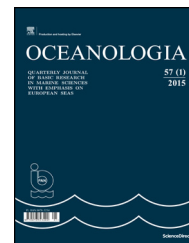




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ORIGINAL RESEARCH ARTICLE

# New simple statistical formulas for estimating surface concentrations of suspended particulate matter (SPM) and particulate organic carbon (POC) from remote-sensing reflectance in the southern Baltic Sea<sup>☆</sup>

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**Summary** In a step taken towards improving the new system for the satellite monitoring of the Baltic Sea environment, officially started in Poland recently (*SatBałtyk System*, see <http://www.satbaaltyk.pl>), a new set of simple statistical formulas was derived. These combine the empirically determined spectral values of remote-sensing reflectance  $R_{rs}(\lambda)$  with the mass concentrations of suspended particulate matter (SPM) and particulate organic carbon (POC) in southern Baltic surface waters. The new formulas are based on 73 empirical data sets gathered during 4 research cruises on board *r/v Oceania* during spring and late summer in the open waters of the southern Baltic and coastal regions of the Gulf of Gdańsk. Correlations of SPM and POC concentrations with reflectance or reflectance ratios in various spectral bands were tested. Several variants of candidate statistical relationships, which can be used later in the construction of simple local remote sensing algorithms for the waters in question, are introduced here. These relationships utilise either absolute values of  $R_{rs}$  at a selected waveband, mostly from the yellow, red or near

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infrared part of the light spectrum, or  $R_{rs}$  ratios for two different wavebands, mostly ratios of blue to yellow, blue to red and blue to infrared or green to yellow and green to red spectral band. From the numerous simple approximate relationships established, the following two, characterised by large correlation coefficients  $r^2$  and small standard error factors  $X$ , may serve as examples: SPM [ $\text{g m}^{-3}$ ] =  $1480(R_{rs}(710))^{0.902}$  (with the factors  $r^2 = 0.86$ ;  $X = 1.26$ ) (the unit of  $R_{rs}(\lambda)$  is [ $\text{sr}^{-1}$ ]) and POC [ $\text{g m}^{-3}$ ] =  $0.814(R_{rs}(555)/R_{rs}(589))^{-4.42}$  ( $r^2 = 0.75$ ;  $X = 1.37$ ). From the practical standpoint, taking into consideration light wavelengths that are close to or concurrent with the currently available spectral bands used in satellite observations of the Baltic Sea, another two formulas (using the same spectral ratio) are worth pointing out: SPM [ $\text{g m}^{-3}$ ] =  $2.6(R_{rs}(490)/R_{rs}(625))^{-1.29}$  ( $r^2 = 0.86$ ;  $X = 1.25$ ) and POC [ $\text{g m}^{-3}$ ] =  $0.774(R_{rs}(490)/R_{rs}(625))^{-1.18}$  ( $r^2 = 0.66$ ;  $X = 1.44$ ). The paper also presents a number of intermediate statistical relationships between SPM and POC concentrations,  $R_{rs}$  spectra and light backscattering coefficients in order to illustrate the simplified physical justification for some of the observed direct statistical relationships, presented as the main content of this work.

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## 1. Introduction

In recent decades there has been significant progress in passive remote-sensing techniques that retrieve information on seawater composition imprinted in the colour of oceans and seas (see, for example, a series of reports by [International Ocean-Colour Coordination Group – IOCCG Report 16 \(2015\)](#) or earlier reports and the references cited therein). To make full use of the potential of these techniques, there is obviously a need to mathematically relate the quantity that describes sea colour precisely, i.e. the remote-sensing reflectance, with the various biogeochemical characteristics describing the concentrations and composition of substances present in surface waters. In practice this can be done in many ways, either directly or indirectly by using the water's inherent optical properties (IOPs) as a “link” between the sea's colour and biogeochemistry. One of the biogeochemical characteristics most often studied with remote sensing techniques is the concentration of chlorophyll  $a$ , the quantity used as the basic measure of phytoplankton biomass. Other substances that are also important indicators of different processes taking place in seawater and at the same time influence its colour include phytoplankton pigments other than chlorophyll  $a$ , chromophoric dissolved organic matter (CDOM), suspended particulate matter (SPM) of both organic and inorganic origin, and the main chemical elements from which organic matter is constructed, e.g. carbon. Hence it is mainly the relationships between the concentrations of these substances/elements and the remote-sensing reflectance, often specific to particular seas, that are investigated.

The application of remote-sensing techniques in the Baltic region started in the 1970s (when the first oceanographic satellites became available) and has intensified in the last 20 years. This problem has been addressed by different scientific groups from many countries, not just from states around the Baltic Sea (detailed literature surveys on this topic can be found, for example, in book chapters by [Siegel and Gerth \(2008\)](#), [Berthon et al. \(2008\)](#) or [Kratzer et al. \(2011\)](#); see also [Arst \(2003\)](#)). The brackish waters of the semi-enclosed shelf basin of the Baltic Sea are optically very complex. These waters belong to a broad category of Case

2 waters (according to the classification of [Morel and Prieur \(1977\)](#)), the optical properties of which do not depend only on phytoplankton and its by-products. In Case 2 waters an important role may be also played by suspended matter and CDOM, which generally do not co-vary with chlorophyll  $a$  concentration. Indeed, Baltic waters are an exceptional example of Case 2 waters, since they are much richer in both allogenic and autogenic CDOM than other shelf seas (see e.g. [Kowalczyk \(1999\)](#)). Consequently, optical relationships, models and algorithms derived as being either universal/global, or even local but for other marine environments, are often unsuitable for Baltic Sea remote sensing (see e.g. a work by [Darecki and Stramski \(2004\)](#), in which the performances of different chlorophyll  $a$  algorithms in the Baltic Sea are compared). The derivation of local algorithms thus appears to be indispensable. In the last 10 years or so, the application of neural network algorithms has become a common practical approach to the remote sensing of the Baltic and other European seas (see e.g. [Doerffer and Schiller \(2006\)](#)). Such algorithms use the artificial neural network inversion procedure to derive various independently varying in-water constituents, such as chlorophyll  $a$  (or pigment index), SPM and CDOM. The input for such algorithms is usually multispectral information (specific to the satellite sensors under consideration) on either top of atmosphere radiances or remote sensing reflectances. Recent evaluations and comparisons of different variants of such algorithms applied to Baltic data acquired using a medium resolution imaging spectrometer (MERIS) can be found, for example, in [Beltran-Abaunza et al. \(2014\)](#) or [D'Alimonte et al. \(2014\)](#). Another observation from the literature survey may be that particulate organic carbon (POC) has not yet become a common ocean colour data product for the Baltic Sea region, despite the already demonstrated fact that SPM can be treated as its effective tracer ([Ferrari et al., 2003](#)).

In common with many other scientific groups and institutions working on the optics of Baltic Sea waters, a group of scientists from Poland has also been deeply involved in this topic in recent decades ([Dera and B. Woźniak, 2010](#) and the extensive list of citations therein). The Polish team has also undertaken comprehensive studies with the aim of developing

practical methods for the remote sensing of this demanding marine environment (see e.g. Darecki et al., 2008; B. Woźniak et al., 2008, 2011a,b; M. Woźniak et al., 2014). The *SatBaltyk System*<sup>1</sup>, a new complex system for the satellite monitoring of the Baltic Sea developed by this research team (B. Woźniak et al., 2011a,b), was officially inaugurated in Poland recently. In order to expand the set of its existing algorithm formulas, new studies focusing on different characteristics of suspended matter are being conducted by the authors of this and a previous paper (S.B. Woźniak, 2014). The latter paper presented the first set of simple local empirical formulas for the southern Baltic area. Among other things, these formulas enable the mass concentration of suspended particulate matter (SPM) or particulate organic carbon (POC) to be estimated as a function of selected seawater IOPs, such as the coefficient of light backscattering by suspended particles  $b_{bp}(\lambda)$  or the coefficient of light absorption by the sum of all substances suspended and dissolved in seawater  $a_n(\lambda)$ . Such formulas can be applied as the final step in a local empirical multistage algorithm for estimating the biogeochemical characteristics of suspended substances. Obviously, coefficients  $b_{bp}$  and/or  $a_n$  have first to be estimated from remote-sensing reflectance spectra  $R_{rs}(\lambda)$ . In the previous work (S.B. Woźniak, 2014) it was suggested that SPM and POC concentrations could be estimated in a relatively simple way as direct functions of  $R_{rs}(\lambda)$ , mostly for red wavelengths of light. But this suggestion was based solely on analyses of modelled reflectance spectra obtained as a result of simplified radiative energy transfer modelling. Moreover, these analyses were performed only for a limited number of light wavebands.

The main objective of the current work was to use the newly acquired empirical data to establish a new, improved set of statistical formulas that would enable SPM and also POC concentrations in southern Baltic Sea surface waters to be estimated simply and directly on the basis of spectral values of the remote-sensing reflectance  $R_{rs}(\lambda)$  at chosen wavelength or from reflectance spectral ratio. The  $R_{rs}(\lambda)$  data used for these analyses are determined from in situ optical measurements performed at over a dozen of spectral bands covering the range from UV, through visible, to near infrared. The analyses presented here are not limited only to the bands corresponding to current or past satellite sensors. On the contrary, all the available spectral information is used. The new simple statistical formulas established in this way, together with our earlier results (S.B. Woźniak et al., 2014), can later serve as elements for constructing new local empirical remote sensing algorithms.

<sup>1</sup> The *SatBaltyk System* has been developed within the framework of the project entitled “The Satellite Monitoring of the Baltic Sea Environment” (Project No. POIG.01.01.02-22-011/09). The project is being implemented within the framework of the Innovative Economy Operational Programme, Priority axis 1: Research and development of modern technologies, Action 1.1: Supported scientific research for the construction of a knowledge-based economy. Executors of the project are the Institute of Oceanology, Polish Academy of Sciences, Sopot (coordinator); the Institute of Oceanography, University of Gdańsk; the University of Szczecin; and the Pomeranian Academy, Słupsk.

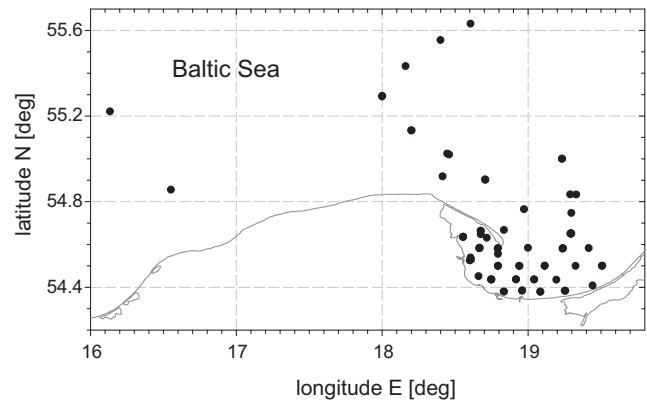


Figure 1 Location of the sampling stations in the southern Baltic Sea.

## 2. Material and methods

The empirical measurements used in this work were performed during 4 research cruises of *r/v Oceania* in spring and late summer (April and September 2011, September 2012 and May 2013), at 73 sampling stations. The positions of these sampling stations in the open waters of the southern Baltic Sea and in the Gulf of Gdańsk are shown in Fig. 1.

### 2.1. Analyses of SPM and POC concentrations

Discrete water samples for laboratory analyses of the biogeochemical properties of suspended matter were taken from the surface layer (ca 1 m depth) in 20 L Niskin bottles. In general, we applied the same laboratory methods as those we had used and described previously (see S.B. Woźniak et al. (2011, 2014)). The concentration of suspended particulate matter (SPM), defined as the dry mass of particles per unit volume of seawater and expressed in  $[g\ m^{-3}]$ , was determined using a standard gravimetric technique. We used specially prepared GF/F filters (25 mm diameter) pre-combusted at 450°C for 4 h, pre-washed with pure deionised and particle-free water (to prevent the loss of filter material during the filtration of the main sample), then dried and pre-weighed. Measured volumes of seawater (generally between 150 and 1000 mL) were filtered immediately after sample collection. At the end of filtration, the filters were rinsed with about 30 mL of deionised water to remove sea salt (the salinity of our samples was on average 6.7, and did not exceed 7.3). The filters together with their particle load were dried and stored in a freezer for later analysis at the land-based laboratory. The dry mass of particles collected on the filters was measured with a Radwag WAX110 microbalance (resolution 0.01 mg). Three replicate filters were measured in each sample. The reproducibility of replicates (defined as the ratio of the standard deviation to the average value and expressed as a percentage) was on average 6%; for 90% of individual samples it was no greater than 13%.

The concentration of particulate organic carbon (POC), expressed in  $[g\ m^{-3}]$ , was determined by high temperature combustion. Samples were collected at sea by filtration in the same way as for the SPM analyses, by using separate sets of pre-combusted GF/F filters (three replicates per water sample). The filters were dried and stored until later analysis at

the land-based laboratory with a Perkin Elmer CHN 2400 instrument. The reproducibility of the POC replicate measurements was on average 11%; for 90% of individual samples it was no greater than 26%.

## 2.2. Determination of remote-sensing reflectance

Values of the remote-sensing reflectance  $R_{rs}(\lambda)$  [ $\text{sr}^{-1}$ ] were obtained from vertical profiles of the spectral upward radiance  $L_u(z, \lambda)$  (measured in water) and the spectral downward irradiance  $E_d(0^+, \lambda)$  (above the sea surface) measured simultaneously. These quantities were measured in 17 spectral channels (centred at wavelengths  $\lambda$  of 340, 380, 395, 412, 443, 465, 490, 510, 532, 555, 565, 589, 625, 665, 683, 710 and 765 nm) with a Compact Optical Profiling System (C-OPS) (Biospherical Instruments Inc.).  $R_{rs}(\lambda)$  was calculated as the ratio of the water-leaving radiance just above the water surface  $L_w(0^+, \lambda)$  to the downward irradiance measured above the water  $E_d(0^+, \lambda)$ . The water-leaving radiance  $L_w(0^+, \lambda)$  was obtained from estimated values of the upward radiance just below the water surface  $L_u(0^-, \lambda)$ , which were propagated through the water–air interface using a factor of 0.544 calculated from the “ $n^2$  law for radiance” (see e.g. Mobley (1994)). Thus, the practical formula for  $R_{rs}(\lambda)$  is as follows:

$$R_{rs}(\lambda) = \frac{L_w(0^+, \lambda)}{E_d(0^+, \lambda)} = 0.544 \frac{L_u(0^-, \lambda)}{E_d(0^+, \lambda)}. \quad (1)$$

To obtain  $L_u(0^-, \lambda)$ , measurements of the profiles of upwelling radiance  $L_u(z, \lambda)$  were extrapolated from a subsurface layer of 0.5–2 m to a depth “just below the sea surface” (“0<sup>-</sup>”) using the attenuation coefficient for upward radiance  $K_{Lu}(z, \lambda)$ , calculated as the local slope of  $\ln[L_u(z, \lambda)]$  measured over a depth interval spanning a few metres in the surface layer. The thickness of this depth interval depended on the extent to which the surface layer was homogeneous (typically about 3 m). The correction for the self-shading effect in the upward radiance just below the sea surface  $L_u(0^-, \lambda)$  was also applied to all data according to Gordon and Ding (1992) and Zibordi and Ferrari (1995). The C-OPS system was equipped with a shadow band radiometer, and ratios of the direct to diffuse light used in the self-shading corrections were determined using this system as well.

## 2.3. Light backscattering measurements

The light backscattering coefficients of  $b_b(\lambda)$  [ $\text{m}^{-1}$ ] were estimated from in situ measurements performed in the surface layer (ca 1 m depth) using a spectral backscattering meter (HOBI Labs Hydroscat-4 instrument) at four light wavelengths (420, 488, 550 and 620 nm). The raw data from the instrument, i.e. the volume scattering functions at an angle of 140°, were used for estimating  $b_b(\lambda)$  according to the method described in Maffione and Dana (1997) and Dana and Maffione (2002). A correction for the incomplete recovery of backscattered light in highly attenuating waters (the so-called sigma-correction) was applied in accordance with the instrument User’s Manual (HOBI Labs, 2008) using data on absorption and attenuation coefficients measured with a separate instrument (WET Labs ac-9). To obtain the backscattering coefficients of particles,  $b_{bp}(\lambda)$  [ $\text{m}^{-1}$ ], the

theoretical values of the backscattering coefficient of pure water were subtracted according to Morel (1974).

## 2.4. Measurements of additional biogeochemical parameters

This work also refers to biogeochemical parameters describing the variability of the seawater samples other than SPM and POC concentrations. They are the concentration of the organic fraction of SPM, i.e. particulate organic matter (POM) and the concentration of the main photosynthetic pigment, chlorophyll *a* (Chl *a*) (additional measurements also followed protocols described in more detail in S.B. Woźniak et al. (2011)). To determine the POM concentration, the same GF/F filters utilised earlier for SPM concentration analyses were placed in a furnace, kept there for 4 h at a temperature of 450°C and then re-weighed. The POM concentration was calculated from the loss of mass of the sample retained by the filter. Here, the total chlorophyll *a* concentration (Chl *a*) was represented by the sum of chlorophyll *a*, allomer and epimer, chlorophyllide *a* and phaeophytin *a*; it was determined with the use of high performance liquid chromatography (HPLC).

## 2.5. Statistical analyses

The empirical data were statistically analysed, as a result of which approximate relationships between the target quantities were obtained. These simple relationships take the form of best-fit power functions ( $y = C_1 x^{C_2}$ ), found using least square linear regression applied to log-transformed variables. For each formula established in this way we give the square of the correlation coefficient  $r^2$  calculated for log-transformed variables and also a set of the standard statistical descriptors of estimation errors, such as the root mean square error between observed and predicted values (RMSE), the mean normalised bias (MNB) and the normalised root mean square error (NRMSE). All these standard descriptors will be given later in the relevant tables for readers who would like to compare our results with others published in the literature. But since the fitting was performed on log-transformed variables, when discussing the quality of the fit we also present and pay special attention to another statistical quantity, the standard error factor  $X$ . Being an element of so-called logarithmic statistics, this can be determined according to the formula:

$$X = 10^{\sigma_{\log}}; \sigma_{\log} = \left[ \frac{1}{n-1} \sum_{i=1}^n \left( \log \left( \frac{P_i}{O_i} \right) - \frac{1}{n} \sum_{j=1}^n \log \left( \frac{P_j}{O_j} \right) \right)^2 \right]^{1/2}, \quad (2)$$

where  $P_i$  stands for values predicted using the approximate formula,  $O_i$  represents empirical values and  $n$  is the number of samples. The standard error factor  $X$  allows one to quantify the range of the statistical error calculated according to logarithmic statistics. This range extends from the value of  $\sigma_- = (1/X) - 1$  to the value of  $\sigma_+ = X - 1$ . Note also, that because of the method used for data approximation (linear regression applied to the log-transformed variables), the systematic error according to logarithmic statistics is always equal to 0; for this reason we make no further mention of it.

**Table 1** Variability ranges of selected biogeochemical characteristics of suspended particulate matter in surface water samples and selected optical properties of water at stations from the southern Baltic Sea analysed in this paper.

Quantity	Minimum value	Maximum value	Average value	Standard deviation (coefficient of variation)	Number of samples
SPM [ $\text{g m}^{-3}$ ]	0.568	9.81	1.77	1.59 (90%)	73
POC [ $\text{g m}^{-3}$ ]	0.145	2.37	0.555	0.438 (79%)	73
POM [ $\text{g m}^{-3}$ ]	0.447	5.39	1.41	0.961 (68%)	73
Chl <i>a</i> [ $\text{mg m}^{-3}$ ]	0.442	36.1	5.79	7.39 (128%)	71
POC/SPM [g:g]	0.16	0.563	0.322	0.073 (23%)	73
POM/SPM [g:g]	0.506	1.05	0.859	0.127 (15%)	73
Chl <i>a</i> /SPM [g:g]	$6.94 \times 10^{-4}$	$9.19 \times 10^{-3}$	$3.02 \times 10^{-3}$	$1.56 \times 10^{-3}$ (52%)	71
$b_{bp}(488)$ [ $\text{m}^{-1}$ ]	$2.7 \times 10^{-3}$	$8.58 \times 10^{-2}$	$1.27 \times 10^{-2}$	$1.27 \times 10^{-2}$ (100%)	73
$b_{bp}(620)$ [ $\text{m}^{-1}$ ]	$2.06 \times 10^{-3}$	$8.17 \times 10^{-2}$	$1.03 \times 10^{-2}$	$1.19 \times 10^{-2}$ (115%)	73
$R_{rs}(490)$ [ $\text{sr}^{-1}$ ]	$1.12 \times 10^{-3}$	$2.84 \times 10^{-3}$	$1.71 \times 10^{-3}$	$3.47 \times 10^{-4}$ (20%)	73
$R_{rs}(625)$ [ $\text{sr}^{-1}$ ]	$4.12 \times 10^{-4}$	$5.12 \times 10^{-3}$	$1.19 \times 10^{-3}$	$7.44 \times 10^{-4}$ (62%)	73
$R_{rs}(710)$ [ $\text{sr}^{-1}$ ]	$1.63 \times 10^{-4}$	$4.11 \times 10^{-3}$	$5.81 \times 10^{-4}$	$6.08 \times 10^{-4}$ (105%)	73

### 3. Results and discussion

#### 3.1. General characterisation of the empirical dataset

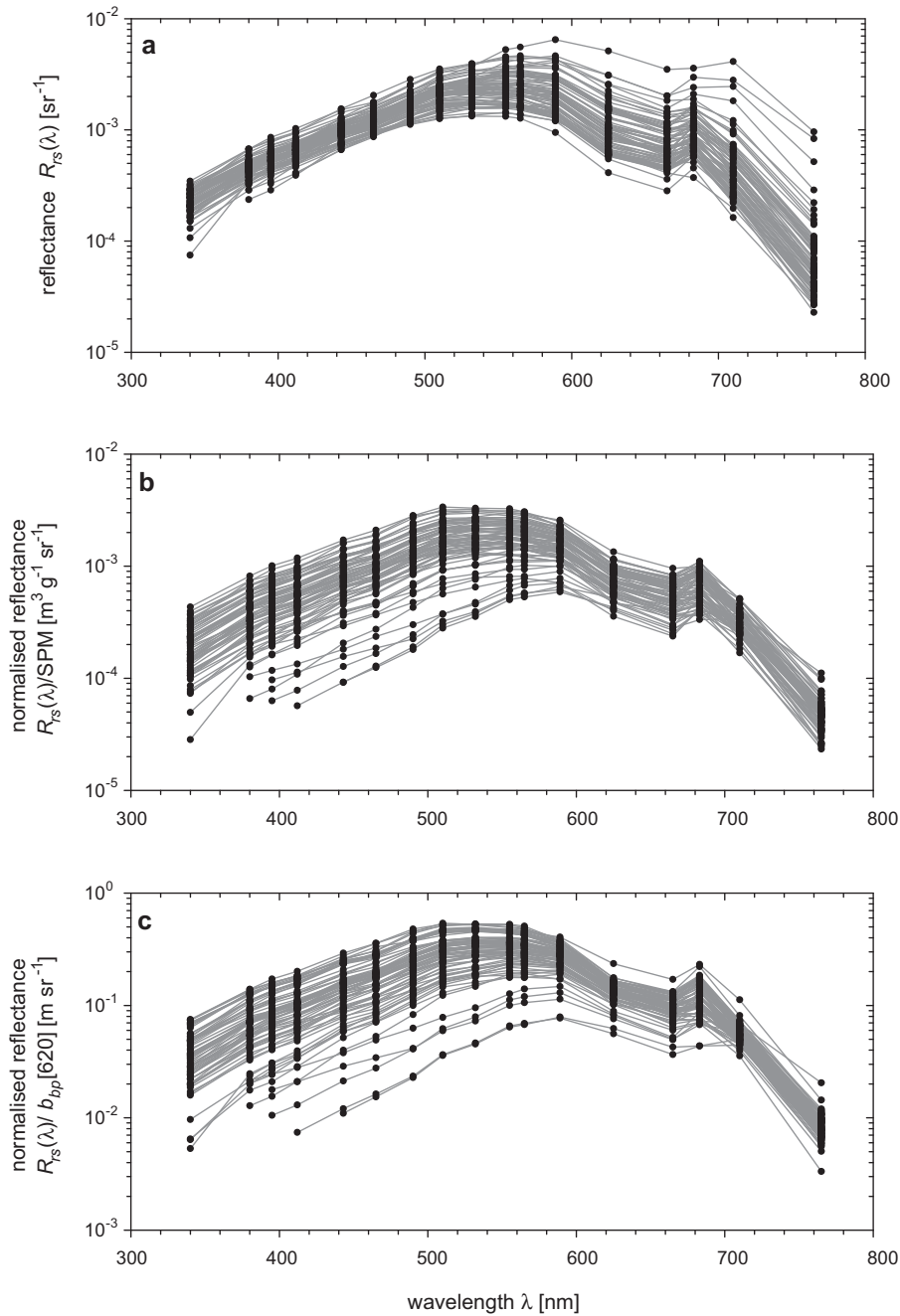
The empirical material, though not large in terms of sample number ( $n = 73$ ) and having been acquired only in spring and late summer, is characterised by a relatively large variability in the target biogeochemical and optical quantities (see Table 1) (this is undoubtedly a consequence of measurements and water sampling performed over different coastal and open sea areas). Both the absolute mass concentration of suspended particulate matter (SPM) and the concentration of organic carbon (POC), the latter an important constituent of the organic fraction of suspended matter, varied over more than one order of magnitude in terms of the maximum to minimum range. The corresponding coefficients of variation CV (defined as the ratio of the standard deviation to the average value) were 90% for SPM and 79% for POC. The concentration of chlorophyll *a* (Chl *a*) in our samples varied even more: the CV was almost 130%. In contrast, the changes in the proportions (ratios) of these biogeochemical quantities were relatively small. Such ratios may help to characterise the variability in suspended matter composition. For example, the average ratio of POC to SPM was 0.32, but its variability, characterised by CV, was only 23%. In the case of the POM to SPM ratio, the average value was 0.86, and the corresponding CV was 15%. These values show that in all the water samples, SPM was dominated by matter of organic origin. This is characteristic of the surface waters of the southern Baltic Sea (see e.g. S.B. Woźniak et al. (2011)). The variability of the optical quantities was also significant: that of the backscattering coefficients of particles  $b_{bp}(\lambda)$  was substantial over the entire spectral range. For  $\lambda = 488$  nm the maximum to minimum variation was more than 30-fold, while for  $\lambda = 620$  nm it was more than 40-fold. The corresponding CVs were 100% and 115% respectively. The variability of the remote-sensing reflectance  $R_{rs}(\lambda)$ , a quantity influenced by both suspended and dissolved substances in seawater, was spectrally diverse: it was the smallest in the bands of the blue part of the spectrum (e.g. CV = 20% for  $R_{rs}(490)$ ), and distinctively larger in the bands of the red and infrared parts of

the spectrum (e.g. CV of 62% for  $R_{rs}(625)$  and 105% for  $R_{rs}(710)$ ). The complete set of remote-sensing reflectance spectra that we registered in the southern Baltic Sea is presented in Fig. 2a. An important observation regarding the nature of the spectral variability of  $R_{rs}(\lambda)$  may be made if we normalise the values of that quantity by dividing them by SPM concentration or the coefficient  $b_{bp}$ . Two sets of curves normalised in this way are presented in panels b and c in Fig. 2. While the absolute values of  $R_{rs}(\lambda)$  varied mostly in the  $\lambda > 600$  nm range, the variability of the normalised curves within that spectral range was the smallest. For example, the CVs calculated for the normalised value of  $R_{rs}(\lambda)/\text{SPM}$  at bands 625 and 710 nm were only 27% and 23%, whereas at 490 nm CV was as high as 45%. All this generally agrees with the qualitative expectation that in the spectral range of red and infrared light, the SPM concentration should exert the greatest influence on the absolute values of reflectance  $R_{rs}$  (through light backscattering), whereas the influence of light absorption by CDOM in this spectral range is small and negligible. Hence, the spectral bands from the red and infrared parts of the spectrum should be the most suitable for establishing simple statistical relationships between  $R_{rs}$  and  $b_{bp}$  or SPM concentration.

#### 3.2. Statistical formulas

The statistical analyses yielded two separate sets of several different spectral variants of formulas, which enable the SPM and POC concentrations to be roughly estimated on the basis of either the absolute values of remote-sensing reflectance or the reflectance ratios at two spectral bands. These formulas are presented in tabular form and will be discussed in detail later in the text. At this point, it should be mentioned that these tables contain not only the best spectral variants from the statistical point of view, but also other ones, slightly inferior but still, we believe, acceptably accurate. This has been done deliberately, in order to give potential users of our formulas the opportunity to select the spectral variant in accordance with the measurement or data collection techniques that are available to them.

Table 2 contains formulas that permit a rough estimate of SPM and POC concentrations based on absolute values of the



**Figure 2** Empirically derived spectra of remote-sensing reflectance  $R_{rs}(\lambda)$  (a) and the same spectra normalised to values of SPM (b) or  $b_{bp}(620)$  (c) for all ( $n = 73$ ) the sampling stations analysed in this work.

remote-sensing reflectance  $R_{rs}(\lambda_i)$  at the chosen spectral band. The different spectral variants in Table 2 all satisfy the following condition: the correlation coefficient  $r^2$  calculated for the relationship between the logarithms of the empirical variables under consideration (e.g. between  $\log(\text{SPM})$  and  $\log(R_{rs}(555))$ ) has to be equal to or greater than 0.5. Based on this criterion, we obtained a listing suggesting that for rough estimates of the SPM concentration one can use as many as 8 of the 17 spectral bands analysed. These are all bands available from the 555–765 nm range. The corresponding standard error factors  $X$  for these formulas range from 1.26 to 1.51. The same criterion applied to POC vs.  $R_{rs}(\lambda_i)$  relationships leads to the selection of only 4 spectral

variants, which use bands of 589, 625, 710 and 765 nm. The standard error factors  $X$  for the latter formulas lie between 1.47 and 1.53. Four examples selected from among all the formulas in Table 2 are presented graphically in Fig. 3. The first two examples (Fig. 3a and c) represent formulas using the spectral band at 710 nm. These formulas have the highest correlation coefficients  $r^2$  and the lowest standard error factors  $X$  within each group:

$$\text{SPM} = 1480(R_{rs}(710))^{0.902} \quad (r^2 = 0.86; X = 1.26), \quad (3)$$

$$\text{POC} = 222(R_{rs}(710))^{0.807} \quad (r^2 = 0.63; X = 1.47). \quad (4)$$

**Table 2** The best-fit power functions ( $y = C_1 x^{C_2}$ ) between the concentration of suspended particulate matter SPM or the concentration of particulate organic carbon POC and the absolute magnitude of remote-sensing reflectance  $R_{rs}(\lambda)$  for different spectral bands. The square of the correlation coefficient  $r^2$  (between the log-transformed variables), root mean square error RMSE<sup>a</sup>, mean normalised bias MNB<sup>b</sup>, normalised root mean square error NRMSE<sup>c</sup>, standard error factor  $X$  and number of samples  $n$  are also given for each fitted function. Examples discussed in more detail in the text are marked in bold.

Relationship	$C_1$	$C_2$	$r^2$	RMSE [ $\text{g m}^{-3}$ ]	MNB [%]	NRMSE [%]	$X$	$n$
SPM vs. $R_{rs}(555)$	$7.52 \times 10^3$	1.42	0.54	1.23	7.9	39.3	1.51	73
SPM vs. $R_{rs}(565)$	$7.66 \times 10^5$	1.42	0.60	1.15	7.0	37.6	1.47	73
SPM vs. $R_{rs}(589)$	$4.94 \times 10^3$	1.32	0.74	0.915	4.7	31.4	1.36	73
<b>SPM vs. <math>R_{rs}(625)</math></b>	$2.51 \times 10^3$	1.09	<b>0.78</b>	0.72	3.9	28.8	<b>1.33</b>	73
SPM vs. $R_{rs}(665)$	$4.22 \times 10^3$	1.11	0.72	0.813	4.9	32.1	1.38	73
SPM vs. $R_{rs}(683)$	$7.33 \times 10^3$	1.23	0.73	0.697	4.9	32.3	1.37	73
<b>SPM vs. <math>R_{rs}(710)</math></b>	$1.48 \times 10^3$	0.902	<b>0.86</b>	0.383	3.6	22.9	<b>1.26</b>	73
SPM vs. $R_{rs}(765)$	$2 \times 10^3$	0.754	0.83	0.502	3.0	24.5	1.29	73
POC vs. $R_{rs}(589)$	$6.97 \times 10^2$	1.19	0.55	0.3	9.6	51.8	1.53	73
<b>POC vs. <math>R_{rs}(625)</math></b>	$3.46 \times 10^2$	0.97	<b>0.57</b>	0.281	9.1	50.1	<b>1.51</b>	73
<b>POC vs. <math>R_{rs}(710)</math></b>	$2.22 \times 10^2$	0.807	<b>0.63</b>	0.239	7.6	43.0	<b>1.47</b>	73
POC vs. $R_{rs}(765)$	$2.85 \times 10^2$	0.672	0.61	0.246	8.0	44.3	1.49	73

$$^a \text{RMSE} = \left[ \frac{1}{n-1} \sum_{i=1}^n (P_i - O_i)^2 \right]^{1/2}$$

$$^b \text{MNB} = \frac{1}{n} \sum_{i=1}^n \left( \frac{P_i - O_i}{O_i} \right)$$

$$^c \text{NRMSE} = \left[ \frac{1}{n-1} \sum_{i=1}^n \left( \frac{P_i - O_i}{O_i} - \text{MNB} \right)^2 \right]^{1/2} \text{ where } P_i \text{ and } O_i \text{ are predicted and observed values, respectively.}$$

The other two examples represent the 625 nm band (Fig. 3b and d). They have slightly inferior statistical parameters compared to formulas (3) and (4) but are still the best if we consider only the visible part of the light spectrum:

$$\text{SPM} = 2510(R_{rs}(625))^{1.09} \quad (r^2 = 0.78; X = 1.33), \quad (5)$$

$$\text{POC} = 346(R_{rs}(625))^{0.97} \quad (r^2 = 0.57; X = 1.51). \quad (6)$$

The other form of the simple formulas we have determined here are the formulas for estimating SPM and POC concentrations based on the so-called colour ratios, i.e. ratios of  $R_{rs}$  values at two spectral bands ( $R_{rs}(\lambda_i)/R_{rs}(\lambda_j)$ ). The colour ratios are often used in satellite data processing. If the bands are appropriately chosen, more information on the optical properties of seawater constituents “concealed” in the signal reaching the satellite sensor can be used, and also, the influence of potential errors resulting from imperfect atmospheric corrections is minimised to some extent. The available empirical material contained  $R_{rs}(\lambda_i)$  data for 17 different spectral bands: 136 different combinations of the  $R_{rs}(\lambda_i)/R_{rs}(\lambda_j)$  ratio (where  $\lambda_j > \lambda_i$ ) could thus be analysed. For all of these combinations we calculated the correlation coefficients  $r^2$  for the relationships between the logarithms of SPM or POC concentration and the logarithms of  $R_{rs}(\lambda_i)/R_{rs}(\lambda_j)$ . With the  $r^2$  values, additionally presented here in Tables 3 and 4, a group of “statistically promising” spectral combinations of bands was chosen at which the approximate formulas could be established. A selection of the best candidate formulas is presented in Table 5. Among these formulas are 12 variants from which the SPM concentration can be estimated. They have correlation coefficients  $r^2$  ranging between 0.84 and 0.89, and standard error factors

$X$  from 1.23 to 1.28. These formulas generally use ratios of the reflectance at blue or green bands (443, 465, 490, 510 or 532 nm) to the reflectance at either yellow (589 nm), red (625 nm) or infrared (710 nm) bands. With regard to the formulas for estimating POC concentration, another 12 promising examples are presented in the lower part of Table 2. These examples have lower correlation coefficients  $r^2$ , in the range between 0.66 and 0.75, and higher standard error factors  $X$ , ranging from 1.37 to 1.45. Apart from the formulas that use a combination of spectral bands similar to that for estimating SPM concentration, a few different formulas have also appeared in this group. The latter formulas use the following bands in the spectral ratio numerator: 555, 565 and 683 nm (see the last four rows in Table 5). Four examples from the 24 formulas in Table 5 are presented in Fig. 4. The first two examples (Fig. 4a and c) represent two formulas that are characterised by the best statistical parameters within each group:

$$\text{SPM} = 0.95(R_{rs}(490)/R_{rs}(589))^{-1.74} \quad (r^2 = 0.89; X = 1.23), \quad (7)$$

$$\text{POC} = 0.814(R_{rs}(555)/R_{rs}(589))^{-4.42} \quad (r^2 = 0.75; X = 1.37). \quad (8)$$

The other two examples (Fig. 4b and d) are arbitrarily chosen formulas that use the reflectance ratio of  $R_{rs}(490)/R_{rs}(625)$ :

$$\text{SPM} = 2.6(R_{rs}(490)/R_{rs}(625))^{-1.29} \quad (r^2 = 0.86; X = 1.25), \quad (9)$$

$$\text{POC} = 0.774(R_{rs}(490)/R_{rs}(625))^{-1.18} \quad (r^2 = 0.66; X = 1.44). \quad (10)$$





**Table 4** The correlation coefficients  $r^2$  calculated for the relationships between log-transformed POC and the log-transformed spectral remote-sensing reflectance ratio of  $R_{rs}(\lambda_i)/R_{rs}(\lambda_j)$ . Examples of the relatively high  $r^2$  values are marked in bold.

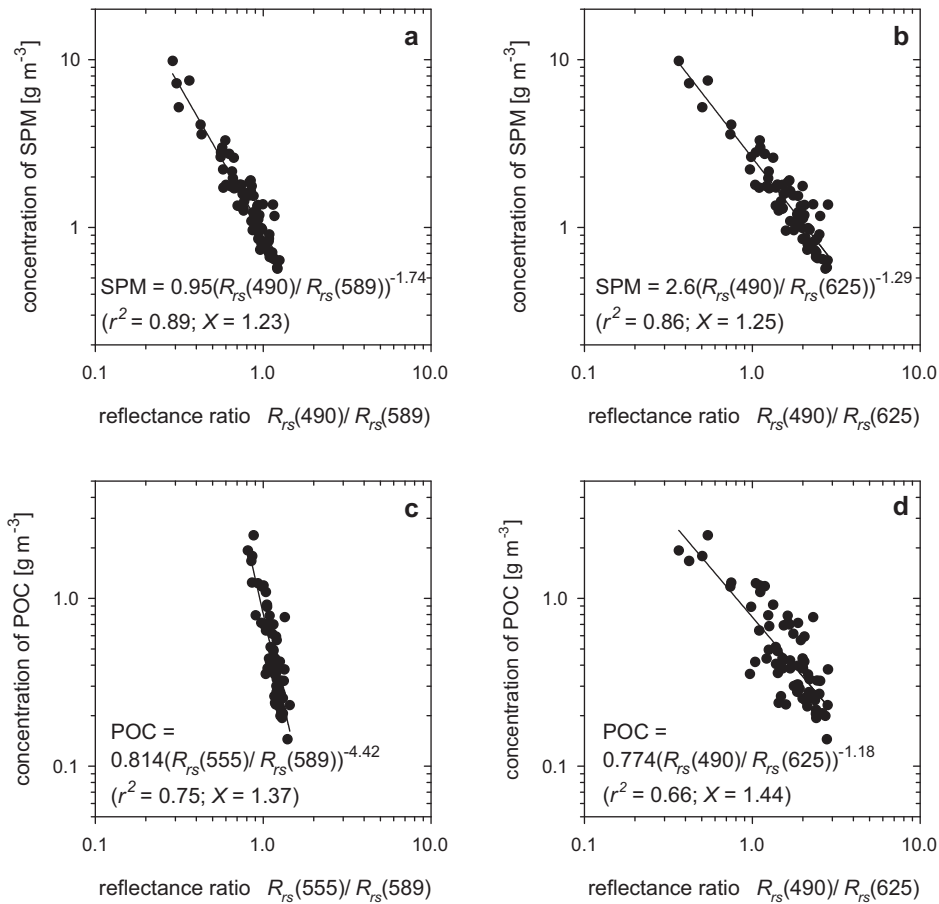
$\lambda_i$ [nm]	$\lambda_j$ [nm]															
	380	395	412	443	465	490	510	532	555	565	589	625	665	683	710	765
340 ( $n = 65$ )	0.12	0.13	0.11	0.07	0.06	0.07	0.12	0.15	0.18	0.19	0.30	0.30	0.24	0.21	0.35	0.34
380 ( $n = 69$ )	–	0.04	0.04	0.02	0.02	0.04	0.10	0.15	0.21	0.24	0.38	0.38	0.30	0.27	0.44	0.43
395 ( $n = 71$ )		–	0.01	0.01	0.01	0.02	0.10	0.16	0.26	0.29	0.44	0.45	0.37	0.35	0.53	0.52
412 ( $n = 72$ )			–	0.01	0.01	0.03	0.16	0.25	0.35	0.38	0.52	0.53	0.44	0.41	0.58	0.57
443 ( $n = 73$ )				–	0.03	0.10	0.37	0.45	0.52	0.54	<b>0.66</b>	0.63	0.55	0.47	0.63	0.61
465 ( $n = 73$ )					–	0.05	0.37	0.52	0.59	0.61	<b>0.72</b>	<b>0.67</b>	0.59	0.50	<b>0.66</b>	0.63
490 ( $n = 73$ )						–	0.61	0.61	0.60	0.61	<b>0.71</b>	<b>0.66</b>	0.57	0.45	0.63	0.61
510 ( $n = 73$ )							–	0.44	0.51	0.53	<b>0.68</b>	0.63	0.52	0.36	0.60	0.57
532 ( $n = 73$ )								–	0.51	0.54	<b>0.72</b>	0.65	0.52	0.33	0.60	0.57
555 ( $n = 73$ )									–	0.55	<b>0.75</b>	<b>0.66</b>	0.46	0.19	0.58	0.55
565 ( $n = 73$ )										–	<b>0.70</b>	0.63	0.40	0.14	0.57	0.53
589 ( $n = 73$ )											–	0.45	0.08	0.00	0.47	0.44
625 ( $n = 73$ )												–	0.39	0.17	0.39	0.38
665 ( $n = 73$ )													–	0.04	0.56	0.49
683 ( $n = 73$ )														–	<b>0.68</b>	0.58
710 ( $n = 73$ )															–	0.21

**Table 5** The best-fit power functions ( $y = C_1 x^{C_2}$ ) between the concentration of suspended particulate matter SPM or the concentration of particulate organic carbon POC and the remote-sensing reflectance ratios  $R_{rs}(\lambda_i)/R_{rs}(\lambda_j)$ . The statistical parameters (as in Table 2) are also given for each fitted function. Examples discussed in more detail in the text are marked in bold.

Relationship	$C_1$	$C_2$	$r^2$	RMSE [ $\text{g m}^{-3}$ ]	MNB [%]	NRMSE [%]	X	n
SPM vs. $R_{rs}(443)/R_{rs}(589)$	0.438	–1.52	0.84	0.625	2.7	22.9	1.27	73
SPM vs. $R_{rs}(443)/R_{rs}(625)$	1.3	–1.17	0.84	0.582	2.8	23.1	1.28	73
SPM vs. $R_{rs}(443)/R_{rs}(710)$	2.79	–0.885	0.84	0.492	2.8	23.4	1.28	73
SPM vs. $R_{rs}(465)/R_{rs}(589)$	0.559	–1.65	0.86	0.616	2.5	22.1	1.26	73
SPM vs. $R_{rs}(465)/R_{rs}(625)$	1.68	–1.25	0.85	0.527	2.6	22.0	1.26	73
SPM vs. $R_{rs}(465)/R_{rs}(710)$	3.49	–0.925	0.84	0.458	2.3	23.1	1.27	73
<b>SPM vs. <math>R_{rs}(490)/R_{rs}(589)</math></b>	0.95	–1.74	<b>0.89</b>	0.483	2.0	19.7	<b>1.23</b>	73
<b>SPM vs. <math>R_{rs}(490)/R_{rs}(625)</math></b>	2.60	–1.29	<b>0.86</b>	0.429	2.4	21.5	<b>1.25</b>	73
SPM vs. $R_{rs}(510)/R_{rs}(589)$	1.42	–2.11	0.87	0.536	2.4	21.5	1.25	73
SPM vs. $R_{rs}(510)/R_{rs}(625)$	3.98	–1.48	0.84	0.434	2.8	23.5	1.27	73
SPM vs. $R_{rs}(532)/R_{rs}(589)$	1.78	–2.64	0.87	0.512	2.4	21.7	1.25	73
SPM vs. $R_{rs}(532)/R_{rs}(625)$	5.46	–1.71	0.84	0.41	2.9	24.1	1.28	73
POC vs. $R_{rs}(443)/R_{rs}(589)$	0.151	–1.4	0.66	0.265	6.7	38.1	1.45	73
POC vs. $R_{rs}(465)/R_{rs}(589)$	0.183	–1.57	0.72	0.242	5.5	34.0	1.4	73
POC vs. $R_{rs}(465)/R_{rs}(625)$	0.52	–1.16	0.67	0.253	6.4	37.1	1.44	73
POC vs. $R_{rs}(465)/R_{rs}(710)$	1.02	–0.854	0.66	0.247	6.5	36.3	1.45	73
POC vs. $R_{rs}(490)/R_{rs}(589)$	0.306	–1.63	0.71	0.218	5.6	34.3	1.4	73
<b>POC vs. <math>R_{rs}(490)/R_{rs}(625)</math></b>	0.774	–1.18	<b>0.66</b>	0.236	6.7	38.3	<b>1.44</b>	73
POC vs. $R_{rs}(510)/R_{rs}(589)$	0.445	–1.95	0.68	0.218	6.2	36.4	1.43	73
POC vs. $R_{rs}(532)/R_{rs}(589)$	0.554	–2.51	0.72	0.205	5.4	33.7	1.4	73
<b>POC vs. <math>R_{rs}(555)/R_{rs}(589)</math></b>	0.814	–4.42	<b>0.75</b>	0.205	4.7	30.6	<b>1.37</b>	73
POC vs. $R_{rs}(555)/R_{rs}(625)$	2.84	–2.22	0.66	0.241	6.9	40.0	1.45	73
POC vs. $R_{rs}(565)/R_{rs}(589)$	0.826	–5.32	0.7	0.24	5.6	33.9	1.41	73
POC vs. $R_{rs}(683)/R_{rs}(710)$	2.14	–2.17	0.68	0.234	6.6	40.0	1.43	73

These latter formulas, although characterised by statistical parameters inferior to formulas (7) and (8), use spectral bands which are close to or concurrent with bands potentially available for satellite observations of the southern Baltic Sea

(compare, for example, with the spectral bands of MODIS Aqua/Terra). But obviously, the final choice of spectral variants from the different formulas listed in Table 5 should depend on the demands and constraints of potential future users.

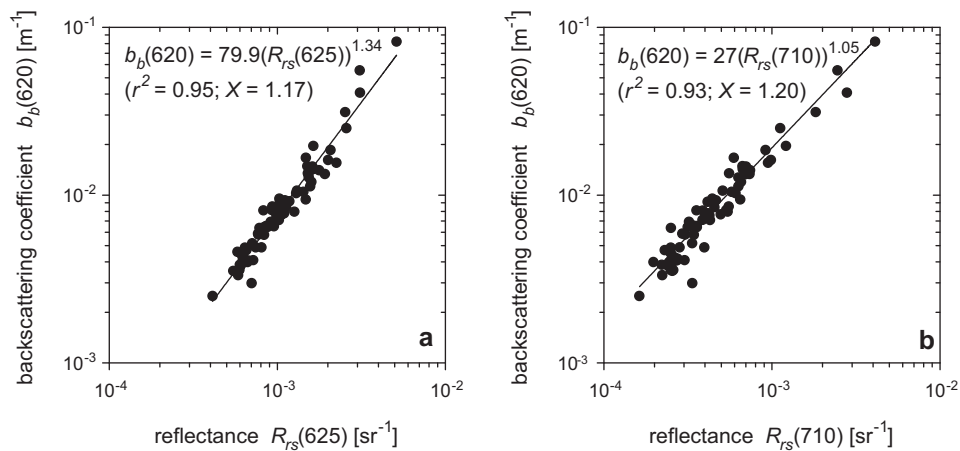


**Figure 4** Examples of empirical relationships between: (a) SPM concentration and the remote-sensing reflectance ratio of  $R_{rs}(490)/R_{rs}(589)$ ; (b) SPM and  $R_{rs}(490)/R_{rs}(625)$ ; (c) POC and  $R_{rs}(555)/R_{rs}(589)$ ; and (d) POC and  $R_{rs}(490)/R_{rs}(625)$ . The black lines represent the best-fit power functions; the formulas and the statistical parameters are given in each panel. For further similar formulas for other spectral variants of remote-sensing reflectance ratios, see Table 5.

### 3.3. Discussion

One can give a simplified physical explanation for some of the formulas presented above, i.e. those which use absolute reflectance values from the red and near infrared spectral

bands, and illustrate it with examples of intermediate statistical relationships. Such relationships between the target quantities and the coefficients describing light backscattering in seawater are presented in the next two figures. Fig. 5 illustrates two correlations between  $R_{rs}(710)$  or  $R_{rs}(625)$  and

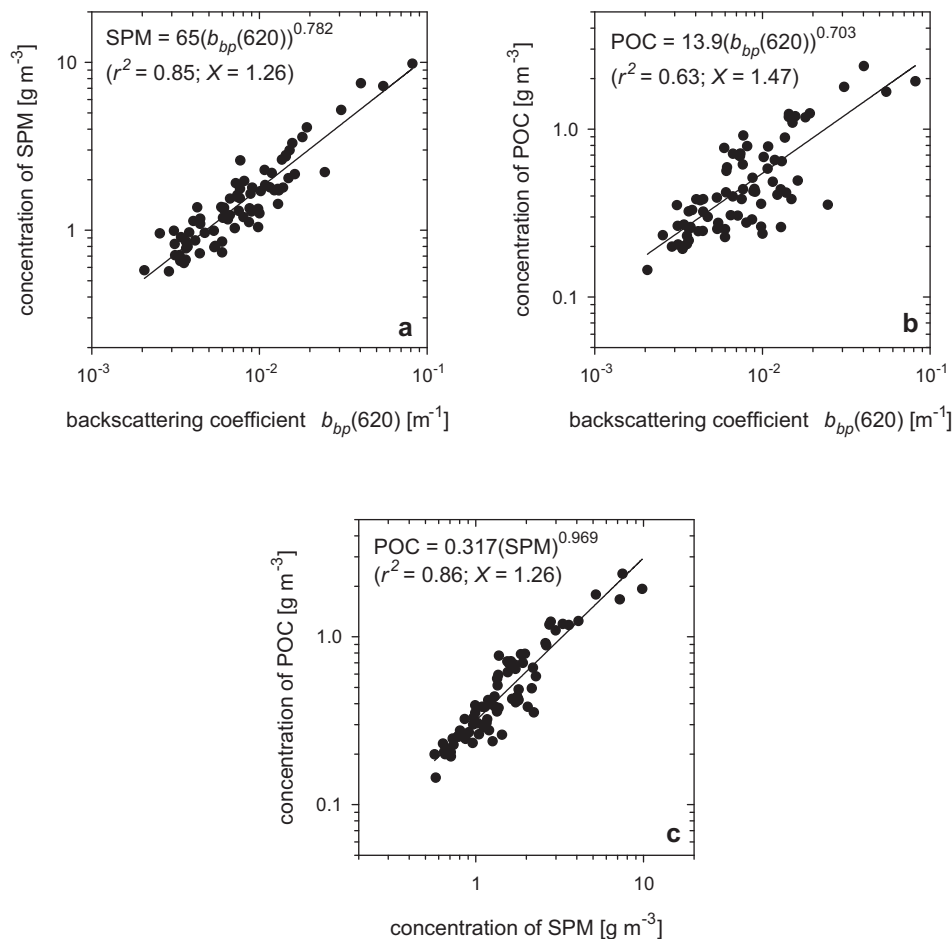


**Figure 5** Examples of empirical relationships between the light backscattering coefficient  $b_b(620)$  and the remote-sensing reflectance  $R_{rs}$  for spectral bands (a) 625 nm and (b) 710 nm. The black lines represent the best-fit power functions; the formulas and the statistical parameters are given in each panel.

light backscattering coefficients in seawater measured in situ at the closest spectral band, i.e.  $b_b(620)$  (the approximation formulas of these relationships are shown in the panels in Fig. 5). The appearance of such correlations is in general agreement with the well-known approximate relation linking  $R_{rs}(\lambda)$  with seawater IOPs, which takes the form:  $R_{rs}(\lambda) \propto b_b(\lambda)/(a(\lambda) + b_b(\lambda))$  (see e.g. Gordon et al., 1988; Lee et al., 1996). Obviously, the light absorption coefficients in seawater  $a(\lambda)$  in the bands from the red and infrared parts of the spectrum are mainly dominated by absorption due to pure molecular water. Hence, this relationship for the particular bands under consideration can be reduced to  $R_{rs}(\lambda) \propto b_b(\lambda)$ . Fig. 6 illustrates relationships between the light backscattering coefficients of particles  $b_{bp}(620)$  (which in southern Baltic conditions is only slightly less than  $b_b(620)$ , due to the relatively small contribution of light backscattering by pure seawater) and SPM and POC concentrations. Comparison of the statistical parameters of all the fits presented in Fig. 6 shows that the approximate relationship POC vs.  $b_{bp}(\lambda)$  (Fig. 6b) is related to the occurrence of stronger relationships between  $b_{bp}(\lambda)$  and the SPM concentration (presented in Fig. 6a as the SPM vs.  $b_b(\lambda)$  relation), and the additional statistical relationship between the concentrations of POC and SPM (Fig. 6c). The latter “local” relationship occurs because southern Baltic surface waters are usually

dominated by suspended matter of organic origin (see e.g. S. B. Woźniak et al., 2011). Here, it is important to stress that the approximate functional relationships presented here are strong and considerable simplifications made in order to achieve practical goals. Detailed analyses of the complicated relationships between light scattering characteristics and the concentration, composition and size distribution of suspended matter can be found in our other works (see e.g. S.B. Woźniak et al., 2010, 2014).

In the case of other approximate statistical relationships, i.e. those which use spectral reflectance ratios, an attempt to give a physical explanation would be much more complicated. In order to do this one would need to perform both qualitative and quantitative analyses using the full physical spectral model of remote-sensing reflectance formation. Such analyses would have to account not only for the influence of light backscattering on reflectance spectra, but also the strongly spectrally diverse influence of the light absorption coefficient, which occurs in different proportions with regard to suspended and dissolved seawater constituents. To carry out such complicated analyses is beyond the scope of this particular work, which is mainly of a statistical nature. Nevertheless, it is worth mentioning one certain fact at this point. The statistical analyses suggest that when SPM concentrations are estimated, the application of colour ratio



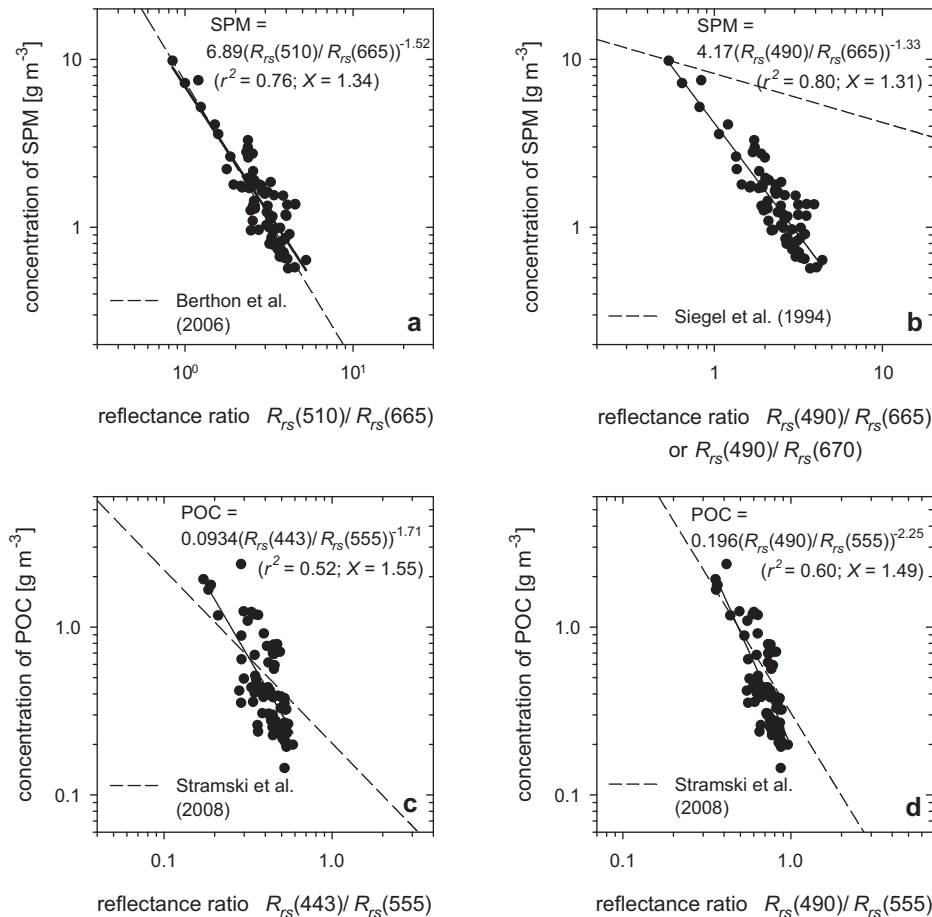
**Figure 6** Examples of empirical relationships between: (a) SPM concentration and coefficient of light backscattering by particles  $b_{bp}(620)$ ; (b) POC and  $b_{bp}(620)$ ; and (c) POC and SPM. The black lines represent the best-fit power functions; the formulas and the statistical parameters are given in each panel.

formulas instead of formulas based on the absolute reflectance at one spectral band alters the accuracy of such an estimate only slightly (compare e.g. the statistical parameters for formulas (3) and (7)). In contrast, when POC is estimated, the differences between these two kinds of formulas are decidedly in favour of colour ratio formulas (compare e.g. the statistical parameters for formulas (4) and (8)). This appears to be in agreement with our earlier observations that in the Baltic Sea conditions POC concentrations exhibit slightly stronger statistical relationships with the light absorption coefficient in the chosen spectral bands than with the light backscattering coefficient (see S.B. Woźniak, 2014).

Among the formulas hitherto shown to be the best examples from the statistical point of view, only a few are directly and quantitatively comparable with the formulas found in the subject literature. One such example is formula (5), which can be compared with the formula given by Ahn et al. (2001). The original formula given by these authors for coastal regions of the Korean peninsula takes the form:  $\text{SPM} [\text{g m}^{-3}] = 647.8(R_{rs}(625))^{0.86}$  (see the additional dashed line in Fig. 3b). The possibility of using the 625 nm band for estimating SPM concentrations agrees qualitatively with our

observations. However, quantitative comparison shows that the formula of Ahn et al., when applied to our Baltic data, predicts slightly different values than our formula (5). In extreme cases (i.e. for the minimum and maximum values of  $R_{rs}(625)$  that we registered) these predictions are up to 1.55 times higher and up to 2.41 times smaller, respectively. In the subject literature there are other works suggesting the possibility of using “red” reflectance bands for estimating SPM concentrations, which also concurs qualitatively with our new results; such citations were given in our earlier work (S.B. Woźniak, 2014).

Further comparisons, albeit done for different variants of new formulas, not those already presented as being the best from the statistical point of view, are shown in Fig. 7. The few formulas presented there combine the SPM concentration with the reflectance ratios of  $R_{rs}(510)/R_{rs}(665)$  or  $R_{rs}(490)/R_{rs}(665)$ , and POC concentration with reflectance ratios of  $R_{rs}(443)/R_{rs}(555)$  or  $R_{rs}(490)/R_{rs}(555)$ . The explicit forms of the new formulas obtained for our data are given in the panels of Fig. 7. They can be compared with the following reflectance ratio based formulas given by other authors, which we have found in the literature: (1) the formula for



**Figure 7** Selected examples of empirical relationships obtained in this work compared with formulas from the literature: (a) relationship between SPM and reflectance ratio of  $R_{rs}(510)/R_{rs}(665)$ ; (b) relationship between SPM and  $R_{rs}(490)/R_{rs}(665)$ ; (c) relationship between POC and  $R_{rs}(443)/R_{rs}(555)$ ; and (d) relationship between POC and  $R_{rs}(490)/R_{rs}(555)$ . The black solid lines represent the best-fit power functions of our southern Baltic Sea data; the formulas and the statistical parameters are given in each panel. The dashed lines in all panels represent formulas from the literature: in panel a it is a formula given for the Baltic Sea by Berthon et al. (2006), in panel b it is a formula given for the Baltic Sea by Siegel et al. (1994), in panels c and d these are the formulas for the southern Pacific and eastern Atlantic Oceans given by Stramski et al. (2008) (for details of the literature formulas, see text).

the Baltic Sea given by Berthon et al. (2006), which after conversion takes the form:  $SPM [g m^{-3}] = 7.396(R_{rs}(510)/R_{rs}(670))^{-1.665}$  (note that this particular formula uses the reflectance ratio of the two spectral bands also pointed out recently by D'Alimonte et al. (2014) as being an effective selection for the simplified neural network inversion of SPM based on MERIS data in the Baltic); (2) the formula also developed for the Baltic Sea by Siegel et al. (1994) but for spectral bands similar to though not identical with ours:  $SPM [g m^{-3}] = 8.22045(R_{rs}(490)/R_{rs}(670))^{-0.29065}$ ; and (3) formulas for POC obtained for the southern Pacific and eastern Atlantic Oceans according to Stramski et al. (2008):  $POC [g m^{-3}] = 0.2032(R_{rs}(443)/R_{rs}(555))^{-1.034}$  and  $POC [g m^{-3}] = 0.3083(R_{rs}(490)/R_{rs}(555))^{-1.639}$ . Comparison of the new SPM formula according to our data with the formula according to Berthon et al. (2006) shows good agreement. Fig. 7a exhibits only small differences in the slopes of the relevant curves. Even in extreme cases, the quantitative differences in predicted SPM values do not exceed a factor of 1.2. In contrast, a marked difference in the slope of the curves can be observed in Fig. 7b when other variant of new formula according to our data is compared with the formula given by Siegel et al. (1994). This difference, unless it is an incorrect interpretation of the literature data on our part, would, in extreme cases, lead to a more than 9-fold difference in predicted SPM values. Other variants of formulas, also given in Siegel et al. (1994), are those for estimating SPM concentration based on colour ratios of 520 to 550 nm, 520 to 670 nm or 665 to 710 nm. Using such (or similar) colour ratios, a rough estimate of the SPM concentration is possible (compare the correlation coefficients  $r^2$  given in Table 3), but they are definitely not the colour ratios that should be regarded as optimal for the Baltic Sea environment in the context of our empirical material. The other two examples presented in Fig. 7 (see panels c and d) relate to the POC concentration calculated with the formulas according to Stramski et al. (2008). Although these formulas were developed for a marine environment different from that of the Baltic Sea, even in extreme cases they show differences of no more than a factor of 1.5. Taking into account these few cases of directly comparable examples, it can be concluded overall that there is a qualitative consistency in the fact that certain reflectance spectral bands can be used for roughly estimating SPM and POC concentrations. In the context of our results, however, the spectral reflectance ratios proposed in the literature often do not seem to be optimal for this purpose in the southern Baltic Sea environment. Nevertheless, for the majority of presented examples (with one notable exception) the quantitative differences even in extreme cases do not exceed a factor of 2.

Finally, one more question should be commented. Even though the variability in the biogeochemical characteristics recorded by us was large (see Section 3.1), it should not be forgotten that the data used here for the derivation of simple statistical formulas were gathered only during two limited periods of the annual phytoplankton activity cycle. The first period was in April and May, when the main annual spring phytoplankton bloom of diatoms and dinoflagellates normally occurs in the Baltic, and the second was in September, which is distinct from the typical occurrence of the important summer annual cyanobacteria bloom (see e.g. discussions in Siegel and Gerth, 2008 or Kratzer et al., 2011 and also the

“classic” work in the Baltic literature by Voipio (1981)). Thus, it is possible that the relationships between SPM, POC and optical properties may differ to some extent at the height of summer or during periods of low phytoplankton activity in autumn and winter. Addressing this problem remains a future task for our group.

#### 4. Final remarks

The new results presented here are in general agreement with earlier observations of other researchers, and also with our own results obtained with the aid of theoretical modelling (see S.B. Woźniak, 2014), that for estimating the concentration of suspended particulate matter (SPM) in surface waters of the southern Baltic Sea one can use simple, direct relationships between that concentration and either absolute values of  $R_{rs}$  at a selected waveband, or alternatively  $R_{rs}$  ratios for two different wavebands (colour ratios). Based on our regionally acquired dataset, we find that the most suitable single bands are those from the long-wave part of the visible light spectrum and from the near infrared (e.g.  $R_{rs}(625)$  or  $R_{rs}(710)$ ), and the most suitable colour ratios are those relating reflectance from the short-wave part of the visible light spectrum to the reflectance from the long-wave part (e.g. ratios of  $R_{rs}(490)/R_{rs}(589)$  or  $R_{rs}(490)/R_{rs}(625)$ ). The standard error factor  $X$  related to such estimates, for the empirical material analysed here, is relatively low, even as low as 1.23. We also find that the use of statistical relationships of a similar form also permits the POC concentration to be roughly estimated for typical southern Baltic conditions. Nevertheless, one should expect that the accuracy of these latter estimates will be inferior compared to the estimated SPM (for the empirical material available here the lowest value of the standard error factor  $X$  was 1.37). Regardless of the relatively small number of empirical data available, we believe that in view of the large variability of our dataset, our quantitative formulas may already adequately describe the approximate relationships that can be established at this level of simplification between SPM and POC concentrations and in situ measured remote-sensing reflectance  $R_{rs}(\lambda)$ , at least for the situations typical of the spring and late summer in the southern Baltic. We consider that both our earlier empirical IOP-based formulas (S.B. Woźniak, 2014) and the new empirical reflectance-based formulas presented here should henceforth be used as a basis for deriving different variants of simple local algorithms for analysing satellite data from the southern Baltic Sea. Once such new algorithms have been derived, they should then be validated against an independent dataset and their performance should be confronted with that of existing algorithms. This will then allow us to make a conscious choice of the most suitable algorithms for the southern Baltic region. This task is especially important in view of the potential input that improved methods of optical remote sensing may have on studies of the dynamics and spatial distribution of organic matter, a topic of major interest to the scientific community studying the Baltic Sea environment (see e.g. Maciejewska and Pempkowiak, 2014, 2015, and the works cited there). Finally, it has to be stressed that potential users of the estimates obtained in the way we propose here should always bear in mind their limited accuracy, which are a consequence of the many simplifications adopted.

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