Algorithms for the remote sensing of the Baltic ecosystem (DESAMBEM). Part 2: Empirical validation*

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The complete text of the paper is available at http://www.iopan.gda.pl/oceanologia/

Abstract

This paper is the second of two articles on the methodology of the remote sensing of the Baltic ecosystem. In Part 1 the authors presented the set of DESAMBEM algorithms for determining the major parameters of this ecosystem on the basis of satellite data (see Woźniak et al. 2008 – this issue). That article discussed in detail the mathematical apparatus of the algorithms. Part 2 presents the effects of the practical application of the algorithms and their validation, the latter based on satellite maps of selected Baltic ecosystem parameters: the distributions of the sea surface temperature (SST), the Photosynthetically Available Radiation (PAR) at the sea surface, the surface concentrations of chlorophyll *a* and the total primary production of organic matter. Particular emphasis was laid on analysing the precision of estimates of these and other parameters of the Baltic ecosystem, determined by remote sensing methods. The errors in these estimates turned out to be relatively small; hence, the set of DESAMBEM algorithms should in the future be utilised as the foundation for the effective satellite monitoring of the state and functioning of the Baltic ecosystem.

1. Introduction

The present article is the second of two dealing with the set of DESAMBEM algorithms for application in the remote sensing of the Baltic ecosystem. These algorithms were derived by scientists from three cooperating institutions[1]: the Institute of Oceanology, Polish Academy of Sciences, Sopot; the Institute of Oceanography, University of Gdańsk; the Institute of Physics, Pomeranian Academy, Słupsk; the Sea Fisheries Institute in Gdynia also played some part in this work. Part 1 (see Woźniak et al. 2008 – this issue) presented the complete mathematical apparatus of the set of DESAMBEM algorithms. This is founded upon a series of component mathematical models and empirical relationships describing a range of important optical, biological and other processes occurring in the atmosphere-sea system in the Baltic Sea region. These processes govern the state and functioning of marine ecosystems, in particular, the supply of solar light energy to them and its utilisation in the photosynthesis of organic matter in marine phytoplankton. Most of these models were developed by our teams of scientists and published at an earlier date.[2]

The set of DESAMBEM algorithms enables the spatial distributions of numerous parameters of the Baltic ecosystem to be estimated directly and

[2]see, for example, Woźniak et al. 1992a,b, 1995, 1997, 2000, 2002a,b, 2003, 2004, 2007a,b; Dera 1995; Kaczmarek & Woźniak 1995; Krężel 1997; Majchrowski & Ostrowska 1999, 2000; Majchrowski et al. 2000, 2007; Ostrowska et al. 2000a,b, 2007; Ficek et al. 2000a,b, 2003, 2004; Ficek 2001; Majchrowski 2001; Ostrowska 2001; Darecki & Stramski 2004; Kowalewski & Krężel 2004; Darecki et al. 2005, in preparation; Krężel et al. 2005, 2008; Woźniak S. B. – in preparation.

indirectly on the basis of the upward flux of radiation recorded by optical sensors operating on board satellites. With the aid of these algorithms it becomes possible to interpret satellite data as information on a great many phenomena taking place in the water. The distributions of the following phenomena and their characteristics can be obtained in the form of maps: sea surface temperature (SST)[3], surface currents and upwelling events, the extent to which riverine waters penetrate into the sea, water transparency, the radiation balance at the sea surface and in the upper layers of the atmosphere, the intensity of UV radiation over the sea and coastal regions, distributions of Photosynthetically Available Radiation (PAR), concentrations of chlorophyll and other pigments in the water, the efficiency of photosynthesis, the primary production of organic matter, the release of oxygen into the sea, and the distribution of phytoplankton blooms (e.g. of toxic blue-green algae). Further extension of these models will make it possible to supply other important information on the marine environment, e.g. pollution assessments.

It is clear from the above that the DESAMBEM algorithm set can play a major part in future studies of the Baltic ecosystem and substantially improve the efficiency of Baltic Sea monitoring. That is why it is important to demonstrate the practical utility of these algorithms by defining the reliability and precision of the Baltic ecosystem parameters estimated with their aid. The primary objective of the present paper (Part 2) is therefore to present an empirical validation of the set of DESAMBEM algorithms for determining the state of the Baltic ecosystem on the basis of remote-sensing data. The errors with which the estimated parameters are encumbered were calculated by comparing the estimated parameters with their values measured in situ in the atmosphere (just above the sea surface) and in the water, or calculated from in vitro measurements in water samples taken from different depths in the Baltic Sea.

2. Principles and experimental material employed in the empirical validation of the DESAMBEM algorithms

The complete set of DESAMBEM algorithms for determining primary production in the Baltic and selected parameters characterising the state and conditions prevailing in Baltic ecosystems were validated on the basis of empirical data of two types: 1 – data from in situ measurements, and 2 – satellite data and selected meteorological parameters. These two types of data are discussed in turn in subsections 2.1 and 2.2. In subsection 2.3

[3]The principal abbreviations and symbols used can be found in the Annex VI in Part 1 of this series of articles (see Woźniak et al. 2008 – this issue).

we then discuss all the validated ecosystem parameters estimated using the DESAMBEM algorithms.

2.1. Empirical in situ data and the methods of measuring them

In contrast to remote-sensing data, the in situ data here include not only parameters measured directly in the sea or the atmosphere but also those measured in vitro in samples of sea water taken from different depths in the sea. Among the many environmental parameters that were investigated, the following were utilised in the empirical validation of the DESAMBEM algorithms:

- $T_M(0)$ – the temperature measured in the thin surface layer of the sea using a CTD probe;
- $E_{c,M}(0^+)$ and $E_{PAR,M}(0^+)$ – the total solar irradiance in the complete spectral range (subscript C) and in the PAR range (400–700 nm), and also the daily doses of those irradiances at the sea surface $\eta_{C,M}(0^+)$ and $\eta_{PAR,M}(0^+)$. These magnitudes were determined on the basis of random in situ measurements with MER 2040 spectrophotometers and RAMSES Hyperspectral Radiometers, and also from continuous pyranometric measurements (from sunrise to sunset) (see Woźniak & Montwiłł 1973, Zibordi & Darecki 2006);
- $C_{a,M}(0)$ – the total concentration of chlorophyll a measured using the traditional spectrophotometric technique in sea water samples taken from depths close to $z = 0$ (see e.g. Strickland & Parsons 1968);
- $C_{a,M}(z)$, $C_{b,M}(z)$, $C_{c,M}(z)$, $C_{PSC,M}(z)$, $C_{phyc,M}(z)$ and $C_{PPC,M}(z)$ – the measured concentrations of different groups of pigments (chlorophyll a, chlorophyll b, chlorophyll c, photosynthetic carotenoids PSC, phycobilins $phyc$ and photoprotecting carotenoids PPC) at different depths in the sea. The concentrations of the chlorophyll pigments and the carotenoids were measured by HPLC (Mantoura & Llewellyn 1983, Stoń & Kosakowska 2002), whereas the phycobilin concentrations were defined by the approximate optical methods described by Ficek et al. (2004) and Majchrowski et al. (2007);
- $a_{pl,M}(\lambda)$ – the spectral coefficients of light absorption by phytoplankton in the spectral range 350–750 nm were measured in vivo using non-extraction methods (see e.g. Tassan & Ferrari 1995, 2002, Ferrari & Tassan 1999) in suitably prepared samples of water containing phytoplankton taken from different depths in the sea. The relevant spectral measurements were performed on a UNICAM UV4-100 spectrophotometer equipped with a LABSPHERE RSA-UC-40 integrating sphere. This is described in detail in Ficek et al. (2004);

- $P_M(z)$ – the primary production measured in situ at different depths in the sea employing the traditional C^{14} technique (see e.g. Steemann Nielsen 1975, Renk 1989).

The measurements of the above-mentioned magnitudes were performed mainly during research cruises of r/v 'Oceania' and r/v 'Baltica' in the Baltic in 2000–05. Empirical data from a few dozen stations were used in the validation of the DESAMBEM algorithms. Different numbers of stations were involved in the measurement of different ecosystem parameters – for details, see the tables in Chapter 3.

2.2. Satellite and meteorological data as input data for the calculations

Satellite data and some meteorological data were included in the set of input data for the DESAMBEM algorithms. Apart from the spatio-temporal parameters defining the position of a point or pixel on the sea, i.e. DOY, GMT, λ_g, φ_g, (the day number of the year, Greenwich Mean Time, longitude and latitude respectively), for which a variety of ecosystem parameters are estimated, the following satellite-derived data are essential in the calculations:

- L_u and τ_a – satellite-derived data, that is, the upward radiance at the satellite level and the aerosol optical thickness. Depending on the retrieval parameters, the upward radiance from various sensors are utilized, e.g. the HRV spectral channel of SEVIRI for the estimation of daily doses of solar irradiance at the sea surface, AVHRR for sea surface temperature and SeaWiFS or MODIS data for ocean colour parameters;

- e, p, T – meteorological data, that is, the water vapour pressure, atmospheric pressure, and air temperature above the sea surface. These meteorological input data were taken from data generated by the operational meteorological model at ICM or from NCEP. They include the ozone data necessary for the atmospheric correction of upwelling radiances; these data were taken from EPTOMS[4].

[4]ICM: Interdisciplinary Centre for Mathematical and Computational Modelling, Warsaw University – http://www.icm.edu.pl/eng/
NCEP – National Centers for Environmental Prediction at NOAA
EPTOMS – Total Ozone Mapping Spectrometer, data provided by NASA

2.3. Estimated parameters and methods of calculation

The input data discussed in section 2.2 were used to calculate, with the aid of the DESAMBEM algorithms, the following parameters characterising the abiotic conditions as well as the state and functioning of the ecosystem:

- SST – the sea surface temperature, determined on the basis of AVHRR data utilising the component subalgorithm of DESAMBEM known as the 'subalgorithm for estimating the Baltic Sea surface temperature' (see subsection 2.2 in Part 1 – Woźniak et al. 2008 – this issue);
- $E_{C,SAT}$ and $E_{PAR,SAT}$ – the solar irradiance at the sea surface in the complete spectral range (subscript C) and in the 400–700 nm range (subscript PAR) respectively, and also $\eta_{C,SAT}$ and $\eta_{PAR,SAT}$ – the respective daily doses of solar radiant energy incident on the sea surface defined for the complete spectral range and for the PAR range – calculated by integrating $E_{C,SAT}$ and $E_{PAR,SAT}$ over time. All these irradiance characteristics were determined on the basis of NOAA data, using the component algorithm of DESAMBEM called the 'subalgorithm for estimating the irradiance at the Baltic Sea surface' (see subsection 2.1 in Part 1 – Woźniak et al. 2008 – this issue);
- $C_{a,SAT}$ – the so-called 'satellite' chlorophyll *a* – strictly speaking, its remotely sensed concentration, which is approximately the mean concentration of this pigment in the top few metres of the sea surface layer. These concentrations were determined on the basis of SeaWiFS data with the site specific atmospheric correction. The DESAMBEM subalgorithm known as the 'subalgorithm for estimating the chlorophyll *a* concentration in the Baltic Sea surface layer' was applied at the end (see subsection 2.3 in Part 1 – Woźniak et al. 2008 – this issue, Darecki et al. – in preparation);
- $C_{a,tot,SAT}$, $C_{b,tot,SAT}$, $C_{c,tot,SAT}$, $C_{PSC,tot,SAT}$, $C_{phyc,tot,SAT}$ and $C_{PPC,tot,SAT}$ – the total contents of chlorophyll *a*, chlorophyll *b*, chlorophyll *c*, photosynthetic carotenoids *PSC*, phycobilins *phyc* and photoprotecting carotenoids *PPC* in the water column under unit area of sea surface in the euphotic zone. These magnitudes were defined on the basis of the remotely determined surface concentrations of chlorophyll *a* and the irradiance conditions at the sea surface, utilising two component subalgorithms of DESAMBEM, namely, the 'subalgorithm for calculating the daily dose of PAR transmitted across a wind-blown sea surface' and the 'subalgorithm for estimating the underwater optical and bio-optical features and photosynthetic primary production in the Baltic Sea' (see subsections 2.4 and 2.5 in Part 1 – Woźniak et al. 2008 – this issue);

- $<a_{pl}>$ – the mean coefficients of light absorption by phytoplankton in the PAR range (400–700 nm) relevant to the surface layer of the sea, defined on the basis of the following remotely sensed magnitudes: surface concentration of chlorophyll *a* and the irradiance conditions; the same subalgorithms are used as for determining the pigment concentrations above;

- $P_{tot,C}$ – the total primary production in the water column under unit area of sea surface. These magnitudes were estimated on the basis of the above-mentioned subalgorithm, the 'subalgorithm for estimating the underwater optical and bio-optical features and photosynthetic primary production in the Baltic Sea'. The input data for calculating $P_{tot,C}$ were the following three remotely sensed values: SST – sea surface temperature, $C_{a,\,SAT}$ – surface concentration of chlorophyll *a*, and the corresponding irradiances: the daily mean $PAR(0^-)$ or the dose of this irradiance $\eta_{PAR}(0^-)$ in the PAR spectral range (400–700 nm) just beneath the sea surface.

Because of the different spatial resolutions of the input data, all the calculations detailed above were performed only after they had been standardized to a grid with a resolution of 1×1 km.

As we mentioned in Part 1, the mathematical structure of the DESAMBEM algorithm set is highly complex. This applies above all to its 'underwater part', which is based on the 'light-photosynthesis' model used for calculating the primary production of organic matter in the sea. That is why the example of the maps of the remotely estimated primary production in the entire Baltic, presented at the beginning of Chapter 3, were compiled using a simplified version of the DESAMBEM algorithm set, an approach that did not introduce any significant inaccuracies. Nevertheless, the precision of these ecosystem parameter estimates obtained from satellite data, set out in subsections 3.1 to 3.5, was analysed using the complete mathematical apparatus.

The simplification of the full version of the DESAMBEM algorithm set involved replacing, with a suitably straightforward functional expression, a series of complicated model formulae describing the dependence of the total primary production P_{tot} (that is, the total production of organic matter in the water column under unit area of sea surface) on three parameters: the sea surface temperature $T_M(0)$, surface concentration of chlorophyll $C_a(0)$ and PAR irradiance just beneath the sea surface $E_{PAR,\,M}(0^-)$. This expression, giving a good approximation of the primary production determined with the aid of the full version of the 'light-photosynthesis' model for the Baltic, was obtained by non-linear regression in the form of the following polynomial:

$$\left.\begin{aligned} &\varsigma = \sum_{j=0}^{5}\left[\sum_{i=0}^{5} A_{T,i,j}\big(\log(C_a(0))\big)^i\right] \times \log\left(E_{PAR}(0^-)\right)^j \\ &P_{tot} = 10^{\varsigma} \end{aligned}\right\}, \qquad (1)$$

where the various magnitudes are expressed in the following units: P_{tot} [mgC m^{-2} s^{-1}], $C_a(0)$ [mg tot chl$a$ m^{-3}], $E_{PAR}(0^-)$ [μEin m^{-2} s^{-1}], whereas $\mathrm{A}_{T,\,i,\,j}$ is expressed by the coefficients of these polynomials determined for various fixed temperatures from *temp* = 0°C to *temp* = 30°C in 1°C steps. For lack of space in this article, we do not give the values of these coefficients (they are contained in an internal IO PAS document – see Ficek et al. 2005).

According to our analysis of the precision of approximating expression (1), the values of P_{tot} it yields, given the ranges of variability of sea surface temperature, sub-surface irradiance and surface concentration of chlorophyll usual in the Baltic, do not in most cases deviate by more than 4% from P_{tot} calculated with the non-approximated version of the light-photosynthesis model for the Baltic (the mean statistical error is ± 3.8%).

A further limitation on the direct applicability of the DESAMBEM algorithms for estimating ecosystem parameters at any time and for any position in the Baltic on the basis of satellite data is that the use of visual and thermal infrared satellite data is restricted by cloud cover. Nevertheless, this limitation had to be overcome in the empirical validation of these algorithms. To reconstruct data in areas temporarily covered by clouds, different methods of estimation are used, which are based on data received in cloud-free situations not far distant in space and/or time (Addink & Stein 1999, Beckers & Rixen 2003, Alvera-Azcárate et al. 2005). One commonly used procedure is *cokriging* interpolation. But as this is a time-consuming procedure, a combination of *kriging* interpolation and linear regression was used for the purposes of the DESAMBEM project (Urbański et al. 2005). Gap-filling then involved combining data from the pixels surrounding the image under scrutiny and data from another image, not far distant with respect to the recording time, and also well correlated, with the area of estimation at least partly cloud-free. Both images were randomly sampled, with stratification based on a cloud mask in order to obtain sufficient complementary data for the area of estimation. Estimation was carried out for the cloudy area, extended by a buffer zone of 5 km. To prevent an artificial border from being set up between the estimated and real data, a fuzzy algorithm was applied to mix them in the buffer zone. Cloud-free images were used to validate the suggested method. Different masks of real cloudiness were used to eliminate certain data, after which estimated values were related to real ones. For 75% of the estimated values the difference between the estimated and real temperature did not exceed 3.7% of the real value. In real situations inaccurate cloud masks may increase the error of estimation.

To fill the gaps due to clouds on the chlorophyll concentration maps derived from SeaWiFS data, the above procedure was modified slightly (Bratke et al. 2005). In the presence of haze the atmospheric correction of visual bands is not accurate, so complementary data were sampled from a map of minimum chlorophyll concentrations calculated over a few days and passed through a median filter. Such a map was usually better correlated with the filled one than any of the daily chlorophyll concentration maps. In addition, a power function was used in the regression. The error of estimation was less than 30% for most of the simulations used in the validation procedure.

3. Estimations using the algorithms: empirical validation and error assessment

Figures 1 to 3 give examples of the practical application of the DESAMBEM algorithms – maps of remotely sensed ecosystem parameters: PAR irradiance at the sea surface PAR, the sea surface temperature SST, surface concentration of chlorophyll a $C_a(0)$ and total primary production P_{tot}. The maps refer to situations with different distributions of the surface parameters and with different amount of areas covered by clouds. The figures also present results of data reconstruction in areas temporarily covered by clouds, as described in the previous paragraph. Figures 1–3 present maps of the surface concentration of chlorophyll a $C_a(0)$ and total primary production P_{tot} showing the areas covered by clouds (the white gaps in Figures 1–3 c and e) and the same maps with reconstructed data in the gaps due to cloud cover (Figures 1–3 d and f). The advantage of data reconstruction is clearly visible, especially in Figure 3 with a significant percentage of the cloud covered area in the central Baltic. Such reconstruction significantly improves the efficiency of remote sensing techniques in marine ecosystem monitoring by ensuring their continuously in time and space. On the other hand it has to be pointed out that in many situations the reconstructed data can be more or less false. Because of the nature of the applied numerical calculations, the local concentration of a parameter or its locally spatial distribution can differ from the real values: see the example in Figure 3, where the distribution of the chlorophyll a concentration in the Gulf of Riga is probably false, especially when compared to the distribution in the

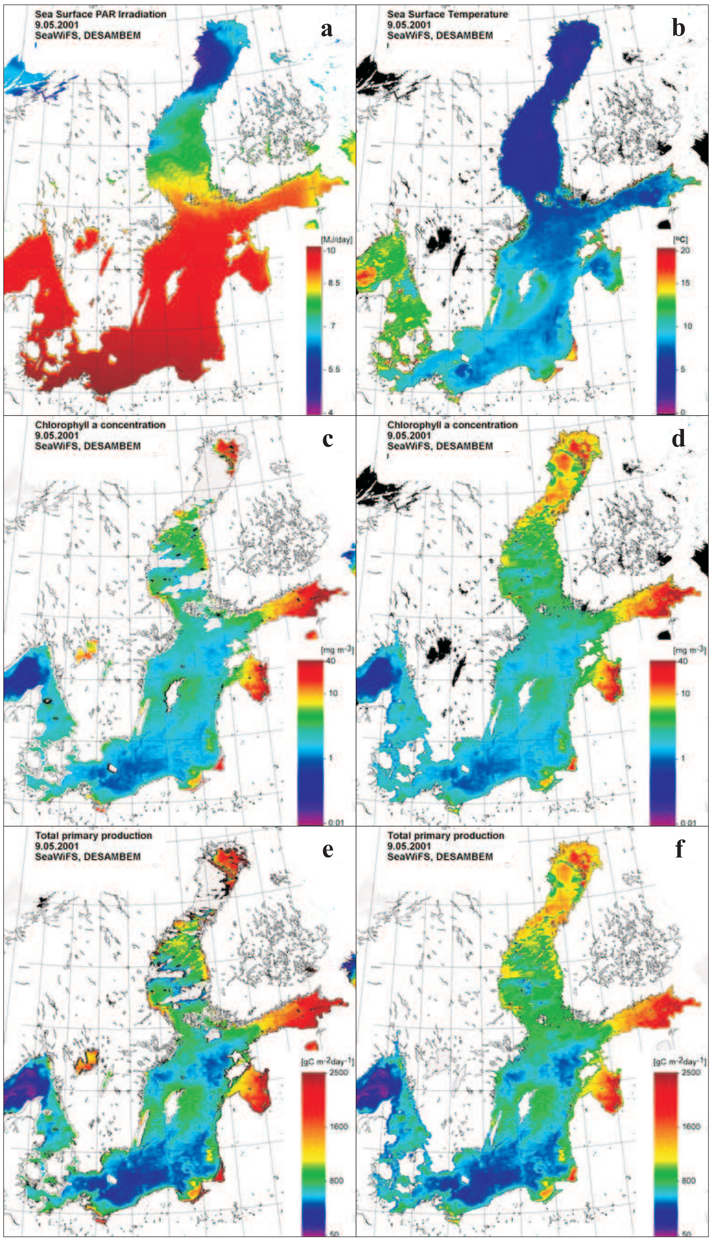

Figure 1. Example of the remotely sensed distribution of 4 selected parameters of the Baltic ecosystem on 9 May 2001 calculated from the DESAMBEM algorithms:

a) PAR irradiance at the sea surface PAR;

b) the sea surface temperature SST;

c) surface concentration of chlorophyll a $C_a(0)$ for the cloud-free area;

d) surface concentration of chlorophyll a $C_a(0)$ for the whole Baltic, with data reconstructed in the gaps due to cloud cover;

e) total primary production P_{tot} for the cloud-free area;

f) total primary production P_{tot} for the whole Baltic, with data reconstructed in the gaps due to cloud cover

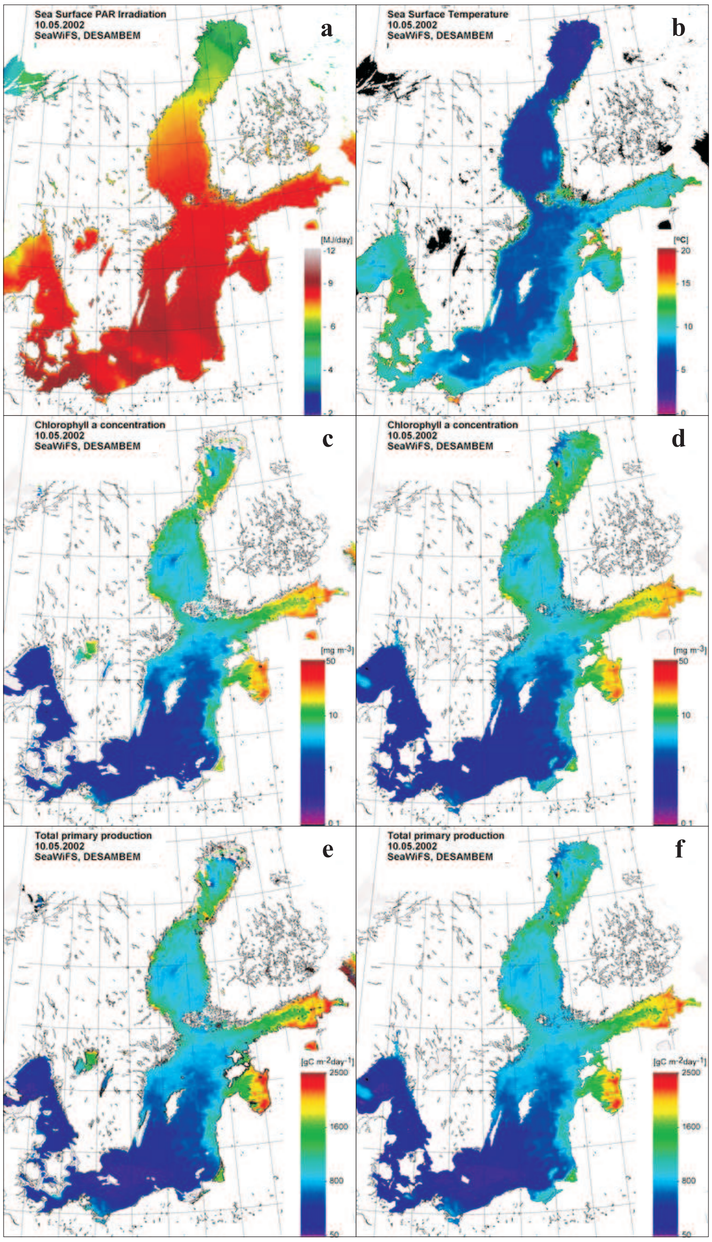

Figure 2. Example of the remotely sensed distribution of 4 selected parameters of the Baltic ecosystem on 10 May 2002 calculated from the DESAMBEM algorithms:

a) PAR irradiance at the sea surface PAR;
b) the sea surface temperature SST;
c) surface concentration of chlorophyll a $C_a(0)$ for the cloud-free area;
d) surface concentration of chlorophyll a $C_a(0)$ for the whole Baltic, with data reconstructed in the gaps due to cloud cover;
e) total primary production P_{tot} for the cloud-free area;
f) total primary production P_{tot} for the whole Baltic, with data reconstructed in the gaps due to cloud cover

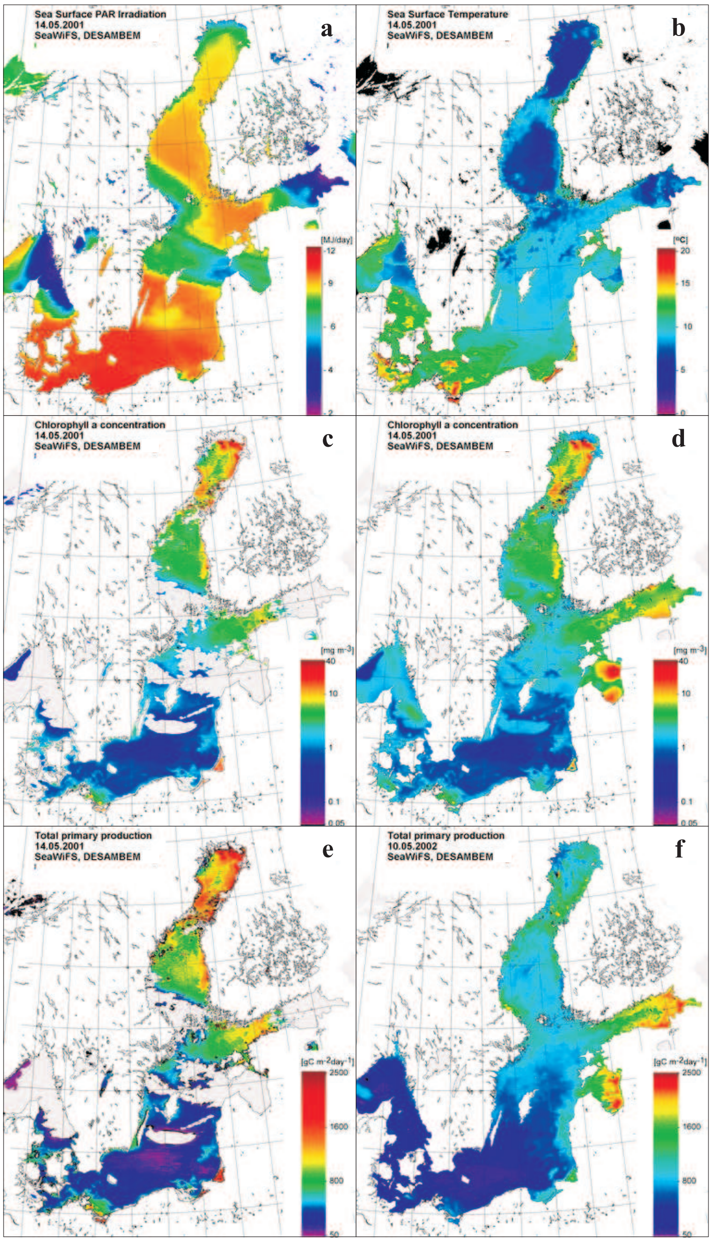

Figure 3. Example of the remotely sensed distribution of 4 selected parameters of the Baltic ecosystem on 14 May 2001 calculated from the DESAMBEM algorithms:

a) PAR irradiance at the sea surface PAR;
b) the sea surface temperature SST;
c) surface concentration of chlorophyll a $C_a(0)$ for the cloud-free area;
d) surface concentration of chlorophyll a $C_a(0)$ for the whole Baltic, with data reconstructed in the gaps due to cloud cover;
e) total primary production P_{tot} for the cloud-free area;
f) total primary production P_{tot} for the whole Baltic, with data reconstructed in the gaps due to cloud cover

same area in Figures 1 and 2. However, in our opinion this does not significantly limit the potential results, especially in a large-scale analysis – in the above example, the average concentration for the whole area is still similar; with some experience, such cases are easily detected and eliminated. The problem of data reconstruction in cloud-covered areas is very complex and exceeds the scope of this work. The authors plan to publish a paper on this particular problem in the near future.

Summarising, it can be assumed that these maps illustrate the Nature of the Baltic Sea in a comprehensive and spatially detailed manner, which is not possible with data obtained solely by means of traditional shipboard measuring techniques. In the future, therefore, tangible benefits will accrue from the satellite monitoring of the sea, as regards not only oceanographic knowledge but also the wider aspects of the Earth's natural history. But the 'quality' of this knowledge will depend on the precision and accuracy of these satellite measurements.

The empirical validation of such satellite-retrieved characteristics of the Baltic ecosystem is the main purpose of this work; the detailed analysis of the performance of the DESAMBEM algorithms will now be presened.

In order to assess the accuracy of our set of algorithms for determining the parameters of the Baltic ecosystem, we compared the values of these parameters determined from satellite data with those measured in situ and in water samples. For these comparisons the relevant errors of these satellite estimations were calculated in accordance with the principles of arithmetic and logarithmic statistics:

Absolute mean error (systematic): $< \varepsilon' > = N^{-1} \sum_i \varepsilon'_i$
(where $\varepsilon'_i = (X_{i,C} - X_{i,M})$)

Relative mean error (systematic): $< \varepsilon > = N^{-1} \sum_i \varepsilon_i$
(where $\varepsilon_i = (X_{i,C} - X_{i,M})/X_{i,M}$)

Standard deviation (statistical error) of ε': $\sigma_{\varepsilon'} = \sqrt{\frac{1}{N}(\sum(\varepsilon'_i - < \varepsilon' >)^2)}$

Standard deviation (statistical error) of ε: $\sigma_{\varepsilon} = \sqrt{\frac{1}{N}(\sum(\varepsilon_i - < \varepsilon >)^2)}$

Mean logarithmic error: $< \varepsilon >_g = 10^{[< \log(X_{i,C}/X_{i,M}) >]} - 1$

Standard error factor: $x = 10^{\sigma \log}$

Statistical logarithmic errors: $\sigma_+ = x - 1,\ \sigma_- = \frac{1}{x} - 1$,
where $X_{i,M}$ – measured values; $X_{i,C}$ – estimated values
(the subscript M stands for 'measured', C for 'calculated');

$< \log(X_{i,C}/X_{i,M}) >$ – mean of $\log(X_{i,C}/X_{i,M})$;

$\sigma_{\log}$ – standard deviation of the set $\log(X_{i,C}/X_{i,M})$.

The following aspects were taken into account in the assessment of the remotely sensed ecosystem parameters:

- for sea surface temperature – the relevant absolute errors determined by arithmetic statistics;
- for the other ecosystem parameters – the relevant relative errors determined by both arithmetic and logarithmic statistics.

In view of the considerable volume of estimated material concerning the abiotic conditions and the complexity of the states and functioning of the Baltic ecosystem, we shall here discuss the validation only of its major parameters, namely, the sea surface temperature, sea surface irradiance, surface concentration of chlorophyll *a*, total concentrations of various other groups of phytoplankton pigments in the water, mean values of the coefficient of light absorption by phytoplankton in the 400–700 nm range in the surface water of the sea, and the total primary production in the water column below unit area of sea surface.

3.1. Sea surface temperature

Figure 4 and Table 1 give the results of the validation of satellite estimations of sea surface temperature. The figure compares the remotely sensed values of this temperature (SST) with values measured in situ ($T_{M\ \text{in situ}}$) at particular measurement stations. The calculated errors (systematic and statistical according to arithmetic statistics) are in the region of 1°C or less. As far as diagnosing the state of the Baltic ecosystem

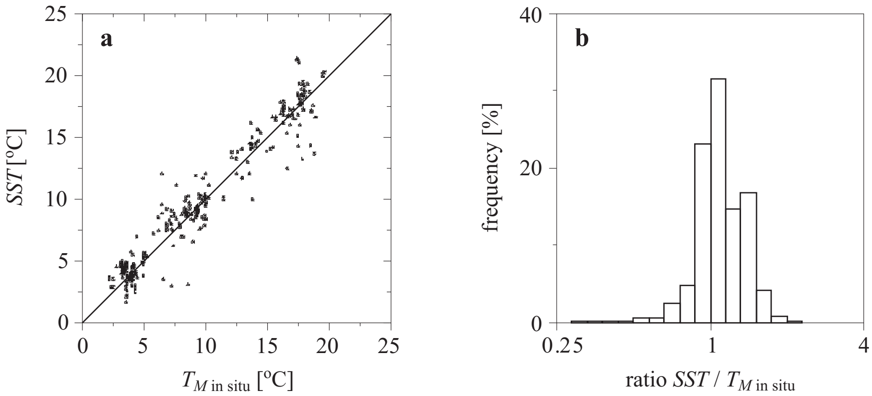

Figure 4. Comparison of sea surface temperatures: measured ($T_{M\ \text{in situ}}$) and calculated (SST) from AVHRR data:
a) relationship between measured and calculated temperatures;
b) probability density distribution of the ratio of the remotely retrived SST to the in situ measured $T_{M\ \text{in situ}}$

Table 1. Relative errors in estimating the sea surface temperature from AVHRR data

No. of data	Arithmetic statistics	
	systematic error $<\varepsilon'>$ [°C]	statistical error $\sigma_{\varepsilon'}$ [°C]
579	0.371	±1.09

is concerned, this level of accuracy is satisfactory, the more so that the error probably stems from the fact that the satellite records the mean temperature of a whole pixel (an area of 1 km^2), and not that of the particular point at sea where the in situ measurement was made.

3.2. Sea surface irradiance

Figures 5–8 and Tables 2–5 show the results of the validation of the sea surface irradiances – total E_{tot} and PAR (i.e. in the spectral range from 400 to 700 nm) and the daily doses of these irradiances.

While the results are similar for the irradiance characteristics with respect to the total and PAR radiation, they differ fundamentally in regard to the signal integration time. In the case of instantaneous irradiances (Figures 5 and 6), the possible systematic errors are very low (see the systematic errors according to logarithmic statistics in Tables 2 and 3), but the statistical errors are high ($\sigma_- > 40\%$, $\sigma_+ > 70\%$). These considerable

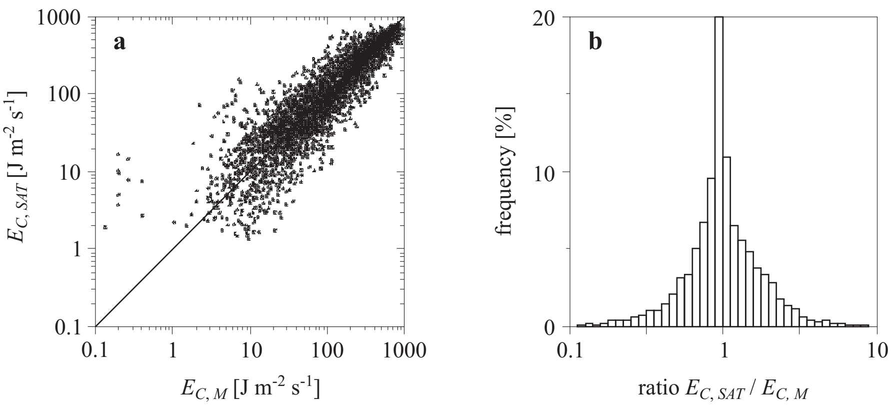

Figure 5. Comparison of sea surface irradiances in the full spectral range measured ($E_{C,M}$) and determined from satellite observations ($E_{C,SAT}$):
a) relationship between measured and calculated irradiance values;
b) probability density distribution of the ratio of the remotely measured sea surface irradiance to the in situ measured sea surface irradiance in the full spectral range

Table 2. Relative errors in estimating the sea surface irradiances over the full spectral range on the basis of satellite data

No. of data	Arithmetic statistics		Logarithmic statistics			
	systematic error $< \varepsilon >$ [%]	statistical error σ_ε [%]	systematic error $< \varepsilon >_g$ [%]	standard error factor x	statistical error σ_- [%]	statistical error σ_+ [%]
3991	28.7	239	0.650	1.80	−44.41	79.9

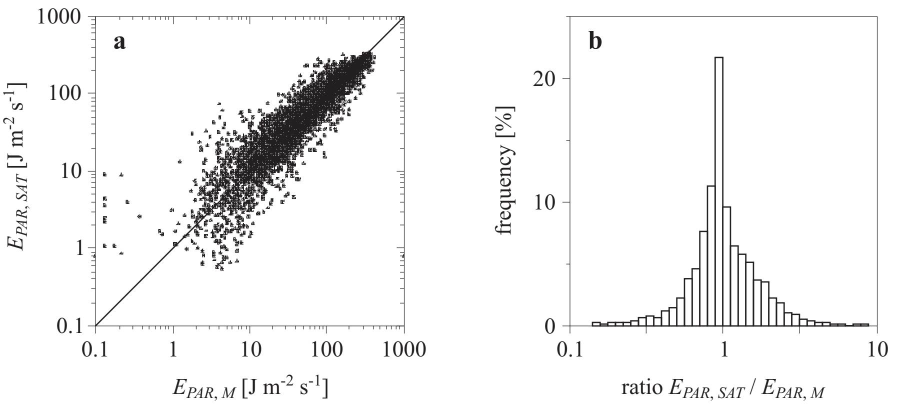

Figure 6. Comparison of sea surface irradiances in the PAR spectral range measured ($E_{PAR,M}$) and determined from satellite observations ($E_{PAR,SAT}$):
a) relationship between measured and calculated irradiance values;
b) probability density distribution of the ratio of the remotely measured sea surface irradiance to the in situ measured sea surface irradiance in the PAR spectral range

Table 3. Relative errors in estimating the sea surface irradiances in the PAR spectral range on the basis of satellite data

No. of data	Arithmetic statistics		Logarithmic statistics			
	systematic error $< \varepsilon >$ [%]	statistical error σ_ε [%]	systematic error $< \varepsilon >_g$ [%]	standard error factor x	statistical error σ_- [%]	statistical error σ_+ [%]
3991	22.2	175	0.914	1.71	−41.6	71.1

errors do not, however, appear to be inherent in satellite measurement techniques. More likely, they are due to the fact that the remotely sensed instantaneous irradiance is the irradiance averaged over the 1 km^2 area of sea covered by one pixel of the METEOSAT satellite, whereas the irradiance measured in situ at the sea surface is that at a random point in the

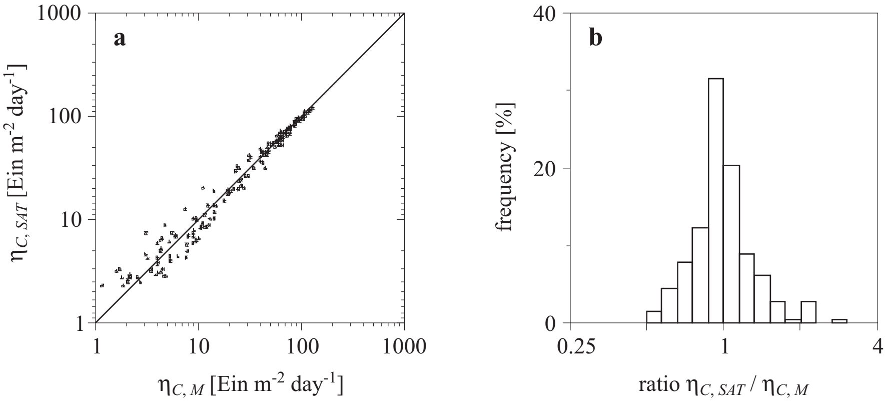

Figure 7. Comparison of daily sea surface irradiance doses in the full spectral range measured (η_M) and determined from satellite observations ($\eta_{C,\,SAT}$):
a) relationship between measured and calculated daily irradiance doses;
b) probability density distribution of the ratio of the remotely measured daily surface irradiance dose to the in situ measured daily surface irradiance dose in the full spectral range

Table 4. Relative errors in estimating the sea surface irradiance doses in the full spectral range on the basis of satellite data

No. of data	Arithmetic statistics		Logarithmic statistics			
	systematic error $<\varepsilon>$ [%]	statistical error σ_ε [%]	systematic error $<\varepsilon>_g$ [%]	standard error factor x	statistical error σ_- [%]	σ_+ [%]
179	2.66	1.98	−0.879	1.26	−20.7	26.1

Table 5. Relative errors in estimating the sea surface irradiance doses in the PAR spectral range on the basis of satellite data

No. of data	Arithmetic statistics		Logarithmic statistics			
	systematic error $<\varepsilon>$ [%]	statistical error σ_ε [%]	systematic error $<\varepsilon>_g$ [%]	standard error factor x	statistical error σ_- [%]	σ_+ [%]
219	2.44	23.3	0.245	1.22	−18.3	22.3

area covered by that pixel. The errors in the daily irradiance doses are considerably smaller, however (Figures 5 and 6): on average, the systematic errors of these estimated doses are c. 20% (see Tables 4 and 5 – logarithmic statistics).

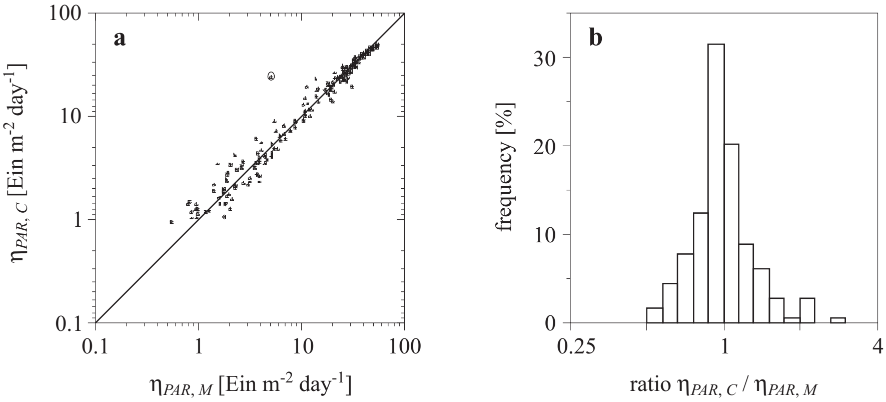

Figure 8. Comparison of daily sea surface irradiance doses in the PAR spectral range measured ($\eta_{PAR,M}$) and determined from satellite observations ($\eta_{PAR,SAT}$):
a) relationship between measured and calculated daily irradiance doses;
b) probability density distribution of the ratio of the remotely measured daily surface irradiance dose to the in situ measured daily surface irradiance dose in the PAR spectral range

3.3. Surface chlorophyll concentration

The analysis of the remotely estimated surface concentration of chlorophyll *a* C_a was carried out jointly for the entire experimental material, i.e. for 171 images, and separately for the three following, different weather situations (the relevant numbers of images are given in Table 6):

- 'certain cloud-free images' – when the measurement was made in a cloud-free region, and the satellite map indicated that similar conditions prevailed over a large area of sea greater than that of a SeaWiFS pixel;
- 'probable cloud-free images' – when the measurement was made in a cloud-free region, but partial cloudiness was possible in the area of a SeaWiFS pixel;
- 'overcast images' – when the measurement was made in a cloudy region and the cloud covered a substantial area of the Baltic, precluding a direct estimate of the chlorophyll concentration from SeaWiFS data.

In the first two cases the surface concentrations of chlorophyll *a* $C_{a,SAT}$ were estimated using the DESAMBEM subalgorithm on the basis of SeaWiFS data, but in the third, $C_{a,SAT}$ was determined by means of the appropriate interpolation of the estimates as above, in time-space, using the results described (Bradtke et al. 2005).

Table 6. Specification of the empirical material used to validate the remotely estimated surface concentration of chlorophyll *a*

	No. of data			
	certain cloud-free images	probable cloud-free images	overcast images	total images
Total	64	86	21	171
Without serious errors (see the explanation in the text)	64	80	16	160

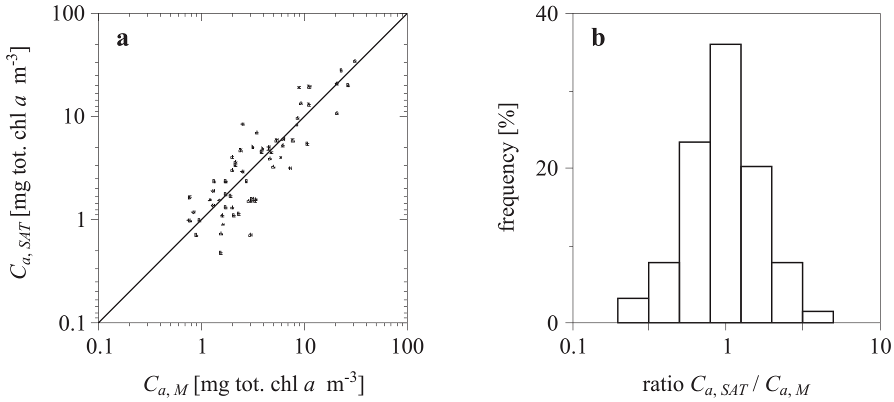

Figure 9. Comparison of surface chlorophyll *a* concentrations measured ($C_{a,M}$) and determined from satellite observations ($C_{a,SAT}$) for certain cloud-free images:
a) relationship between surface chlorophyll *a* concentrations measured ($C_{a,M}$) and determined from satellite observations ($C_{a,SAT}$);
b) probability density distribution of the ratio of the remotely measured chlorophyll *a* concentrations to the in situ measured chlorophyll *a* concentrations for certain cloud-free images

Table 7. Relative errors in estimating the surface chlorophyll *a* concentrations on the basis of satellite data for certain cloud-free images

Arithmetic statistics		Logarithmic statistics			
systematic error $< \varepsilon >$ [%]	statistical error σ_ε [%]	systematic error $< \varepsilon >_{\rm g}$ [%]	standard error factor x	statistical error σ_- [%]	statistical error σ_+ [%]
9.93	56.6	−3.16	1.68	−40.5	68.1

The results of the error analyses are presented as follows: (1) for 'certain cloud-free images' – Figure 9 and Table 7; (2) for 'probable cloud-free

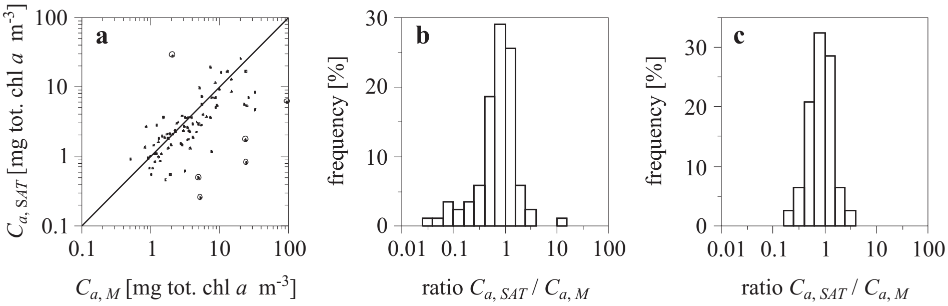

Figure 10. Comparison of surface chlorophyll a concentrations measured ($C_{a,M}$) and determined from satellite observations ($C_{a,SAT}$) for probable cloud-free images:

a) relationship between surface chlorophyll a concentrations measured ($C_{a,M}$) and determined from satellite observations ($C_{a,SAT}$) (points in circles – serious errors);

b) probability density distribution of the ratio of the remotely measured chlorophyll a concentrations to the in situ measured chlorophyll a concentrations for all probable cloud-free images;

c) probability density distribution of the ratio of the remotely measured chlorophyll a concentrations to the in situ measured chlorophyll a concentrations with the exclusion of serious errors

Table 8. Relative errors in estimating the surface chlorophyll a concentrations on the basis of satellite data for probable cloud-free images

	Arithmetic statistics		Logarithmic statistics			
	systematic error $<\varepsilon>$ [%]	statistical error σ_ε [%]	systematic error $<\varepsilon>_g$ [%]	standard error factor x	statistical error σ_- [%]	statistical error σ_+ [%]
All	2.19	149.6	−30.8	2.50	−59.9	150
Without serious errors (see the explanation in the text)	−7.68	55.0	−17.4	1.72	−42.0	72.4

images' – Figure 10 and Table 8; (3) for 'overcast images' – Figure 11 and Table 9; (4) for all the points validated – Figure 12 and Table 10. Validation was performed twice in all cases: once, in order to assess the errors for all the points in the sets of empirical material to be validated, then again to assess the errors in those sets, now 'reduced' by those empirical points, which were judged to be results encumbered by serious errors. When the results with serious errors were being singled out, the distributions of the probability densities of the error magnitudes were also taken into consideration on the assumption that they ought to resemble Gaussian, log-normal distributions.

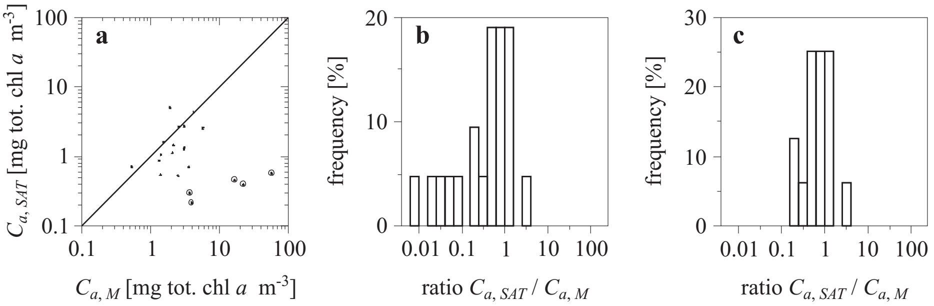

Figure 11. Comparison of surface chlorophyll a concentrations measured ($C_{a,\,M}$) and determined from satellite observations ($C_{a,\,SAT}$) for overcast images:

a) relationship between surface chlorophyll a concentrations measured ($C_{a,\,M}$) and determined from satellite observations ($C_{a,\,SAT}$) (points in circles – serious errors);

b) probability density distribution of the ratio of the remotely measured chlorophyll a concentrations to the in situ measured chlorophyll a concentrations for all overcast images;

c) probability density distribution of the ratio of the remotely measured chlorophyll a concentrations to the in situ measured chlorophyll a concentrations with the exclusion of serious errors

Table 9. Relative errors in estimating the surface chlorophyll a concentrations on the basis of satellite data for overcast images

	Arithmetic statistics		Logarithmic statistics			
	systematic error $<\varepsilon>$ [%]	statistical error σ_ε [%]	systematic error $<\varepsilon>_g$ [%]	standard error factor x	statistical error σ_- [%]	σ_+ [%]
All	39.0	60.7	−69.5	4.57	−78.1	357
Without serious errors	−21.1	59.0	−38.3	1.96	−48.9	95.8

According to the data in the Figures and Tables, the validations indicate that the surface chlorophyll a concentrations estimated with the DESAMBEM subalgorithm are encumbered with relatively small errors (once the serious errors have been eliminated). So for all the weather types considered, the standard error factor (after elimination of serious errors) is no greater than 2, which corresponds to values of the relevant errors of $\sigma_- \approx 50\%$ and $\sigma_+ \approx 100\%$. These values are the limits accepted as being the typical methodological errors inherent in the various experimental techniques for determining the phytoplankton pigment concentrations in sea waters. In fact, the precision of satellite methods for estimating chlorophyll

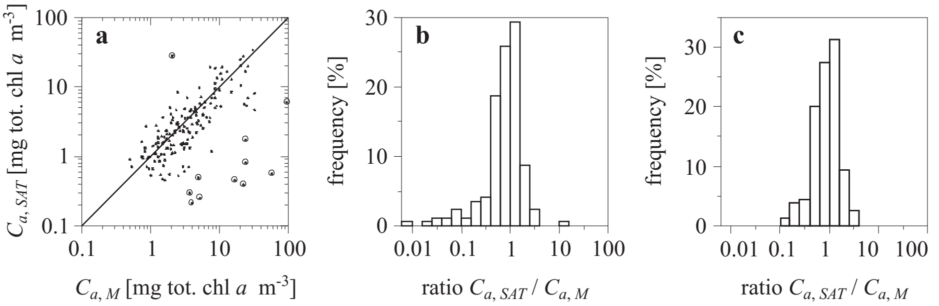

Figure 12. Comparison of surface chlorophyll a concentrations measured ($C_{a,M}$) and determined from satellite observations ($C_{a,SAT}$) for all images:

a) relationship between surface chlorophyll a concentrations measured ($C_{a,M}$) and determined from satellite observations ($C_{a,SAT}$) (points in circles – serious errors);

b) probability density distribution of the ratio of the remotely measured chlorophyll a concentrations to the in situ measured chlorophyll a concentrations for all images;

c) probability density distribution of the ratio of the remotely measured chlorophyll a concentrations to the in situ measured chlorophyll a concentrations with the exclusion of serious errors

Table 10. Relative errors in estimating the surface chlorophyll a concentrations for all images on the basis of satellite data for all images

	Arithmetic statistics		Logarithmic statistics			
	systematic error $<\varepsilon>$ [%]	statistical error σ_ε [%]	systematic error $<\varepsilon>_g$ [%]	standard error factor x	statistical error σ_- [%]	σ_+ [%]
All	−0.03	114	−29.0	2.60	−61.6	160
Without serious errors	−1.98	56.7	−16.8	1.82	−45.0	81.9

concentrations is actually better than that suggested by the error levels given here. This is because, as we mentioned earlier, in situ measurements are point measurements, whereas the satellite estimates refer to chlorophyll concentrations averaged over the area of a whole SeaWiFS pixel.

3.4. Other quantitative characteristics of phytoplankton pigments

The next of the validated magnitudes to be determined with the DESAMBEM algorithm was the mean coefficient of light absorption in the

PAR range (400–700 nm) by phytoplankton in the surface water. It is defined as:

$$< a_{pl} >= \frac{1}{300\,\mathrm{nm}} \int_{400\,\mathrm{nm}}^{700\,\mathrm{nm}} a_{pl}(\lambda) d\lambda. \tag{2}$$

Table 11 sets out the results of the validation of this parameter. As in the case of the estimated chlorophyll concentrations, the systematic error in the magnitudes of absorption is not great.

Table 11. Relative errors in the estimation of the surface coefficient of light absorption $< a_{pl} >$ by algae

No. of data	Arithmetic statistics		Logarithmic statistics			
	systematic error $< \varepsilon >$ [%]	statistical error σ_ε [%]	systematic error $< \varepsilon >_g$ [%]	standard error factor x	statistical error σ_- [%]	σ_+ [%]
19	−38.9	±40.3	−50.5	2.00	−49.9	99.7

The DESAMBEM algorithm was also used for the remote estimation of the concentrations of various phytoplankton pigments $C_{a,\,tot,\,SAT}$, $C_{b,\,tot,\,SAT}$, $C_{c,\,tot,\,SAT}$, $C_{PSC,\,tot,\,SAT}$, $C_{phyc,\,tot,\,SAT}$, $C_{PPC,\,tot,\,SAT}$. Table 12 shows the results of the validation of these quantitative characteristics of phytoplankton: the estimation errors are relatively low. The standard error factor for these values is close to or less than the conventional boundary value of 2.

Table 12. Relative errors in the estimation of the total concentration C of different pigments in the euphotic zone (N – number of data)

Pigment	N	Arithmetic statistics		Logarithmic statistics			
		systematic error $< \varepsilon >$ [%]	statistical error σ_ε [%]	systematic error $< \varepsilon >_g$ [%]	standard error factor x	statistical error σ_- [%]	σ_+ [%]
$C_{a,\,tot,\,SAT}$	35	−18.7	±48.6	−31.1	1.84	−45.7	84.0
$C_{b,\,tot,\,SAT}$	33	18.2	±77.5	−4.72	1.98	−49.4	97.8
$C_{c,\,tot,\,SAT}$	33	28.3	±74.5	9.05	1.83	−45.3	82.8
$C_{PSC,\,tot,\,SAT}$	33	53.5	±110	21.4	2.04	−50.9	104
$C_{phyc,\,tot,\,SAT}$	33	11.5	±54.7	−1.18	1.67	−39.9	66.6
$C_{PPC,\,tot,\,SAT}$	20	−41.9	±45.2	−54.2	2.01	−50.1	100

3.5. Total primary production in the water column

The final magnitude to be verified was the total primary production P_{tot} in the water column beneath unit area of sea water. P_{tot} is calculated by numerically integrating the vertical distributions of production $P(z)$ (both measured and modelled) over depth:

$$P_{tot} = \int_{0}^{z_{\max}} P(z)dz, \tag{3}$$

where the depth limit $z_{\max}$ in these calculations was taken to be 1.5 times the depth of the euphotic zone, i.e. $z_{\max} = 1.5 z_e$. Below the boundary depth $z_{\max}$ thus defined, the production $P(z > z_{\max})$ is relatively small (i.e. $P(z > z_{\max}) \approx 0$) and has no significant effect on the magnitude of the total production P_{tot} in a water column in the Baltic.

Figure 13 and Table 13 show the results of this validation obtained for 83 measurement points. The errors in the estimated total production P_{tot} are clearly relatively small and comparable with the methodological errors inherent in the measurement of primary production using the traditional C^{14} techniques. For the time being we regard these results as satisfactory, but in the future we intend to modify and make more precise our models for this parameter, above all in order to reduce the level of the systematic errors.

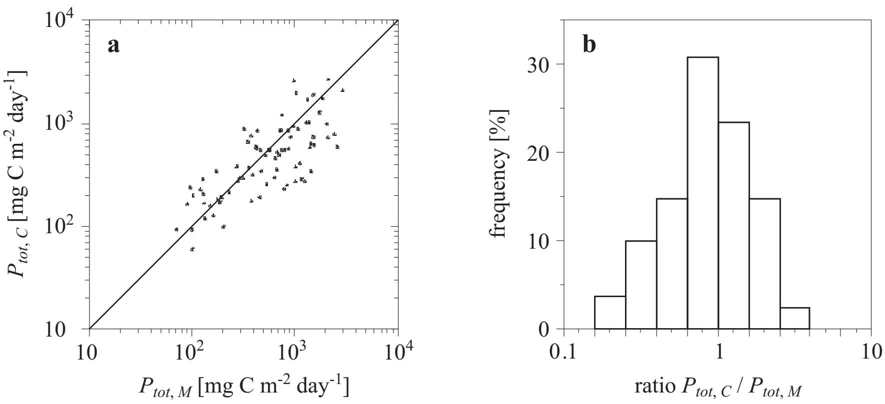

Figure 13. Comparison of daily primary production in the water column ($P_{tot,\,M}$) and determined from satellite observations ($P_{tot,\,C}$):
a) relationship between measured and calculated primary production;
b) probability density distribution of the ratio of the remotely measured daily primary production to the in situ measured daily primary production

Table 13. Relative errors in estimating the daily primary production in the water column on the basis of satellite data

No. of data	Arithmetic statistics		Logarithmic statistics			
	systematic error $<\varepsilon>$ [%]	statistical error σ_ε [%]	systematic error $<\varepsilon>_g$ [%]	standard error factor x	statistical error σ_- [%]	σ_+ [%]
81	2.00	60.6	−14.6	1.71	−41.7	71.7

4. Summary

In the course of the investigations presented in the two parts of this article (Part 1 – Woźniak et al. 2008, this issue), we worked out a number of detailed mathematical models and statistical regularities describing the transport of solar radiation in the atmosphere-sea system, its absorption in the water and its utilisation in the process of photosynthesis. This led to the derivation of the set of DESAMBEM algorithms, which enable a series of important parameters of the Baltic ecosystem, among others, the biotic and abiotic conditions prevailing in the Baltic and the state and functioning of its ecosystem, to be defined on the basis of available satellite information. The data yielded by the processing of satellite images in accordance with the DESAMBEM algorithm were compared with data obtained by means of in situ studies and measurements from on board ship. The two sets of data turned out to be very similar, as testified by the relatively small errors of estimation. We can therefore recommend the utilisation of satellite images to investigate different aspects of the Baltic ecosystem, such as the cleanliness of the waters and their degree of eutrophication. Our research has shown that with the aid of satellite data, a range of phenomena occurring in Baltic waters can be monitored. These data can therefore be used in the systematic construction of maps of the spatial distributions of many parameters indicating the state of this environment, including the sea surface temperature, surface and rising currents (upwelling events), the extent of penetration of riverine waters into the Baltic, water transparency, the radiation balance between the sea surface and the upper layers of the atmosphere, the intensity of UV radiation over the sea and in coastal areas, the distributions of Photosynthetically Available Radiation (PAR), the concentrations of chlorophyll and other pigments in the water, the efficiency of photosynthesis, the primary production of organic matter and release of oxygen, and the distribution of phytoplankton blooms (including that of toxic blue-green algae). In the future it will be possible to supply other essential information about the Baltic environment, e.g. for assessing pollution or monitoring environmental disasters such as spills of crude oil or other environmentally harmful substances.

We regard the current state of advancement of our modelling of light and photosynthesis in the Baltic and the derivation of algorithms for the remote diagnosis of the states of the Baltic ecosystem as satisfactory. The precision of these algorithms is in no way inferior to that of published algorithms applicable to other regions of the World Ocean (Campbell et al. 2002, Carr et al. 2006). The satellite methods of monitoring the state and functioning of the Baltic ecosystem, developed and presented here, are therefore ready to be applied in practice. Nonetheless, further specification of some of the blocks in the DESAMBEM algorithm set is possible and is included in our research plans.

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