into account the "package effect" more thoroughly (Alcantara et al., 2016).

A weak correlation (about 50%) can be explained not only by the imperfection of the algorithm, but also by the vertical distribution profile of the algae. Since the samples were taken from a depth of 0.1 m, they could contain higher or lower concentrations of pigments than the depth averaged (effective) concentration in the photic zone, which affects the reflectance. At the same time, due to the large range of chlorophyll *a* concentration variability in samples (1 – 30 mg/m^3), a significant change in the reflectance spectral shape and the calculated values of the unknown parameters can be observed. Acquisition of new data for different seasons, together with further modification and improvement of the bio-optical model, algorithm, and measuring equipment, will allow to obtain better correlations of field and model data.

5. CONCLUSIONS

Analysis of the reflectance spectral shape features show strong seasonal variations, corresponding to natural processes in dynamic and thermal structure of the reservoir. In June the reflectance was almost uniformly distributed and influenced mainly by nonliving organic matter. In August the main optically significant component of water was phytoplankton, contributing to both absorption and backscattering, while reflectance values were in average two times higher than in June. Solution of the inverse problem of biooptics for such conditions requires an instrument with wide ranges of adaptation.

The proposed regional bio-optical algorithm is the first attempt to solve the inverse problem of bio-optics for the waters of the Gorky reservoir. The advantages of this algorithm are the usage of mathematical model and the possibility to verify the results with a data of laboratory analysis of water samples. At the same time, the current error of the algorithm tested on 20 water samples is about 50%.

The ways to improve the accuracy of the proposed algorithm are the further optimizing the mathematical approaches of the algorithm, and field observations of the environmental parameters used in the algorithm. The latter include the spectral absorption and backscattering characteristics of the water components of the studied water body, and their distribution profiles with connection to the wind-wave situation.

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FIGURES

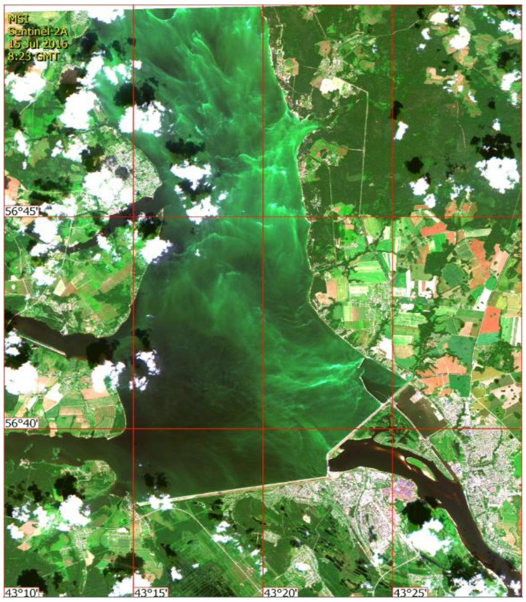

Figure 1. Cyanobacteria bloom in July 2016 in the southern part of the Gorky reservoir. Sentinel 2 quasi-truecolor image

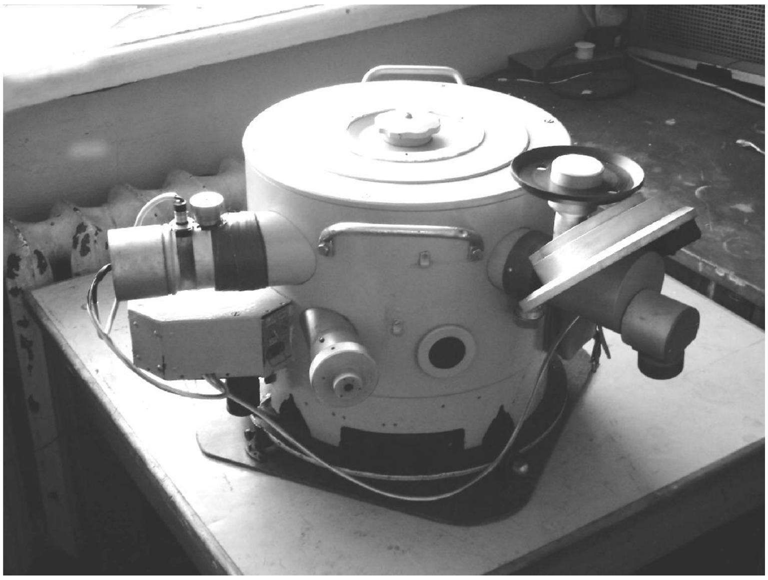

Figure 2. Spectrophotometer for water reflectance measurements (MHI RAS Marine Optics and Biophysics Department)

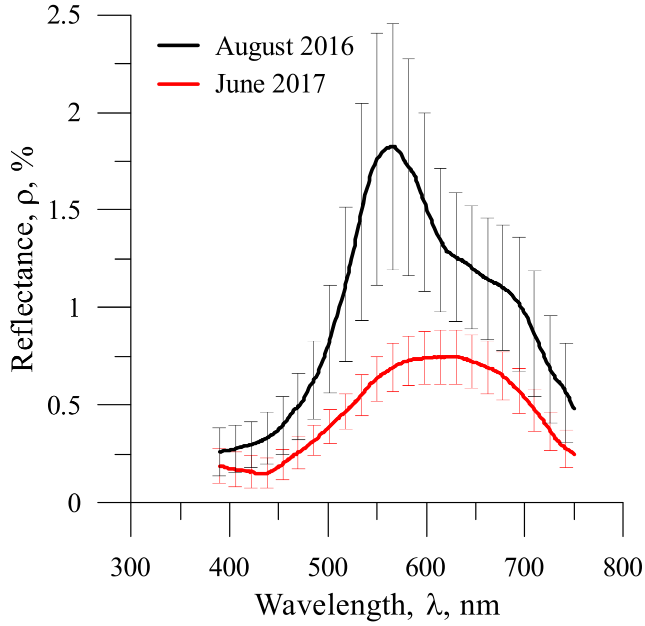

Figure 3. Average reflectance spectra (lines) and standard deviation (grey fill) obtained at the Gorky reservoir

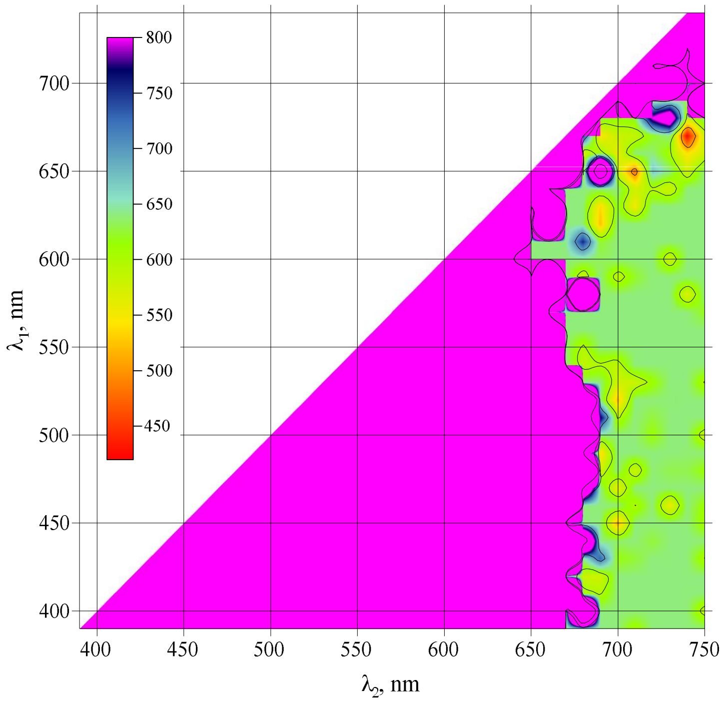

Figure 4. Residual $(C_{Chl} - C_{Chl0})^2$ depending on border wavelengths λ_1 and λ_2 for pigments concentration spectral site

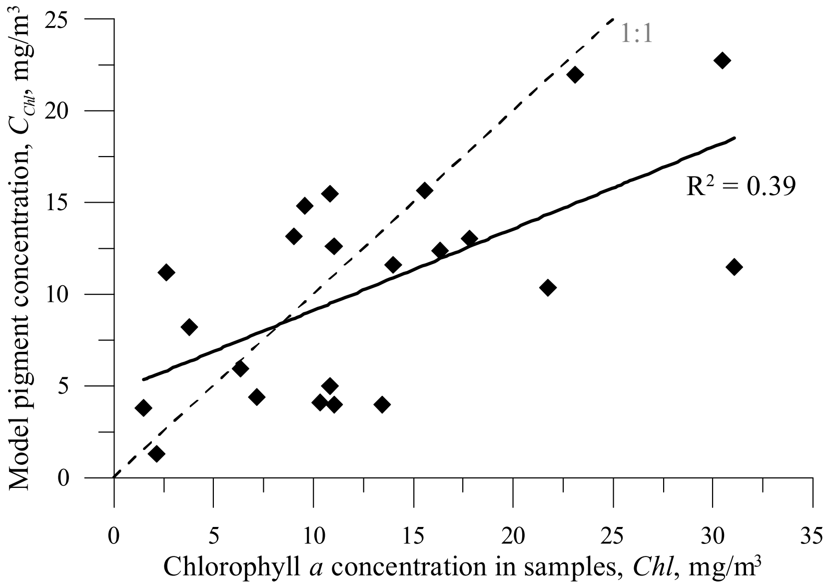

Figure 5. Comparison of calculated pigment concentration with chlorophyll *a* concentration obtained from samples analyses