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Original article

Features of Results of Optical Observations of the Black Sea from Space in Summer 2015

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Abstract
Purpose. The study aims to analyze the results of satellite observations of the Black Sea in summer 2015 during the period of increased chlorophyll *a* concentration in its deep-water region.
Methods and Results. We analyzed NASA archive products from MODIS and VIIRS optical data updated during the 2022 archive reprocessing. To ensure reliable conclusions, we compared synchronous observations from Aqua, Terra and Suomi NPP satellites and analyzed spectral dependencies of sea surface reflectance. Additionally, we compared chlorophyll *a* concentration estimates in the sea near-surface layer using two different methods: the standard NASA processing method and an alternative approach based on calculating the phytoplankton-related light absorption coefficient. This value is calculated using the GIOP (Generalized ocean color inversion model for retrieving marine Inherent Optical Properties) procedure and is included in the NASA archive among other products.
Conclusions. Analysis of satellite observations revealed the need to account for significant errors and distortions. After excluding erroneous data, we found that chlorophyll *a* concentrations in the eastern deep-water region at the end of summer 2015 reached anomalously high values of ~ 1–2 mg/m^3.

Keywords: Black Sea, satellite observations, chlorophyll *a* concentration, optical characteristics, light absorption, MODIS, VIIRS, GIOP, phytoplankton, yellow substance

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Introduction

Modern space-based optical instruments, operating in continuous global survey mode for marine regions, measure radiation emitted into space at multiple wavelengths in the visible spectrum. This enables separate analysis of atmospheric and water parameter variations, allowing their numerical values to be determined. A key parameter in this context is the chlorophyll *a* (C_a) concentration in the near-surface layer of the sea [1, 2]. This study analyzes C_a concentration estimates in the Black Sea during summer 2015.

We analyzed standard data products from the MODIS and VIIRS instruments on the Aqua, Terra and Suomi NPP satellites, sourced from the NASA archive. Satellite data analysis often encounters significant errors or limitations. These include instrumental errors during radiation detection, as well as effects from sun glint, atmospheric interference and regional seawater optical properties. Thus, careful quality control of data and results is essential.

The simplest way to improve the reliability of results is to exclude distorted data. NASA's processing system removes only data segments with gross errors. An effective method for verifying satellite data reliability is the comparative analysis of synchronous observations from different satellites [3]. Additionally, comparing C_a estimates derived from NASA's standard processing method with those from an alternative method based on the phytoplankton-related light absorption coefficient is valuable. This coefficient is calculated using the GIOP method [1] and is included among other products in the NASA archive. Another indicator of data errors is the presence of unphysical negative values of remote sensing reflectance in the short-wavelength spectral range.

These approaches to satellite data analysis were applied to study the C_a concentration anomaly in the Black Sea during summer 2015. This phenomenon was first reported in [4], which documented C_a concentrations reaching 5 mg/m³. However, that study relied solely on standard Ca estimates from the NASA archive, derived from Aqua satellite data, without rigorous validation. Typically, in summer, C_a concentrations in the near-surface layer of the Black Sea's deep-water region do not exceed 0.5 mg/m³ [5–8]. Given the significance of the phenomenon described in [4], its findings require further verification using data from all three instruments after excluding erroneous data. The absence of direct *in situ* measurements for validating satellite data underscores the importance of thorough data analysis.

This study aims to conduct a thorough analysis of Black Sea satellite data from summer 2015 to investigate elevated chlorophyll *a* concentrations in the deep-water region.

Materials and methods

The analysis below includes Black Sea observations from MODIS on Aqua and Terra satellites (MODIS-A and MODIS-T) and VIIRS on the Suomi NPP satellite. We analyzed standard Level-2 and Level-3 data products from the NASA archive (https://oceancolor.gsfc.nasa.gov/data/), updated in late 2022 (https://oceancolor.gsfc.nasa.gov/data/reprocessing/r2022). During the update, a modernized processing system was applied, resulting to final noticeable differences compared to the previous version of the corresponding data. We used the NASA-developed specialized program SeaWiFS Data Analysis System (SeaDAS, version 9.0 (https://seadas.gsfc.nasa.gov/)) for data format conversion, array compilation and pseudo-color image preparation.

The NASA archive provides data on numerous atmospheric and marine parameters, including C_a, spectral values of the sea surface reflectance coefficient ($R_{rs}(\lambda)$), indicators of backscattering and light absorption as well as components of the absorption index due to phytoplankton and yellow substance (together with detritus). For C_a analysis, we used data from two methods: NASA's standard processing method and an alternative method based on the phytoplankton-related light absorption coefficient.

C_a values in the NASA archive are calculated using a function of the $R_{rs}(\lambda)$ ratio for different pairs of light wavelengths λ selected based on the spectral region of maximum $R_{rs}(\lambda)$. This function is designed to reflect the statistical variability of water optical properties in the World Ocean [9, 10]. In general, such an approach cannot ensure accurate accounting of all the diverse variable factors affecting space-measured radiation under their independent variability [11, 12]. As experience shows, C_a estimates for the Black Sea waters in the NASA archive have low accuracy [8, 13, 14]. The effects associated with the contribution of yellow substance to light absorption in water can be one of the main sources of errors [15–17]. Thus, we also consider the results of C_a estimates calculated using the model in [18] by the following formula:

$$C_{a1} = 222 \cdot a_{ph}(443)^{1.64},$$

where $a_{ph}(\lambda)$ is phytoplankton-conditioned component of the light absorption coefficient in the sea at a wavelength of 443 nm.

The $a_{ph}(\lambda)$ value is calculated using the GIOP method and is included in the NASA archive among the other products. The GIOP method relies on modeling empirical $R_{rs}(\lambda)$ values obtained during atmospheric correction. In this case, we use physical models describing the $R_{rs}(\lambda)$ dependence on the light wavelength and on the content of main impurities in the water or their optical properties at a fixed λ. The solution is derived by minimizing differences between empirical and modeled $R_{rs}(\lambda)$ spectra. The key feature of this method is the separate quantification of light absorption components associated with yellow substance and phytoplankton. A detailed discussion of the physical meaning and limitations of the possibilities of applying various methods for determining C_a from satellite measurements is provided in [1, 2, 15–17, 19]. Comparing C_a estimates from two methods enhances the reliability of results.

The initial data for C_a calculations are spectral $R_{rs}(\lambda)$ values obtained during the elimination of atmospheric interference. To ensure reliable conclusions, it is necessary to take into account that various kinds of errors and distortions can occur in the empirical $R_{rs}(\lambda)$ values [1] [20–24]. These errors may arise from complex

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[1] Papkova, A.S., 2023. [*Accounting for the Influence of Dust Aerosols on the Restoration of the Spectral Brightness Coefficient of the Black Sea Based on Satellite Data*]. Thesis of Cand. Phys.-Math. Sci. Sevastopol: FRC Marine Hydrophysical Institute of the Russian Academy of Sciences, 117 p. (in Russian).

atmospheric correction, sun glint, instrument calibration errors, etc. In the GIOP method, distortions in R_{rs} values increase discrepancies between their empirical and modeled values. Thus, only data that have undergone rigorous quality control should be analyzed. Different methods and criteria can be used to select suitable data based on research objectives and data characteristics. NASA's satellite data processing includes operations to identify and exclude distorted data. The final results are Level-3 products. During preparation, all relevant reliability control criteria for specific data segments are applied. A description of the aforementioned criteria is available at https://oceancolor.gsfc.nasa.gov/resources/atbd/ocl2flags/.

Evidence from the Black Sea observations suggests that NASA's quality control system eliminates gross errors. To enhance result reliability, our methodology involves comparing data from instruments installed on three different satellites. Additionally, we analyze $R_{rs}(\lambda)$ spectral dependencies, assess discrepancies between empirical and modeled $R_{rs}(\lambda)$ spectra and compare C_a estimates from two computational methods.

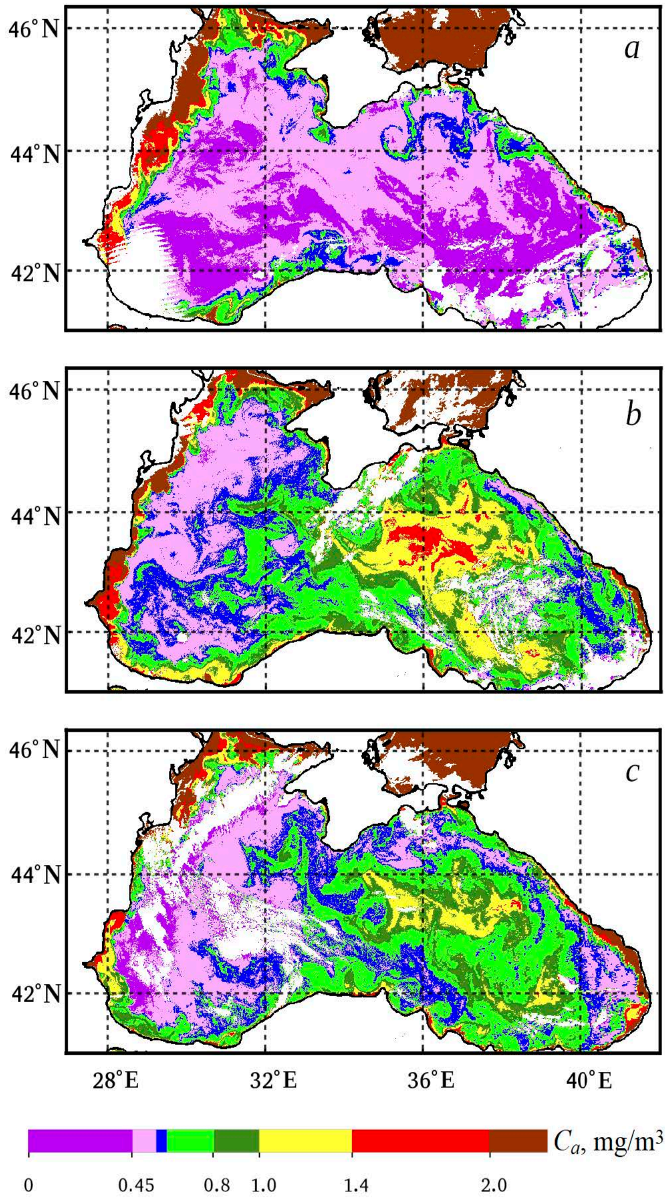
Results and discussion

Fig. 1 shows the results of the Black Sea satellite observations in summer 2015. These include C_a estimates derived from standard NASA archive processing of MODIS-A instrument data. C_a estimates in the NASA archive for the Black Sea are approximate, but this is not critical for our analysis if data with gross errors, as noted in [13], are excluded. At the beginning of summer, no anomalies are observed, but in August, C_a in the eastern sea center reaches ~ 1–2 mg/m^3. Data from [4] for August 31 indicate that C_a exceeded 5 mg/m^3. The highest C_a values, exceeding 1 mg/m^3, are concentrated in an irregularly shaped region at ~ 43–44°N, 35–39°E. Such high C_a levels are very unusual; thus, additional analysis accounting for potential interference and errors is necessary.

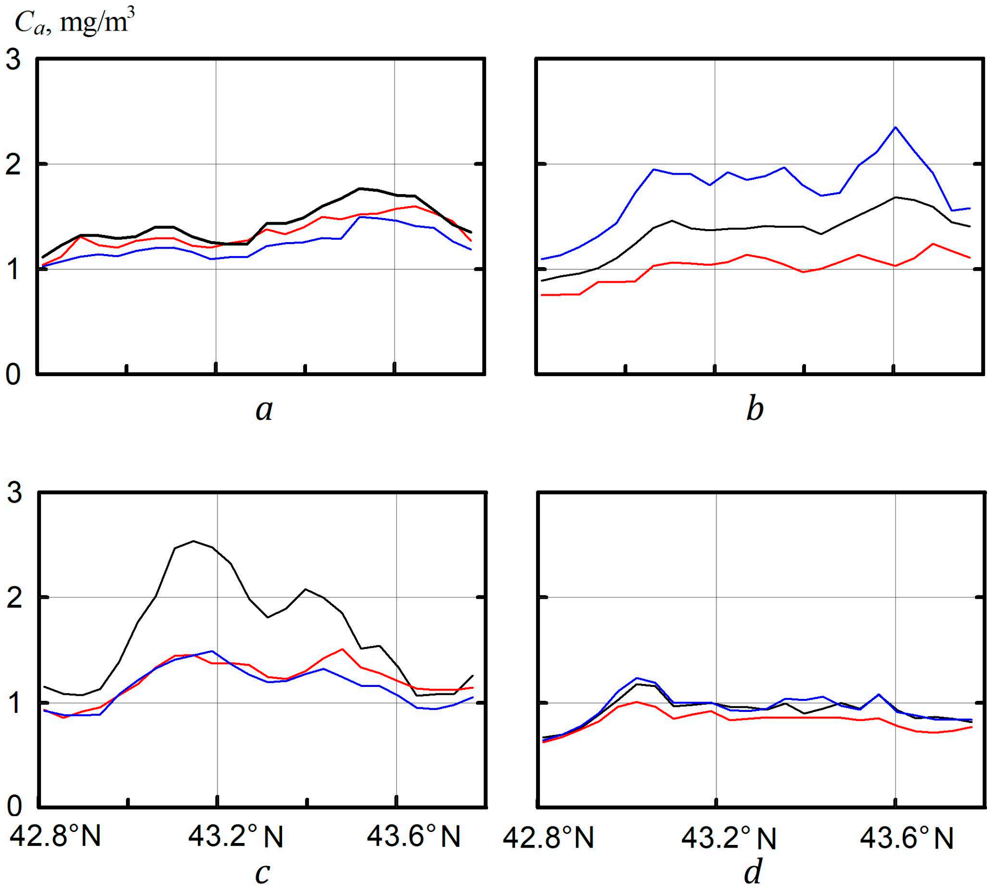
To this end, we examine C_a estimates from different days using data from MODIS-A, MODIS-T and VIIRS instruments. Fig. 2 demonstrates standard Level-3m data products in format denoted by C_a from the NASA archive for a single satellite pass over the Black Sea region. These data are averaged over a 4 km regular coordinate grid. C_a variations with latitude are shown at longitudes 36.19°E (Fig. 2, *a*, *c*), 35.81°E (Fig. 2, *b*) and 37.35°E (Fig. 2, *d*).

C_a values in Fig. 2 exceed significantly typical values for the Black Sea in summer, usually below 0.5 mg/m^3. On August 27, as well as on September 3, similar results were observed from all three instruments. On these days, the C_a values do not exceed 2.0 mg/m^3. Differences between August 27 and September 3 results are small and can reflect natural C_a variations in the sea.

Results differ significantly for August 29 and 31 data. On August 29, results from all three instruments vary widely, with VIIRS data reaching ~ 2.4 mg/m^3. On August 31, the MODIS-T and VIIRS instruments showed similar results, with C_a not exceeding 1.5 mg/m^3, while MODIS-A reported C_a at ~ 2.5 mg/m^3.



F i g. 1. Results of C_a determining in the near-surface layer of the Black Sea based on the MODIS-A data for 17.07.2015 (*a*), 27.08.2015 (*b*) and 03.09.2015 (*c*)



F i g. 2. Comparison of the results of C_a determining based on the MODIS-A (black curve), MODIS-T (red curve) and VIIRS (blue curve) data for 27.08.2015 (*a*), 29.08.2015 (*b*), 31.08.2015 (*c*) and 03.09.2015 (*d*)

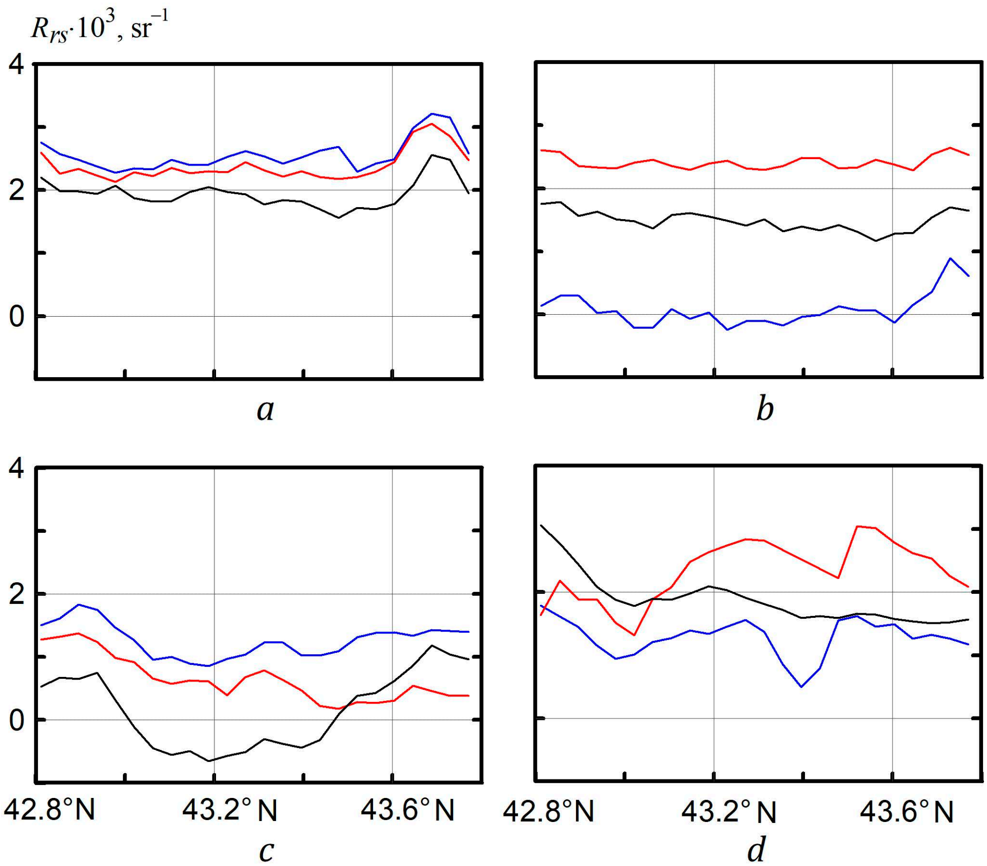
Elevated C_a values were observed at coordinates 43.60°N, 35.81°E from VIIRS on August 29 and 43.1458°N, 36.1875°E from MODIS-A on August 31. Table provides C_a values from all three instruments on the Level-3m data grid. The table data are representative; the highest C_a values are lower than reported in [4], but this difference is not due to the spatial location of the data. As noted above, comparing the 2022-updated and previous NASA archive data shows that the 2022 reprocessing resulted in differences compared to earlier data, explaining this discrepancy.

The results are evident from graphs of sea surface reflectance coefficient $R_{rs}(\lambda)$ derived from MODIS and VIIRS data at radiation wavelengths λ equal to 412 and 410 nm, respectively. Hereafter, these wavelengths are denoted as λ_1. The graphs in Fig. 2 and 3 are derived from the same data. The $R_{rs}(\lambda_1)$ values at the two points specified earlier are presented in Table. The $R_{rs}(\lambda_1)$ values from different instruments show poor agreement. This indicates errors and distortions due to challenges in determining $R_{rs}(\lambda)$.

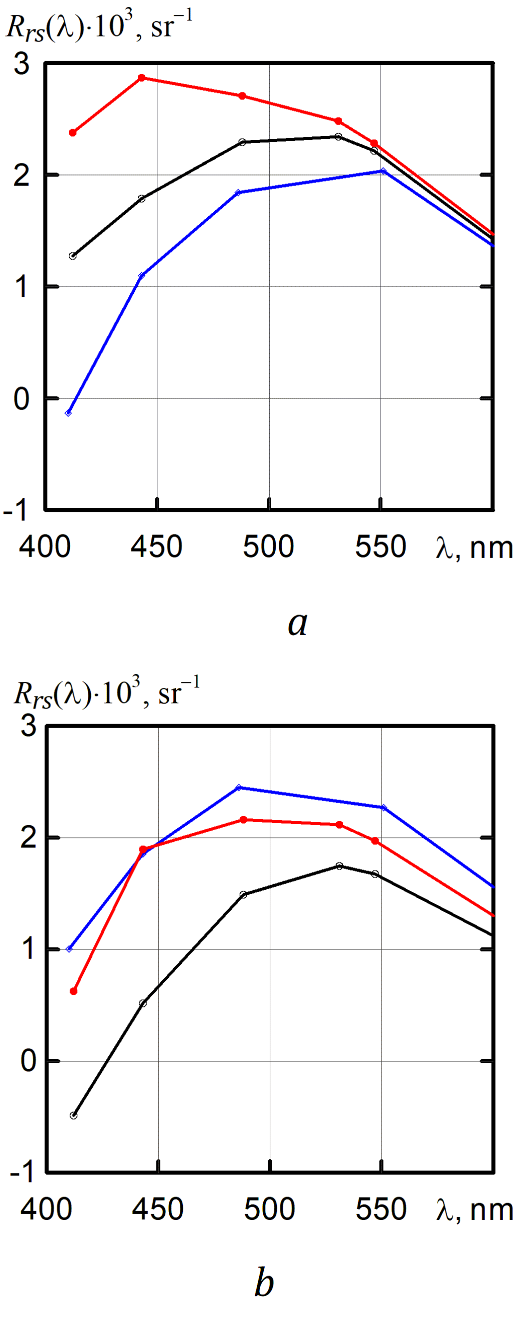
Results of determining C_a and $R_{rs}(\lambda_1)$ at certain points based on the data from various instruments

Date	Instrument	C_a, mg/m^3	$R_{rs}(\lambda_1)$, sr^{-1}
29.08.2015	MODIS-A	1.69	0.00128
	MODIS-T	1.03	0.00238
	VIIRS	2.35	−0.00013
31.08.2015	MODIS-A	2.54	−0.00049
	MODIS-T	1.45	0.00063
	VIIRS	1.45	0.00089

The key features in Fig. 3 graphs are unphysical negative $R_{rs}(\lambda_1)$ values from VIIRS on August 29 and MODIS-A on August 31, coinciding with the highest C_a values in Fig. 2. At the same time, conditions on August 27 and September 3 were more favorable, with $R_{rs}(\lambda_1) > 0$ from all three instruments. Notably, NASA's satellite data processing system for Level-3 data preparation does not exclude data with negative $R_{rs}(\lambda)$ values.



F i g. 3. Results of determining sea surface reflectance $R_{rs}(\lambda_1)$ based on the MODIS-A (black curve), MODIS-T (red curve) and VIIRS (blue curve) data for 27.08.2015 (*a*), 29.08.2015 (*b*), 31.08.2015 (*c*) and 03.09.2015 (*d*)



F i g. 4. Empirical $R_{rs}(\lambda)$ spectral dependencies obtained from the MODIS-A (black curve), MODIS-T (red curve) and VIIRS (blue curve) data for 29.08.2015 (*a*) and 31.08.2015 (*b*)

The $R_{rs}(\lambda)$ values are obtained during initial data processing and atmospheric correction. When determining the value of C_a, wavelengths $\lambda < 443$ nm are not used directly, as distortions are most pronounced in this spectral range. Elsewhere in the spectrum, the $R_{rs}(\lambda)$ values may also be distorted, though less noticeably.

To illustrate the Table data, full $R_{rs}(\lambda)$ spectra are demonstrated in Fig. 4. Differences in C_a estimates from different instruments result from $R_{rs}(\lambda)$ differences caused by distorting factors. $R_{rs}(\lambda)$ values cannot be negative, so measurements with $R_{rs}(\lambda_1) < 0$ are unsuitable. As shown in Fig. 4, negative $R_{rs}(\lambda_1)$ values indicate a distorted spectrum, leading to overestimated C_a values.

Thus, excluding data with negative $R_{rs}(\lambda_1)$ values, the remaining C_a values do not exceed 2.0 mg/m^3. Notably, the conclusion of anomalously high C_a in [4] relied on MODIS-Aqua data from August 31, but excluding these data leaves results from two other instruments without losing useful information. This was not taken into account in [4], resulting in overestimated C_a values.

Due to the contribution of yellow substance to light absorption, C_a values from the NASA archive for the Black Sea often differ from actual values [8, 13, 14]. Thus, it is valuable to evaluate an alternative approach using the GIOP method [1, 19]. In this approach, C_a is calculated using the phytoplankton-related light absorption coefficient $a_{ph}(443)$. The results obtained in this case are denoted as C_{a1}.

Since the GIOP method involves instability or ambiguity in solving the multidimensional optimization problem, the obtained results are more sensitive to $R_{rs}(\lambda)$ inaccuracies than standard C_a estimates. Therefore, the obtained C_{a1} values often show clear distortions or questionable reliability. Overall, the situation as a whole during the period under consideration was unfavorable. Nevertheless, conditions for successful GIOP application may exist in specific data subsets where at least one instrument's readings lack significant distortions.

For example, one can analyze a homogeneous region identified from the Black Sea survey conducted using the MODIS-A instrument, where no significant local fluctuations in measurement results (with sizes ~ 1 km) are observed between adjacent spatial resolution elements. This region, characterized by elevated C_a concentrations, spans ~ 5 × 5 km, with its center located at ~ 37.33°E, 43.18°N. It includes 23 data points in Level-2 format, each with a spatial resolution of ~ 1 km.

We present a comparison of chlorophyll *a* concentration estimates derived from various satellite measurement methods for this selected area on September 3, 2015: $\langle C_a \rangle = 1.013$ mg/m^3; $\langle C_a \rangle = 1.055$ mg/m^3; $\langle a_{ph}(443) \rangle = 0.038$ m^{-1}; $\langle a_{dg}(443) \rangle = 0.061$ m^{-1}; $\sigma(C_a) = 0.051$ mg/m^3; $\sigma(C_{a1}) = 0.128$ mg/m^3.

Here, $\langle x \rangle$ and $\sigma(x)$ represent the mean value and standard deviation of the quantity x; $a_{dg}(443)$ denotes the light absorption coefficient at $\lambda = 443$ nm due to yellow substance (with detritus). The reliability of these results is supported by the implementation of the GIOP method within the study area, where the errors in the model reconstruction of the $R_{rs}(\lambda)$ empirical spectra do not exceed a few percent.

The standard deviation values mentioned above further confirm the reliability of the obtained results.

The GIOP method cannot be applied to the survey results from the eastern Black Sea on September 3, obtained by MODIS-T and VIIRS instruments due to the significant distorting effect of sun glint.

When determining C_a concentration using the GIOP method, a value of C_{a1} ~ 1.0 mg/m^3 was obtained, consistent with the result from NASA's standard method. In terms of concentration level, C_a ~ C_{a1} ~ 1.0 mg/m^3 turned out to be lower than the C_a values observed on other days, possibly due to a natural decline in the anomalous concentrations observed on August 31 by September 3. Nevertheless, the level of C_a ~ 1.0 mg/m^3 remains notably high for the summer season. The agreement between C_a and C_{a1} at 1.0 mg/m^3 was previously reported in [17], attributed to the identical values of $a_{\mathrm{ph}}(443)$ and $a_{\mathrm{dg}}(443)$. Different methods for calculating C_a from satellite data rely on distinct physical principles, which may introduce varying sources of error in the results. Consequently, the agreement between results from different methods provides indirect confirmation of minimal distortions in the analyzed data segment.

Conclusion

In analyzing chlorophyll *a* concentrations in the Black Sea derived from satellite measurements during summer 2015, sourced from the NASA archive, we identified the need to account for significant errors and distortions. Indicators of errors included discrepancies between data processing products from the MODIS and VIIRS optical instruments on the Aqua, Terra and Suomi NPP satellites, as well as physically implausible negative values of $R_{\mathrm{rs}}(\lambda)$ in the short-wavelength spectral range. Additionally, we compared chlorophyll *a* concentrations in the sea surface layer estimated using two calculation methods: NASA's standard operational processing method and an alternative approach based on calculating the phytoplankton-related component of the light absorption coefficient.

After excluding erroneous data from the analysis, it was found that over a large area in the eastern deep-water region of the Black Sea in late summer 2015, chlorophyll *a* concentrations derived from satellite data exhibited anomalously high values, ranging from ~ 1–2 mg/m^3.

It should be noted that the described 2015 anomaly is not entirely unique. Similar events occurred in 2001, 2012 and 2019. The most likely cause of the 2015 anomaly was an intense and prolonged storm wind.

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Sergey N. Korolev – preparation of data and graphic illustrations, discussion of applied methods of data analysis and the results obtained, final design of materials for publication

The authors have read and approved the final manuscript.
The authors declare that they have no conflict of interest.