Regional algorithms for the estimation of chlorophyll and suspended matter concentration in the Gulf of Finland from MODIS-Aqua satellite data

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Abstract

Validation of algorithms for the retrieval of concentrations of chlorophyll (Chl) and total suspended matter (TSM) in the Gulf of Finland from satellite ocean colour data was carried out using field measurement data from summer 2012 and 2013. These data included spectral values of the remote sensing reflectance $R_{rs}(\lambda)$.

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Chl and TSM concentrations. Testing of the existing algorithms (OC4v4, OC3M, and the Baltic regional algorithms developed by Polish specialists) showed that all of them overestimated Chl several times. The new regional algorithms were developed on the basis of measured values of $R_{rs}(\lambda)$, Chl and TSM (40 stations in total). Direct comparison of Chl and TSM values, obtained from MODIS-Aqua data with the algorithms developed here, with their in situ values showed reasonable agreement. The spatial distributions of Chl and TSM concentrations were constructed from MODIS-Aqua data. Errors of the atmospheric correction were analysed.

1. Introduction

The aim of our studies is to derive regional algorithms for calculating chlorophyll and suspended matter concentrations in surface waters of the Gulf of Finland from satellite ocean colour scanner data. The Gulf of Finland is strongly influenced by river runoff, primarily from the Neva (2/3 of the total runoff), and this influence is evident not only in the low salinity ($<10$ PSU) but also in their optical properties of these waters. The standard algorithms for calculating bio-optical characteristics from satellite ocean colour scanners, designed mainly on the basis of data measured in ocean waters (http://oceancolor.gsfc.nasa.gov), do not take into account regional specificity and may give rise to large errors in such waters. Regional algorithms, based on data measured in situ in a given area, are needed (http://optics.ocean.ru). Such measurements were carried out in the expeditions organised by the Russian State Hydrometeorological University (RSHU) in the summers of 2012 and 2013.

2. Material and methods

2.1. Study area and stations

The field studies were carried out on the yacht CENTAURUS II during 21–28 July 2012 and 20 July–02 August 2013; 15 stations were set up in 2012 and 26 in 2013. The positions of the station are given on maps showing the spatial distributions of Chl concentration from MODIS-Aqua data on 22 July 2012 and 27 July 2013 derived by a standard MODIS algorithm (Figure 1a,b). According to these maps, Chl values on the most of stations were $>10$ and even 20 mg m$^{-3}$. In fact, the Chl concentration, directly measured in the study area, varied from 1.2 to 23.7 mg m$^{-3}$ in 2012 and from 1.6 to 18.6 mg m$^{-3}$ in 2013.

The Secchi depth varied from 1.8 m in the eastern part of the Gulf of Finland near the Neva Bay to 4.0 m in the open part of the Gulf. Station M2 of 26 July 2013 (Figure 1b) was rejected owing to the inconsistency of
Figure 1. Location of stations in 2012 (a) and 2013 (b). The maps show the distributions of chlorophyll concentration derived from satellite data of MODIS-Aqua on 22 July 2012 and 27 July 2013 using a standard algorithm (http://oceancolor.gsfc.nasa.gov)

the measured Chl value with other values on that day; the remaining 40 stations were used for the derivation of the Chl regional algorithm.

The spectral radiance reflectance was measured, the surface irradiance at 554 nm for controlling the illumination conditions continuously recorded and photographs of clouds taken at each station. Some of the stations were located directly under the passing MODIS-Aqua and VIIRS satellite scanners. Such measurements provided us with data for evaluating the atmospheric correction errors.

2.2. Floating spectroradiometer

This instrument measures the spectral upwelling radiance just beneath the sea surface and the spectral downwelling irradiance just above the sea
surface (Artemiev et al. 2000). The spectral range is 390–700 nm, spectral resolution – 2 nm, the scan time – 15 s. The accuracy of measurement of absolute values of the radiance and irradiance is about 5%.

Figure 2 shows the spectroradiometer during measurements. The measurements are taken at drift stations. The device drifts with the drogue at a distance of 30–50 m from the ship to avoid the influence of the ship’s hull, and 20–30 scans are run during 15–20 min.

![Figure 2. The spectroradiometer used for the measurements](image)

The measurement data are processed with a specially developed computer program. The subsurface radiance reflectance \( \rho(\lambda) \) is calculated from

\[
\rho(\lambda) = \pi L_u(\lambda) / E_d(\lambda),
\]

where \( L_u(\lambda) \) and \( E_d(\lambda) \) are the upwelling radiance and downwelling irradiance just beneath the sea surface.

The calculated values of \( \rho(\lambda) \) were used to develop bio-optical algorithms and also to validate of the atmospheric correction algorithms if the measurements were performed simultaneously with satellite observations.

2.3. Measurement of chlorophyll and suspended matter concentrations

Chlorophyll concentration was measured by a spectrophotometric method with 90% aqueous acetone solution. For calculating the chlorophyll \( a \)
Regional algorithms for the estimation of chlorophyll concentration, data for the wavelengths of 630, 645, 663 and 750 nm were used (Report 1966).

The total suspended matter (TSM) concentration was determined by filtering the water sample (volume 1 l) through a pre-weighed membrane filter (pore size 0.45 µm) and subsequently weighing the rinsed and dried filters (PNDF 2004).

2.4. Satellite data

For deriving the bio-optical algorithms, Level 2 satellite data from MODIS-Aqua with a spatial resolution of 1 km were used. These data include values of the spectral remote sensing reflectance \( R_{rs}(\lambda_i) \) from 412 to 869 nm, chlorophyll concentration, aerosol optical thickness and so-called ‘flags’, indicating the quality of the satellite image and some of its characteristics (land, clouds) (http://oceancolor.gsfc.nasa.gov/). The spectral subsurface radiance reflectance \( \rho(\lambda) \), introduced above, is related to \( R_{rs}(\lambda) \) by the formula (Lee et al. 1998)

\[
\rho(\lambda) = \frac{R_{rs}(\lambda)}{[0.165 + 0.497 R_{rs}(\lambda)]}. \tag{2}
\]

Data from a new colour scanner VIIRS, having only five spectral bands in the visible spectral region (410, 443, 486, 551 and 671 nm), were used for the validation of the atmospheric correction algorithm. Development of the VIIRS bio-optical algorithm for the Gulf of Finland requires special study (see section 4.3).

3. Results

3.1. Spectra of the subsurface radiance reflectance

Examples of the spectral subsurface reflectance \( \rho(\lambda) \), measured by a floating spectroradiometer during the expeditions in 2012 and 2013, are given in Figure 3. The measured spectra are similar in shape, but there are considerable differences in the absolute values of \( \rho(\lambda) \) that can be directly related to the different chlorophyll concentrations (see the numbers by the curves).

The chlorophyll absorption manifests itself in the red part of the spectrum – the minima near 680 nm are caused by the red absorption maximum of chlorophyll \( a \). The blue maximum of the pigment absorption near 440 nm is not seen owing to the strong absorption of coloured organic matter (‘yellow substance’), which causes a sharp decrease of \( \rho(\lambda) \) towards shorter wavelengths after the maximum at 560–580 nm.

Another feature of the spectra of \( \rho(\lambda) \), observed in both 2012 and in 2013, is the minimum near 620 nm, which presumably corresponds to the
Figure 3. Examples of the spectral subsurface reflectance $\rho(\lambda)$ measured with the floating spectroradiometer during the expeditions in 2012 (a) and 2013 (b). a: 1 – St. 3L, 2 – St. 2L, 3 – St. 4F5, 4 – St. 4L; b: 1 – St. 2F5, 2 – St. V1, 3 – St. 10F (see Figure 1). The numbers in parentheses indicate chlorophyll concentration maximum absorption of phycocyanin; the maximum near 650 nm between the two minima at 620 and 680 nm may be reinforced by the fluorescence of phycocyanin at 650 nm.

It should be noted that this pigment is peculiar to blue-green algae (cyanobacteria). Cyanobacterial blooms in the Baltic Sea, especially in the Gulf of Finland, occur every year and can give rise to very high chlorophyll concentrations there (Reinart & Kutser 2006).

In 2013, the measurements were performed both in the open part of the Gulf and in the eastern part near Neva Bay. The spectra of $\rho(\lambda)$ near Neva Bay differ markedly from those in the open part as a result of the substantial turbidity and high content of yellow substance (Figure 4).

Figure 4. Spectra of $\rho(\lambda)$ measured near Neva Bay in 2013: diamonds, St. TSP2-1; circles, St. TSP2-2. The numbers in parentheses indicate chlorophyll concentration.
An anomalous increase in $\rho(\lambda)$ is observed in the red part of the spectrum where the absorption by yellow substance decreases; the minimum at 620 nm and the maximum at 650 nm are retained – they are indicative of the blue-green algae bloom.

3.2. A regional algorithm for calculating the chlorophyll concentration

Regional algorithms for calculating the chlorophyll concentration in the Baltic Sea have been developed in several papers, in particular by specialists from the Institute of Oceanology, Polish Academy of Sciences (Darecki & Stramski 2004, Darecki et al. 2008, Woźniak et al. 2008). The applicability of these algorithms for determining Chl concentration in the Gulf of Finland was tested with our field data; the results are discussed in section 4.1.

We derived several algorithms in different forms specifically for the Gulf of Finland. After various tests, the input parameter was selected as $X = \log[R_{rs}(547)/R_{rs}(531)]$, where 547 and 531 nm are the effective wavelengths of the MODIS-Aqua spectral bands (see section 4.3). The regression equations were derived as Chl vs. $X$ and log Chl vs. $X$ with formulae of the first- and second-order:

#1 $\text{Chl} = 183X - 7.73$;
#2 $\text{Chl} = 277X - 12.21$;
#3 $\text{Chl} = 207X - 8.19$;
#4 $\text{Chl} = 1.65 - 72.6X + 1850X^2$;
#5 $\log \text{Chl} = 11.5X - 0.29$;
#6 $\log \text{Chl} = 18.4X - 0.52$;
#7 $\log \text{Chl} = 13.4X - 0.27$;
#8 $\log \text{Chl} = -0.50 + 19.8X - 42.7X^2$.

Algorithms #1, #5 ($n = 15$) and #2, #6 ($n = 25$) were derived by using data from the expeditions of 2012 and 2013 respectively. The equations for these years differ clearly from each other, but Student’s test shows that the differences between the regression coefficients of equations #1 and #2, #5 and #6 are not statistically significant in both cases. Equations #3, #4 and #7, #8 were derived for the combined data set ($n = 40$).

The evaluation parameters for the above algorithms are given in Table 1; Figures 5 and 6 show the results in graphical form. The standard errors for algorithms #4 and #8 are equal to 3.26 mg m$^{-3}$ and 3.37 mg m$^{-3}$.
Table 1. Comparison between the Chl averages – measured, and calculated using algorithms #1–#8 (Chl\text{meas} and Chl\text{calc}, mg m\text{−3}); the standard errors \(s\) of Chl calculation [mg m\text{−3}]; coefficients of determination \(r^2\); the averaged ‘calculated/measured’ ratios and their ranges

<table>
<thead>
<tr>
<th>#algorithm</th>
<th>Chl\text{meas}</th>
<th>Chl\text{calc}</th>
<th>(s)</th>
<th>(r^2)</th>
<th>calc/meas</th>
<th>range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.25</td>
<td>4.27</td>
<td>3.20</td>
<td>0.68</td>
<td>1.05</td>
<td>0.09–2.4</td>
</tr>
<tr>
<td>2</td>
<td>6.33</td>
<td>6.31</td>
<td>3.32</td>
<td>0.45</td>
<td>1.24</td>
<td>0.54–2.4</td>
</tr>
<tr>
<td>3</td>
<td>5.55</td>
<td>5.55</td>
<td>3.43</td>
<td>0.52</td>
<td>1.25</td>
<td>0.10–2.9</td>
</tr>
<tr>
<td>4</td>
<td>5.55</td>
<td>5.53</td>
<td>3.26</td>
<td>0.57</td>
<td>1.30</td>
<td>0.44–3.2</td>
</tr>
<tr>
<td>5</td>
<td>4.25</td>
<td>3.77</td>
<td>2.32</td>
<td>0.94</td>
<td>1.07</td>
<td>0.67–1.8</td>
</tr>
<tr>
<td>6</td>
<td>6.33</td>
<td>5.70</td>
<td>3.32</td>
<td>0.47</td>
<td>1.14</td>
<td>0.45–2.3</td>
</tr>
<tr>
<td>7</td>
<td>5.55</td>
<td>4.91</td>
<td>3.50</td>
<td>0.54</td>
<td>1.13</td>
<td>0.36–2.6</td>
</tr>
<tr>
<td>8</td>
<td>5.55</td>
<td>4.82</td>
<td>3.37</td>
<td>0.57</td>
<td>1.14</td>
<td>0.37–2.7</td>
</tr>
</tbody>
</table>

Figure 5. Dependences of chlorophyll concentration Chl on parameter \(X = \log[R_{rs}(547)/R_{rs}(531)]\) using the different algorithms (specified by the numbers near the curves). a) Chl vs. \(X\); b) log Chl vs. \(X\)

respectively; as seen from Figure 6, both algorithms mostly overestimate Chl values \(< 5\) mg m\text{−3}, but algorithm #8 does so to a lesser degree than algorithm #4. It is also seen that both algorithms underestimate Chl values \(> 5\) mg m\text{−3}, but algorithm #4 to a lesser degree than algorithm #8.

As a result, algorithm #8 underestimates the average value of Chl (about 13%), but the average value of the ratio of Chl\text{calc}/Chl\text{meas} for this algorithm is \(\sim 1.14\); in the case of algorithm #4 the calculated average value of Chl is practically equal to the measured one, but the ratio of Chl\text{calc}/Chl\text{meas} is 1.30. Since most of the waters in the study area have
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Figure 6. Scatter plots of Chl values, calculated (Chl$_{\text{calc}}$) and measured (Chl$_{\text{meas}}$). a) calculated with algorithm #4; b) with algorithm #8. Crosses – data from 2012, diamonds – data from 2013. The solid line shows the perfect agreement.

chlorophyll concentrations $< 5 \text{ mg m}^{-3}$, algorithm #8 was selected as the primary one.

Figure 7 shows the spatial distribution of the chlorophyll concentrations calculated from MODIS-Aqua data on 22 July 2012 and 27 July 2013 using the selected algorithm.

Figure 7. Spatial distributions of the chlorophyll concentrations derived from MODIS-Aqua data of 22 July 2012 (a) and 27 July 2013 (b) using algorithm #8

The maps show no basic differences between the chlorophyll concentration distributions in 2012 and 2013. Most of the study area is occupied by water with chlorophyll concentrations of 2–5 mg m$^{-3}$, but there are heterogeneities within this gradation which may be $> 5$ and even 10 mg m$^{-3}$ as well as lower values. The highest chlorophyll concentrations are recorded
in the eastern part of the Gulf of Finland near Neva Bay and along the southern coast of the Gulf (especially in 2012).

3.3. Regional algorithms for calculating the concentration of suspended matter

The algorithm consists of two parts: first, values of the particle backscattering coefficient $b_{bp}$ are derived from satellite data and then the TSM concentration is calculated from the $b_{bp}$ values with the appropriate regression equation.

Coefficient $b_{bp}$ is computed by using the MODIS standard products of $R_{rs}(531)$, $R_{rs}(547)$ and $K_d(490)$ (http://oceancolor.gsfc.nasa.gov); a brief description of the algorithm is given at (http://optics.ocean.ru) and in more detail by Burenkov et al. (2001).

The regression equation TSM vs. $b_{bp}$ was derived from our field data of 2012 and 2013; the combined data set included 39 stations (15 in 2012, 24 in 2013). The TSM concentration varied from 1.0 mg l$^{-1}$ (St. 19F) to 5.5 mg l$^{-1}$ (St. 3L) in 2012 and from 1.7 mg l$^{-1}$ (St. 10F and 33F) to 4.4 mg l$^{-1}$ (St. 3FG) in 2013. The regression equation was derived in logarithmic form:

$$\log \text{TSM} = 0.79 \log b_{bp} + 1.95,$$

where TSM is expressed in mg l$^{-1}$, $b_{bp}$ in m$^{-1}$.

Figure 8 shows the regression line TSM vs. $b_{bp}$ on a logarithmic scale; Figure 9 is a scatterplot showing TSM$_\text{calc}$ vs. TSM$_\text{meas}$. As seen from the figure, the agreement is rather good: the coefficient of determination $r^2 = 0.61$, the standard error of the regression is equal to 0.62 mg l$^{-1}$; the averages of TSM$_\text{calc}$ and TSM$_\text{meas}$ are close to each other at 2.56 and 2.62 mg l$^{-1}$ respectively; the averaged ratio of TSM$_\text{calc}$/TSM$_\text{meas}$ is equal to 1.03, and the ratio range is 0.72–1.5.

Figure 10 shows the spatial distributions of TSM concentration calculated from MODIS-Aqua data on 22 July 2012 and 27 July 2013 using (3).

One can see a general similarity of these distributions with the distributions of chlorophyll concentration in Figure 7. Such a similarity is to be expected, because there is a common factor determining the distribution of both TSM and chlorophyll: the River Neva carries suspended particles and phytoplankton with chlorophyll and nutrients for primary bioproduction.
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Figure 8. The regression line of TSM vs. $b_{bp}$; crosses – 2012 data, diamonds – 2013 data

Figure 9. Comparison between the calculated (TSM$_{calc}$) and measured (TSM$_{meas}$) TSM values; crosses – data from 2012, diamonds – data from 2013. The solid line shows the perfect agreement

Figure 10. Spatial distributions of TSM concentrations calculated using the equation (3) from MODIS-Aqua data on 22 July 2012 (a) and 27 July 2013 (b)
4. Discussion

4.1. Comparison of the newly developed algorithms with the other Baltic regional algorithms for Chl concentration

We evaluated the applicability of the regional Baltic algorithms by Darecki & Stramski (2004) and Woźniak et al. (2008) for determining chlorophyll concentrations in the Gulf of Finland by using our data set of 2012–2013.

The input parameter of the second of them (the DESAMBEM algorithm – Development of a Satellite Method for Baltic Ecosystem Monitoring) is the ratio $XR = [R_{rs}(490) - R_{rs}(665)]/[R_{rs}(550) - R_{rs}(665)]$, which is completely unsuitable for the Gulf of Finland because of the abnormally high values of $R_{rs}(665)$. The regional parameterisation of MODIS algorithms for chlorophyll retrieval in the Baltic was presented by Darecki & Stramski (2004) in two versions:

- **#9 Baltic_chlor_MODIS**: Chl = $10^{0.4692 - 2.6802X}$, where $X = \log[L_{wn}(443) + L_{wn}(488)/L_{wn}(551)]$

- **#10 Baltic_chlor_a2**: Chl = $10^{0.1520 - 3.0558X}$, where $X = \log \max[L_{wn}(443)/L_{wn}(551), L_{wn}(488)/L_{wn}(551)]$

$L_{wn}(443), L_{wn}(488)$ and $L_{wn}(551)$ are the normalised water-leaving radiances.

The values of $L_{wn}$ are related to $R_{rs}$ by a simple formula: $L_{wn}(\lambda) = F_0(\lambda) R_{rs}(\lambda)$, where $F_0(\lambda)$ is the mean extra-terrestrial solar irradiance (http://oceancolor.gsfc.nasa.gov).

The results of the evaluation of these algorithms are presented in Table 2 and can be compared with the results for algorithms #4 and #8 from Table 1.

Comparing Tables 1 and 2, one can see that algorithms #9 and #10 are inferior to algorithms #4 and #8 in all parameters. Noteworthy is the almost zero value of the coefficient of determination for algorithm #9; it is not high for #10 either. Figure 11 shows that both algorithms greatly overestimate the Chl concentrations of < 5 mg m⁻³ prevailing in the area of our study.

![Table 2. Evaluation parameters of algorithms #9 and #10 (the same as in Table 1)](image)
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**Figure 11.** Comparison between the Chl values measured (Chl\textsubscript{meas}) and calculated (Chl\textsubscript{calc}) using algorithms #9 (a) and #10 (b). The solid line shows the perfect agreement.

### 4.2. Validation of the algorithms with MODIS-Aqua data

Direct comparison of chlorophyll or TSM concentrations, derived from satellite data and measured in situ, is the most compelling evidence for the effectiveness of our algorithm. Of course, the satellite and in situ data should be measured simultaneously, that is, the time interval between them has to be small enough to for the temporal variability to be negligible. For the open ocean, where the waters are sufficiently homogeneous, satellite and ship measurements can be regarded as simultaneous (‘match-up’) if the time difference is not more than 3 hours (Bailey & Werdell 2006).

During our expeditions of 2012 and 2013, the weather conditions (cloudiness) allowed sub-satellite measurements to be performed only on 27 July in 2012 and on 26, 27, 29 July in 2013. Ten stations satisfying the above-mentioned requirements were selected: 3 in 2012 and 7 in 2013. Figure 12 shows the results of the direct comparison of chlorophyll concentrations calculated from satellite data (Chl\textsubscript{calc}) and those measured in situ (Chl\textsubscript{meas}); the satellite data were taken as the averages over 9 pixels around the station.

Table 3 summarises the results of the comparison of Chl values, calculated from the data provided by a floating spectroradiometer and MODIS-Aqua, with the measured ones.

The range of measured Chl values in the analysed subset is large enough – 1.2–11.7 mg m\textsuperscript{-3} (although five stations with the highest chlorophyll values – from 11.8 to 23.7 mg m\textsuperscript{-3} – were not included owing to a lack of satellite data, and the average value decreased from 5.55 to 4.97 mg m\textsuperscript{-3}).
The results of the comparison of the chlorophyll values calculated from MODIS-Aqua data using regional algorithm #8 with values measured in situ. The numbers in parentheses are the chlorophyll concentrations calculated using the standard MODIS algorithm.

**Figure 12.**

**Table 3.** Comparison between the Chl concentrations – measured, and calculated from floating spectroradiometer (in situ) and MODIS-Aqua data using algorithms #8 – #10 and the standard MODIS algorithm OC3M (the same as in Table 1) $n=10$

<table>
<thead>
<tr>
<th>#algorithm</th>
<th>Chl\text{meas}</th>
<th>Chl\text{calc}</th>
<th>s</th>
<th>$r^2$</th>
<th>calc/meas</th>
<th>range</th>
</tr>
</thead>
<tbody>
<tr>
<td>8, in situ</td>
<td>4.97</td>
<td>3.48</td>
<td>3.35</td>
<td>0.692</td>
<td>1.03</td>
<td>0.4–2.2</td>
</tr>
<tr>
<td>8, MODIS</td>
<td>4.97</td>
<td>3.97</td>
<td>3.88</td>
<td>0.122</td>
<td>1.20</td>
<td>0.3–3.0</td>
</tr>
<tr>
<td>9, MODIS</td>
<td>4.97</td>
<td>13.8</td>
<td>11.4</td>
<td>0.532</td>
<td>3.60</td>
<td>0.96–8.5</td>
</tr>
<tr>
<td>10, MODIS</td>
<td>4.97</td>
<td>18.0</td>
<td>17.7</td>
<td>0.118</td>
<td>5.29</td>
<td>1.1–16.0</td>
</tr>
<tr>
<td>OC3M, MODIS</td>
<td>4.97</td>
<td>51.8</td>
<td>63.9</td>
<td>0.882</td>
<td>11.3</td>
<td>3.9–18.7</td>
</tr>
</tbody>
</table>

The range of Chl values, calculated from the floating spectroradiometer data, is narrower (2.1–6.0 mg m$^{-3}$) because, as noted above, our algorithm mostly overestimates Chl values < 5 mg m$^{-3}$ and underestimates Chl values > 5 mg m$^{-3}$. For Chl values derived from MODIS-Aqua data, the range widens (1.1–7.8 mg m$^{-3}$) as a result of errors in the atmospheric correction. The same applies to the mean values of Chl, calculated from the floating spectroradiometer and MODIS-Aqua data (3.48 and 3.97), and to the ratios of Chl\text{calc}/Chl\text{meas} (0.4–2.2 and 0.3–3.0).

The average ratio of Chl\text{calc}/Chl\text{meas} is 1.03±0.62 if data from the floating spectroradiometer are used (recall that for the entire data set it is equal 1.14±0.57 – see Table 1) and 1.20±0.92 for MODIS-Aqua data.
The results of applying the new algorithm to the MODIS data should be considered quite satisfactory, especially in comparison with the results of the standard algorithm. The new regional algorithm gives a maximum 3.6-fold underestimation and a 3-fold overestimation; the average is overestimated by only 20%; the standard algorithm always significantly overestimates chlorophyll concentrations – minimally about 4 times, maximally almost 19 times, and on average more than 11 times.

As can be seen from Table 3, the results with algorithms #9 – Baltic_chlor_MODIS and #10 – Baltic_chlor_a2 (Darecki & Stramski 2004) are better than those obtained with the MODIS_standard but noticeably worse than those using the regional algorithm #8.

The results of the comparison of TSM values, calculated from the floating spectroradiometer and MODIS-Aqua data using the regional algorithm (3), with the measured ones are presented in Table 4 (TSM is not a standard product processed from MODIS-Aqua data).

<table>
<thead>
<tr>
<th>#algorithm</th>
<th>TSM&lt;sub&gt;meas&lt;/sub&gt;</th>
<th>TSM&lt;sub&gt;calc&lt;/sub&gt;</th>
<th>s</th>
<th>$r^2$</th>
<th>calc/meas</th>
<th>range</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3) in situ</td>
<td>2.32</td>
<td>2.25</td>
<td>0.42</td>
<td>0.821</td>
<td>1.04</td>
<td>0.77–1.51</td>
</tr>
<tr>
<td>(3) MODIS</td>
<td>2.32</td>
<td>2.64</td>
<td>0.64</td>
<td>0.608</td>
<td>1.21</td>
<td>0.79–1.59</td>
</tr>
</tbody>
</table>

As seen from Table 4, retrieval from satellite data, as compared with in situ data, results in an increase in errors and a lowering of the coefficient of determination, but the algorithms work acceptably with satellite data – the averaged ratio of the calculated TSM values to the measured ones is 1.21; the maximum overestimation is <60%, and the underestimation is 21%. The errors of the atmospheric correction are analysed in more detail in the next paragraph.

4.3. Validation of the atmospheric correction algorithm

As mentioned above, the values of $\rho(\lambda)$, measured with a floating spectroradiometer, can be used for validating the atmospheric correction algorithm if the measurements are performed simultaneously with satellite observations. For that, we have the 10 stations considered above. Four comparisons between spectra of the remote sensing reflectance $R_{rs}(\lambda)$, measured in situ and retrieved from satellite data of MODIS-Aqua and VIIRS, are shown in Figure 13.
Figure 13. Comparison between the spectra of $R_{rs}(\lambda)$ measured in situ and those retrieved from the satellite data of the MODIS-Aqua and VIIRS scanners.

It is seen that the atmospheric correction is not ideal – the errors are rather great in most cases. But from the practical point of view, only the errors for spectral bands of 531 and 547 nm, used in the bio-optical algorithm, are important. But as Figure 13 shows, the errors for these wavelengths are not so high.

The effect of errors in the input parameter $X$ on the retrieval of Chl concentration with our regional algorithm #8 can be estimated by using the approximation formula

$$\Delta(\log \text{Chl}) = \Delta X (19.8 - 85.4 X), \quad (4)$$

where $\Delta(\log \text{Chl})$ is the error in $\log \text{Chl}$, $\Delta X$ – in the $X$ parameter. The errors in the retrieval of different input parameters of the bio-optical algorithms are presented in Table 5.
Table 5. The errors in retrieval of parameters $X_1$, $X_2$ and $X_3$ from MODIS and VIIRS satellite data as compared with the ones calculated from the floating spectroradiometer (‘measured’) data

<table>
<thead>
<tr>
<th>Quantity</th>
<th>$X_1$</th>
<th>$X_2$</th>
<th>$X_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>range of values</td>
<td>0.046–0.077</td>
<td>0.029–0.086</td>
<td>0.22–0.50</td>
</tr>
<tr>
<td>average</td>
<td>0.060</td>
<td>0.061</td>
<td>0.27</td>
</tr>
<tr>
<td>standard error</td>
<td>0.012</td>
<td>0.11</td>
<td>0.09</td>
</tr>
</tbody>
</table>

One of our objectives was to estimate the effect of the atmospheric correction using different spectral bands on the derived values of the input parameter; the calculation was performed with MODIS-Aqua and VIIRS satellite data (averaged over 9 pixels). For comparison, the values calculated from the floating spectroradiometer data (11 stations in 2012 and 2013) were taken (‘measured’).

Three potential input parameters using different spectral bands of MODIS-Aqua and VIIRS scanners are considered: $X_1 = \log\left[\frac{R_{rs}(547)}{R_{rs}(531)}\right]$, $X_2 = \log\left[\frac{R_{rs}(547)}{R_{rs}(488)}\right]$ and $X_3 = \log\left[\frac{R_{rs}(551)}{R_{rs}(486)}\right]$.

It is seen from Table 5 that the errors increase when using spectral bands of 488 nm (MODIS) or 486 nm (VIIRS) instead of 531 nm. This should be kept in mind when deriving bio-optical algorithms, in particular VIIRS bio-optical algorithms for such a region as the Gulf of Finland.

Our results are in good agreement with data by Darecki & Stramski (2004) for the Baltic Sea, which showed poor agreement between in situ and satellite determinations of the normalised water-leaving radiance $L_{wn}$, especially in the blue spectral region (412–488 nm). The data for 551 nm showed the best agreement (unfortunately, the data for 531 nm was not included for lack of the corresponding spectral channel in the in situ spectroradiometer).

The quality of the atmospheric correction in the Gulf of Finland was checked by Zibordi et al. (2009), but they presented the relative errors for the $L_{wn}$ satellite retrieval, averaged over 100 matchups in different regions (Adriatic Sea, Atlantic Ocean, Persian Gulf) where only 20% were obtained in the Gulf of Finland.

For our regional algorithm #8, formula (5) with data from Table 5 gives the following values of the ratio of Chl$_{calc}$/Chl$_{meas}$: range = 0.52–2.03, average = 1.16, standard error = 0.50. Comparing them with the results of direct estimation given in Tables 1 and 3, one can see there is good agreement between both estimates: the contribution to the errors in Chl retrieval from the atmospheric correction for this data subset makes up on
average an overestimation of 16–17%. These estimates should be considered preliminary, since there were too few data to draw definitive conclusions.

5. Conclusion

The main result of our work is a set of new regional algorithms for estimating chlorophyll (Chl) and suspended matter (TSM) concentrations in surface waters of the Gulf of Finland from MODIS satellite scanner data. The algorithms were developed on the basis of data from field and satellite measurements in the study area in summers of 2012 and 2013 (40 stations); the data measured in situ included spectral values of the remote sensing reflectance $R_{rs}$, Chl and TSM concentrations. Testing of the existing algorithms with field data showed that all of them overestimated chlorophyll concentration several times, in particular, the standard MODIS algorithm (http://oceancolor.gsfc.nasa.gov/) overestimated Chl 4–19 times.

The new regional algorithm for Chl estimation takes the form

$$\log \text{Chl} = -0.50 + 19.8X - 42.7X^2,$$

where $X = \log\left[\frac{R_{rs}(547)}{R_{rs}(531)}\right]$. Its validation with MODIS-Aqua data (10 stations) gave an average relative error of 20%. The bio-optical algorithm #8 contributes to this error $\sim 3\%$ (Table 3) and the atmospheric correction – about 16–17% (see section 4.3).

A new regional relationship between TSM and the particle backscattering coefficient $b_{bp}$ has been derived:

$$\log \text{TSM} = 0.79 \log b_{bp} + 1.95,$$

where TSM is expressed in mg l$^{-1}$ and $b_{bp}$ in m$^{-1}$. It was calculated from the satellite data with using a previously developed algorithm (http://optics.ocean.ru). The coefficient of determination $r^2$ for this regression equation is equal to 0.61, and the standard error is 0.6 mg l$^{-1}$. Testing the new algorithm with MODIS data gave the averaged ratio of calculated TSM to measured TSM of 1.21(0.79 – 1.59); calculation of this ratio using the data from the floating spectroradiometer for the same stations gave a value of 1.04(0.77 – 1.51).

More data from simultaneous field and satellite measurements are needed to refine these algorithms.

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References


