Bio-Optical Characteristics of the Black Sea Coastal Waters near Sevastopol: Assessment of the *MODIS* and *VIIRS* Products Accuracy

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Purpose. The purpose of the work is to evaluate accuracy of the satellite products for the coastal waters near Sevastopol, generated by the standard algorithms based on the *MODIS* and *VIIRS* (installed at the artificial Earth satellites *Aqua* and *Terra,* and at *Suomi NPP*, respectively) data.
Methods and Results. In situ sampling was carried out at the station (44°37'26" N and 33°26'05" E) located at a distance of two miles from the Sevastopol Bay. The chlorophyll *a* concentration was measured by the spectrophotometric method. The spectral light absorption coefficients by optically active components were measured in accordance with the current NASA protocol. The spectroradiometers *MODIS* and *VIIRS* Level-2 data with spatial resolution 1 km in nadir around the *in situ* station (44°37'26" ± 0°00'32" N and 33°26'05" ± 0°00'54" E) were used. The satellite products were processed by the *SeaDAS* 7.5.3 software developed in NASA. The research showed that the standard NASA algorithms being applied to the *MODIS* and *VIIRS* data, yielded incorrect values of the optically active components' content in the Black Sea coastal waters near Sevastopol as compared to the data of *in situ* measurements in the same region: the satellite-derived "chlorophyll *a* concentration" was on average 1.6 times lower in spring, and 1.4 times higher in summer; the contribution of phytoplankton to total light absorption at 443 nm was underestimated in 8.7 times; the light absorption by colored detrital matter was overestimated in 2.2 times.
Conclusions. The NASA standard algorithms are inapplicable to calculating bio-optical indices in the coastal waters of the Black Sea near Sevastopol since they provide incorrect values of the satellite products ($C_{a\text{-s}}$, $a_{\text{ph-s}}(443)$ and $a_{\text{CDM-s}}(443)$). Operative ecological monitoring based on satellite data requires development of a regional algorithm taking into account the seawater optical features in the region and in the coastal zone, in particular.

Keywords: chlorophyll *a*, phytoplankton, colored dissolved organic matter, non-algal particles, remote sensing, *MODIS*, *VIIRS*, Black Sea

Introduction

Remote sensing is actively applied to solve various scientific problems, including operational monitoring of the aquatic ecosystems state. Great advantages of remote sensing are the ability to carry out long-term series of observations with a large spatial coverage.

In aquatic ecosystems, coastal waters deserve distinct consideration, since they are heavily impacted by man-made factors. With river/coastal runoff, suspended and colored dissolved organic matter along with nutrients enters coastal waters, which leads to phytoplankton biomass increase in coastal waters [1]. Phytoplankton, non-algal particles and colored dissolved organic matter are optically active components of the environment (OAC). The OAC content in water and their spectral optical properties (absorption and scattering) [2–4] determine the radiance ascending from the water column, recorded by satellite instruments [5]. The variability of OAC contribution to the total light absorption is one of the reasons for the inaccuracy of modeling satellite products using standard algorithms.

Chlorophyll *a* concentration ($C_{a\text{-}s}$) is one of the standard satellite products used widely as water productivity indicator. To use satellite products, it is important to verify that they characterize the studied water area state correctly. At present, no works with the results of the *MODIS* and *VIIRS* satellite products comparison with *in situ* measurements in the coastal Black Sea waters in different seasons of the year similar in space and time are known.

Long-term data array of regular bio-optical monitoring carried out in the coastal Black Sea waters in the Sevastopol Bay area since 2009 is a unique base for satellite data validation.

The purpose of the present work is to evaluate accuracy of the satellite products for the coastal waters near Sevastopol, generated by the standard algorithms based on the *MODIS* and *VIIRS* (installed at the artificial Earth satellites *Aqua* [1] (*MA*) and *Terra* [2] (*MT*), and *VIIRS* [3] at *Suomi NPP* (*V*) respectively) data. For this purpose, a comparison between the chlorophyll *a* concentration of and the light absorption coefficient of the OAC, calculated from satellite and *in situ* data in the coastal waters of Sevastopol in individual seasons was carried out.

Preliminary results were presented at the All-Russian Scientific Conference [6].

The Material and Methods

The in situ data. As part of regular bio-optical monitoring, samples were taken in the surface layer of the Black Sea at a station located opposite Sevastopol Bay at a distance of two miles from the coast at 44 ° 37'26 "N, 33 ° 26'05" E point. The depth at the station is ~ 62 m.

To determine the chlorophyll *a* concentration ($C_{a\text{-}i}$), a spectrophotometric method was used [7]. Light absorption by particles ($a_{\text{p-i}}(\lambda)$) and colored dissolved organic matter ($a_{\text{CDOM-i}}(\lambda)$) were measured in accordance with the NASA protocol [8, 9]. Seawater samples were gently vacuum filtered (no more than 0.2 atm) onto 25 mm

[1] NASA Goddard Space Flight Center, 2020. *Ocean Color WEB*. [online] Available at: https://oceancolor.gsfc.nasa.gov/data/aqua/ [Accessed: 21 October 2020].

[2] NASA Goddard Space Flight Center, 2020. *Ocean Color WEB*. [online] Available at: https://oceancolor.gsfc.nasa.gov/data/terra/ [Accessed: 21 October 2020].

[3] NASA Goddard Space Flight Center, 2020. *Ocean Color WEB*. [online] Available at: https://oceancolor.gsfc.nasa.gov/data/viirs-snpp/ [Accessed: 21 October 2020].

diameter GF/F type (Whatman) glass fiber filters with pores of 0.7 μm. To obtain a sample of the colored dissolved organic matter, seawater was passed through 47 mm diameter membrane filters with pores of 0.2 μm.

Spectrophotometric measurements were carried out immediately after sampling on dual-beam spectrophotometers: *SPECORD M*40 *(Carl Zeiss Jena)* in 2009–2014 and *LAMBDA* 35 *(PerkinElmer)* with an integrating sphere in 2015–2019.

Light absorption by particles ($a_{p-i}(\lambda)$) was divided into absorption by phytoplankton (($a_{ph-i}(\lambda)$) and absorption by non-algal particles ($a_{NAP-i}(\lambda)$) in-accordance with the general methods [10, 11].

Satellite data. *MODIS* and *VIIRS* Level-2 [4] data with a spatial resolution of 1 km were used.

The following satellite products were used in the analysis:

– chlorophyll *a* concentration (C_{a-s}, mg·m^{-3}), generated based on two standard NASA algorithms: *Ocean chlorophyll algorithm (OCx)* [12] and *Hu color index (CI)* [13];

– light absorption by phytoplankton at 443 nm ($a_{ph-s}(443)$, m^{-1}), generated according to the *NASA Generalized Inherent Optical Property (GIOP)* model [14, 15];

– light absorption by colored detrital matter (colored dissolved organic matter and non-algal particles) at 443 nm ($a_{CDM-s}(443)$, m^{-1}), generated according to the *NASA GIOP* model.

Satellite data processing was carried out using *SeaDAS* 7.5.3 software developed by NASA [5]. Satellite data was sampled from the area around the station. The area is in square-shaped centered at 44°37'26" ± 0°00'32"N and 33°26'05" ± 0°00'54"E. When selecting satellite data, preference was given to those geographically close to the point of field measurements. In the absence of satellite data in the selected area, standard products were obtained by approximating the values of neighboring pixels (at least two adjacent pixels from opposite sides).

Results and Discussion

Comparison of satellite products with *in situ* measurements was carried out throughout the entire annual cycle of phytoplankton development. For this purpose, a data array containing the results of field and satellite measurements was created.

Chlorophyll *a* concentration (C_a). The C_{a-s} calculation error in winter averaged ±38%. Deviations from the results of field measurements were observed both towards higher and towards lower values (Fig. 1, *a*).

A significant deviation of C_{a-s} values from the results of C_{a-i} field measurements was noted in spring. The error nature is clearly expressed: at high values of C_{a-i} ($C_{a-i} > 1.1$ mg·m^{-3}) C_{a-s} was 1.0–5.4 times lower than C_{a-i}. The error in determining C_{a-s} in spring averaged ±35%.

In summer, the nature of the error changed: there was primarily an excess of C_{a-s} values compared to C_{a-i} by 0.36–2.7 times, by 1.4 times on average. The C_a values are small, but the error in C_{a-s} calculation was quite significant ±55% on average.

[4] NASA Goddard Space Flight Center, 2020. *Ocean Level-2 Data Format Specification*. [online] Available at: https://oceancolor.gsfc.nasa.gov/docs/format/l2nc/ [Accessed: 21 October 2020].

[5] NASA Goddard Space Flight Center, 2020. *The Official NASA/OB.DAAC Data Analysis Software*. [online] Available at: https://seadas.gsfc.nasa.gov/ [Accessed: 21 October 2020].
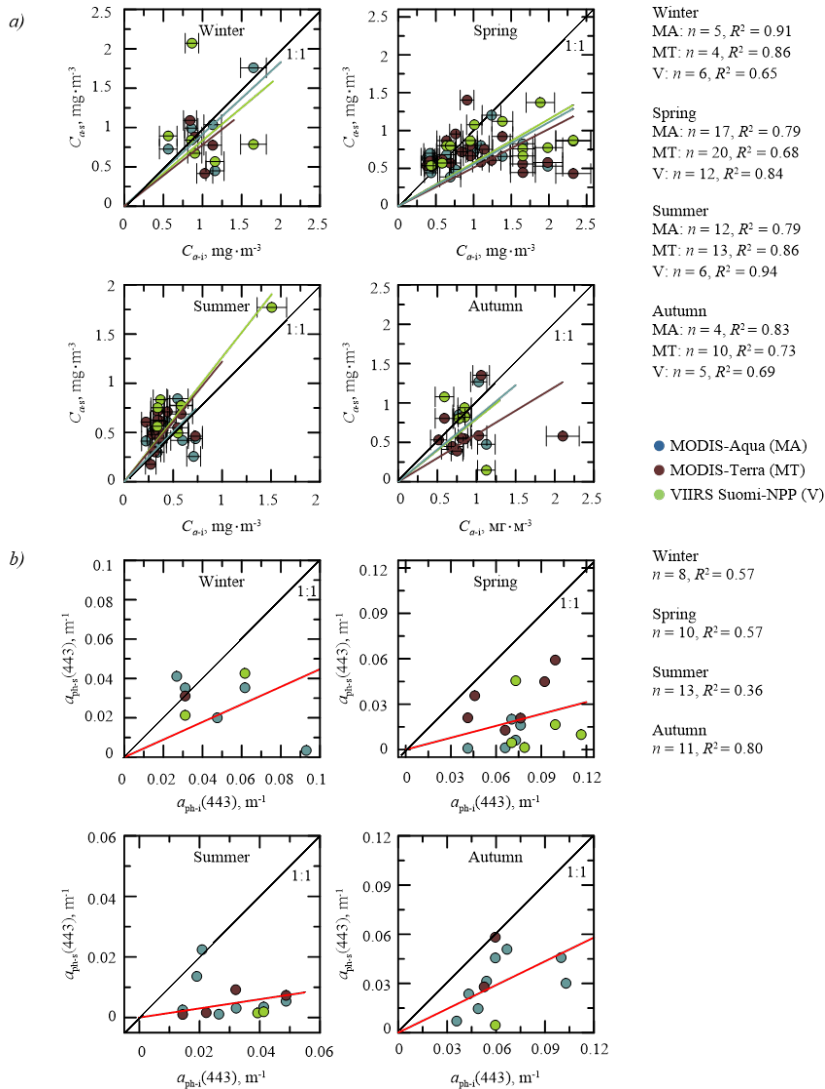
F i g. 1. Comparison of the satellite-derived products $C_{a\text{-s}}$ (*a*) and $a_{ph\text{-s}}(443)$ (*b*) with the results of field bio-optical measurements ($C_{a\text{-i}}$ and $a_{ph\text{-i}}(443)$). Color lines are the linear regression lines; red line is the linear regression for all the spectroradiometers

In autumn, as well as in spring, $C_{a\text{-s}} < C_{a\text{-i}}$ (when $C_{a\text{-i}} > 1.1$ mg·m^{-3}), mainly according to *MT* data. The error in $C_{a\text{-s}}$ determination from the data of all spectroradiometers in that season averaged ±36%.

That is, throughout the year, the $C_{a\text{-s}}$ satellite product is determined with a large relative error (on average ±41%) according to the data of all spectroradiometers, but it is still possible to single out *V* (an average error of ±43% with a sample of 29 values) as the most inaccurate of the considered spectroradiometers and *MA* as the best one (error on average ±38% with a sample of 38 values).

The satellite product $C_{a\text{-s}}$ is generated by two algorithms: *CI* and O*Cx*. For $C_{a\text{-s}}$ below 0.15 mg·m^{-3}, the *CI* algorithm is used, for $C_{a\text{-s}}$ above 0.20 mg·m^{-3} – the O*Cx*

algorithm is applied. With $C_{a\text{-s}}$ values ranging from 0.15 to 0.20 mg·m^{-3}, the *CI* and *OCx* algorithms are combined using a balanced approach. Input data for $C_{a\text{-s}}$ generated by *CI* and *OCx* algorithms are the values of the remote sensing reflectance ($R_{rs}(\lambda)$). Except $R_{rs}(\lambda)$, the *OCx* algorithm includes constant table coefficients a_i.

Use of the same coefficients without taking into account the type of water can be one of the reasons for the occurrence of an error in $C_{a\text{-s}}$ determining at the regional level.

Light absorption by phytoplankton at 443 nm. This coefficient values, obtained from the data of spectroradiometers ($a_{ph\text{-s}}(443)$), during the year is almost always lower than the results of in situ observations ($a_{ph\text{-s}}(443)$). Ranges of $a_{ph\text{-s}}(443)$ variation are, on average, two times narrower than the range of variation of $a_{ph\text{-s}}(443)$ (Fig. 1, *b*). Thus, the light absorption by phytoplankton in the coastal Black Sea waters, generated by standard algorithms from satellite data, is significantly underestimated.

Relationship between C_a and $a_{ph}(443)$. Earlier, for a large array of ocean data, a relationship between C_a and $a_{ph}(\lambda)$ described by a power function [16, 17] was established. The coefficients of this power-law dependence are different both for various water areas [18, 19] and for one water area in different seasons [20, 21].

Relationship between C_a and $a_{ph}(\lambda)$ makes it possible to fairly accurately simulate C_a in terms of light absorption, taking into account the seasonal characteristics of the influence of phytoplankton habitat conditions on the pigment content and light absorption capacity of cells. This approach which consists in the C_a estimation based on $a_{ph}(\lambda)$, is used in the currently actively developing three-channel algorithm [22].

If C_a and $a_{ph}(\lambda)$ are determined correctly, then their relationship should be traced. Fig. 2 shows that the power-law dependence between the data of field observations ($a_{ph\text{-i}}(443)$ and $C_{a\text{-i}}$) is observed in all seasons, while the relationship between satellite products ($a_{ph\text{-s}}(443)$ and $C_{a\text{-s}}$) is almost absent, which indicates the incorrectness of these parameters estimates according to the standard NASA algorithms.
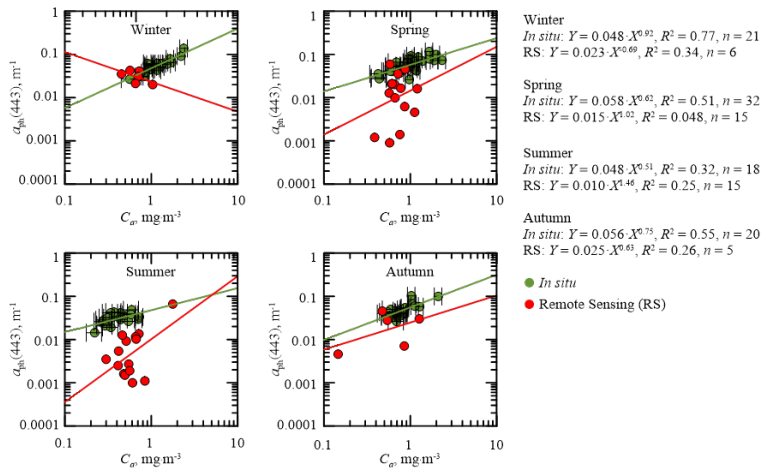
F i g. 2. Relation between $a_{ph}(443)$ and C_a. Color lines denote the regression lines

Light absorption by colored detrital matter at 443 nm. Range of $a_{CDM\text{-s}}(443)$ variability (from 0.010 to 1.02 m^{-1}) during the year is five times greater than

the range of a_{CDM-s} (443) variability (from 0.060 to 0.23 m⁻¹) (Fig. 3, *a*). Error of a_{CDM-s} (443) determination averaged ±160% per year. The smallest errors were observed in spring: the mean relative error of a_{CDM-s} (443) determination was ±82%.
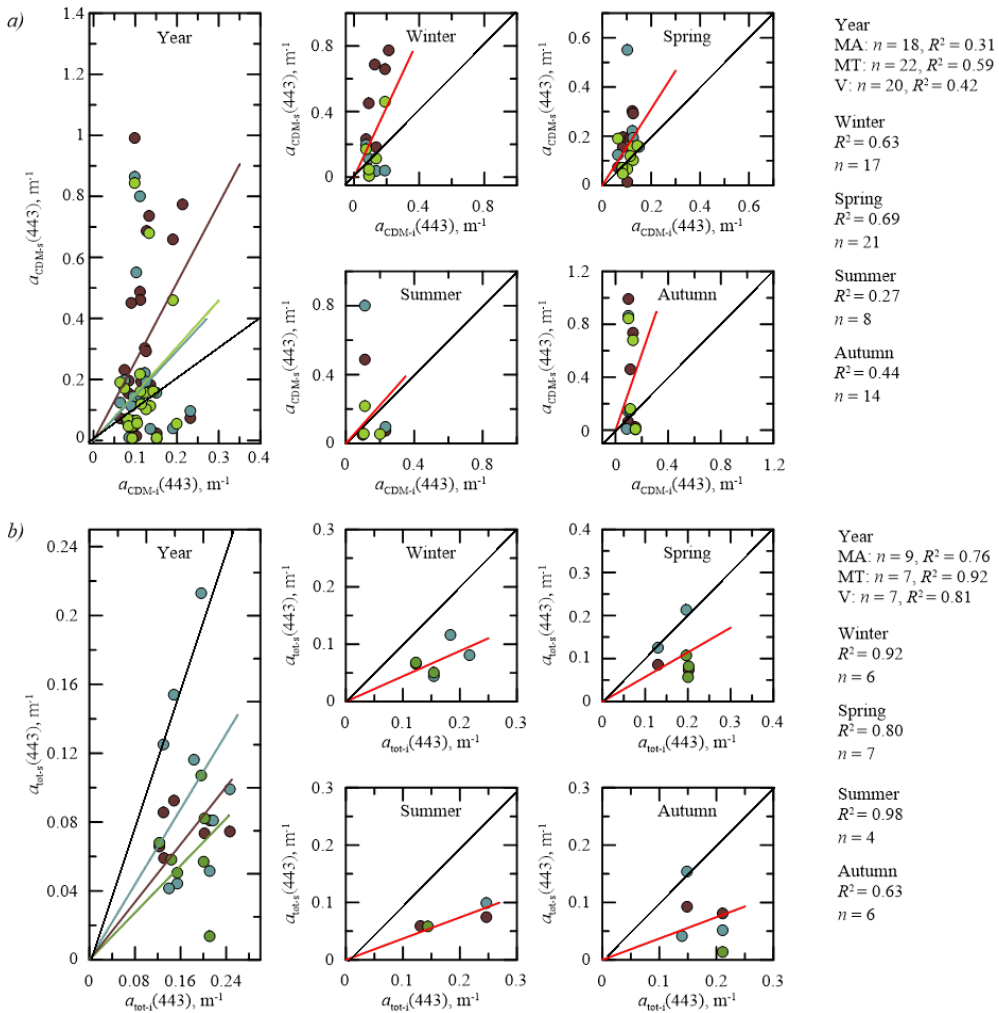
F i g. 3. Comparison of the a_{CDM-s}(443) (*a*) and a_{tot-s}(443) (*b*) values with the results of field measurements (a_{CDM-i}(443) and a_{tot-i}(443)). Designations as in Fig. 1

The satellite products reconstructed from the data of quasi-synchronous measurements by various spectroradiometers were different, but on the whole, the accuracy of determining satellite products throughout the year was comparable: the relative error δ(C$_{a-s}$) was ±38, ±41, ±43% for *MA*; *MT*; *V*, respectively, and (a_{ph-s} (443)) ±64, ±54, ±75%, with the exception of δ(a_{CDM-s}(443)) equal to ±158, ±207, ±117%.

Light absorption by all OACs at 443 nm (a_{tot}(443)). Error in C$_{a-s}$, a_{ph-s}(443) and a_{CDM-s}(443) determination is possibly a consequence of the incorrect separation of the

total light absorption by all OACs into $a_{ph-s}(443)$ and $a_{CDM-s}(443)$. To test this hypothesis, $a_{tot}(443)$ values from spectroradiometer data and *in situ* measurements were compared. The light absorption by pure water at 443 nm ($a_w(443)$, m^{-1}) was not taken into account, since it is constant.

Throughout the year, the difference between the maximum and minimum values according to satellite data (0.014–0.21 m^{-1}) and according to *in situ* measurements (0.051–0.25 m^{-1}) was the same and amounted to 0.20 m^{-1}. At the same time, the range of satellite values was slightly shifted (by 0.037 m^{-1}) relative to the *in situ* data towards smaller values (Fig. 3, *b*).

However, it should be noted that the data comparison in pairs of quasi-synchronous measurements showed that $a_{tot-s}(443)$ is 0.92–4.1 times lower than $a_{tot-i}(443)$. In one case, a significant difference was found between satellite (*V*) data ($a_{tot-s}(443) = 0.014$ m^{-1}) from the results of in situ observations ($a_{tot-i}(443) = 0.21$ m^{-1}). Comparison of all pairs of data revealed that the values of $a_{tot-s}(443)$ do not coincide with $a_{tot-i}(443)$. In this case, according to the data of different spectroradiometers obtained within one day the $a_{tot-s}(443)$ values differ significantly (in 0.57–7.2 times) among themselves. Hence, it follows that the problem lies not in the accuracy of $a_{tot-s}(\lambda)$ dividing into the light absorption indices of the OAC (by phytoplankton and colored dissolved organic matter in total with the non-algal particles), but in its initially inaccurate determination. Comparison showed that the $a_{tot-s}(443)$ estimate is lower than $a_{tot-i}(443)$ in most cases (0.92–15 times, on average 2.9 times).

The OAC contribution to total light absorption according to *in situ* measurements. Relative contribution of individual OACs to the total light absorption varies depending on the wavelength and season and characterizes the optical type of waters [23–26]. The OAC contribution to the total light absorption ($a_{tot-i}(\lambda)$) at 440 and 488 nm in individual seasons in the surface sea layer is shown in Fig. 4.
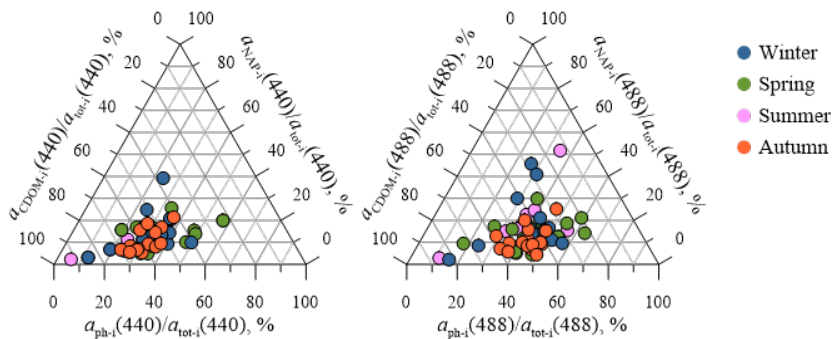
F i g. 4. Contribution of the phytoplankton ($a_{ph-i}(\lambda)/a_{tot-i}(\lambda)$), the colored dissolved organic matter ($a_{CDOM-i}(\lambda)/a_{tot-i}(\lambda)$), and the non-algal particles ($a_{NAP-i}(\lambda)/a_{tot-i}(\lambda)$) to the light absorption budget ($a_{tot-i}(\lambda)$) at 440 nm and 488 nm

For the studied wavelengths, it was found that the light absorption by colored dissolved organic matter prevails over the light absorption by phytoplankton and the light absorption by non-algal particles in all seasons. Throughout the year, the largest contribution of colored dissolved organic matter was noted in autumn. On average, its value was 59 and 47% at 440 and 488 nm, respectively. At 488 nm, the

contribution of phytoplankton to total absorption increases in comparison with the data obtained at 440 nm. Analysis of seasonal dynamics showed that the largest contribution of phytoplankton to the total absorption occurs in spring and averages 35 and 44% at 440 and 488 nm, respectively. The noted seasonal dynamics of the values of the light absorption indices of individual OAC of the medium, as well as their relative contribution to the total light absorption at wavelengths in the radiance range in which the sea brightness is most sensitive to the optical properties of the medium, is probably the cause of gross errors in the OAC estimate using standard algorithms.

The study showed that the considered satellite products incorrectly correlate with the bio-optical indicators of the waters of the considered water area and their ratios (table). Seasonal variation of chlorophyll a concentration is smoothed out: the $C_{a\text{-s}}$ values vary from 0.18–1.8 mg·m^{-3} in summer to 0.39–1.4 mg·m^{-3} in spring, in contrast to the naturally observed increase in $C_{a\text{-i}}$ from minimum values (0.22–1.5 mg·m^{-3}) in summer to maximum (0.38–2.3 mg·m^{-3}) in spring. The $C_{a\text{-s}}$ error, depending on the season, varied from ±34 to ±55%, while it was not of the same type: in spring, the $C_{a\text{-s}}$ values were on average 1.6 times lower than $C_{a\text{-i}}$, and 1.4 times higher in summer.

Ratio of light absorption by the phytoplankton to absorption by the colored detrital matter at 443 nm ($a_{\text{ph}}(443)/a_{\text{CDM}}(443)$)

Value	*in situ*	*MA*	*MT*	*V*
Winter				
Min	12/88	3.0/97	-	31/69
Max	51/49	80/20	-	84/16
Mean	32/68	38/62	50/50*	58/42
Spring				
Min	20/80	1.0/99	7,0/93	2/98
Max	58/42	15/85	81/19	60/40
Mean	38/62	9.0/91	36/64	21/79
Summer				
Min	6.0/94	1/99	0.40/100	3.0/97
Max	37/63	14/86	16/84	55/45
Mean	26/71	7.0/93	8.0/92	18/82
Autumn				
Min	24/76	5.0/95	30/70	–
Max	39/61	88/12	88/12	–
Mean	33/67	45/55	51/49	34/66*

* One data pair.

Inaccuracy in the chlorophyll a concentration determination leads to errors in the determination of many other indicators, the calculations of which are based on this parameter. In particular, this leads to an incorrect estimate of the phytoplankton biomass, primary production and growth rate of plankton microalgae [27, 28]. The $a_{CDM-s}(443)$ values are higher than the $a_{ph-s}(443)$ values (2.2 times on average), and the $a_{ph-s}(443)$ values are lower than the $a_{ph-i}(443)$ (9 times on average) throughout the year, leading to an incorrect result of calculating the relative contribution of phytoplankton and non-algal particles of optically active substances in the medium (*CDOM* and *NAP*), and, consequently, to an error in determining the optical properties of waters, in particular transparency, spectral properties of quantum irradiation penetrating into the water column [4, 24, 29] and photosynthetic potential of microalgae [30–32].

The results of the study indicate that the applied standard algorithms based on bio-optical indicators of Case 1 water [33] are not suitable for calculating satellite products for the coastal Black Sea (in particular, in the area of the Sevastopol Bay).

To use remote sensing data, it is necessary to develop regional algorithms that take into account the seasonal features of the spectral bio-optical indicators of waters and their relationship with the concentration of the main photosynthetically active pigment, chlorophyll *a*, in the region under consideration. In particular, it is possible to adapt the three-channel algorithm [22], which divides the total light absorption into the absorption of the colored dissolved organic matter in the sum with non-algal particles and absorption by phytoplankton. In the calculation by this algorithm, the remote sensing reflectance at 480–560 nm are used, according to which the concentration of chlorophyll *a* is restored, taking into account the relationship between the light absorption by phytoplankton and the chlorophyll *a* concentration [20, 34].

Conclusion

Based on the formed long-term array of natural bio-optical data, the accuracy of satellite products generated from the data of the *MA*, *MT* and *V* spectroradiometers was estimated. The following results were obtained:

1. On average, the relative error of the standard satellite product "chlorophyll *a* concentration", depending on the season, ranged from ±34 to ±55%, while the error was not of the same type: in spring, the C_{a-s} values were on average 1.6 times below C_{a-i}, and in summer – 1.4 times higher.

2. During the study, it was revealed that when calculating satellite products using standard NASA algorithms, the contribution of phytoplankton to total light absorption remains underestimated: on average, the values of light absorption by phytoplankton at 443 nm ($a_{ph-s}(443)$) were nine times less than the results of field measurements. At the same time, the light absorption of colored dissolved organic matter in total with the non-algal particles at 443 nm ($a_{CDM-s}(443)$) was, on average, 2.2 times overestimated.

3. Significant errors in the calculation of satellite products and the difference between the light absorption values of all OACs of water ($a_{tot}(\lambda)$) cast doubt on the applicability of standard algorithms for the sea area under study.

4. Distribution of the OAC contribution to the total light absorption varies throughout the year: the largest *CDOM* contribution at 443 and 488 nm (59 and 47%) occurs in autumn, and the largest $a_{ph-i}(\lambda)$ contribution (35 and 43%) – in the spring.

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