Determination of phytoplankton abundances (Chlorophyll-a) in the optically complex inland water - the Baltic Sea

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Abstract

A novel approach, termed Summed Positive Peaks (SPP), is proposed for determining phytoplankton abundances (Chlorophyll-a, Chl-a) and surface phytoplankton bloom extent in the optically complex Baltic Sea. The SPP approach is established on the basis of a baseline subtraction method using Rayleigh corrected top-of-atmosphere data from the Medium Resolution Imaging Spectrometer (MERIS) measurements. It calculates the reflectance differences between phytoplankton related signals observed in the MERIS red and near infrared (NIR) bands, such as sun-induced chlorophyll fluorescence (SICF) and the backscattering at 709 nm, and considers the summation of the positive line heights for estimating Chl-a concentrations. The SPP algorithm is calibrated against near coincident *in situ* data collected from three types of phytoplankton dominant waters encountered in the Baltic Sea during 2010 (N=379). The validation results show that the algorithm is capable of retrieving Chl-a con-

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centrations ranging from 0.5 to 3 mg m⁻³, with an RMSE of 0.24 mg m⁻³ (R²=0.69, N=264). Additionally, the comparison results with several Chl-a algorithms demonstrates the robustness of the SPP approach and its sensitivity to low to medium biomass waters. Based on the red and NIR reflectance features, a flagging method is also proposed to distinguish intensive surface phytoplankton blooms from the background water.

Keywords: Satellite remote sensing, Phytoplankton abundance, Chlorophyll-a, MERIS, Baltic Sea

1. Introduction

Being an optically active constituent present in natural waters, phytoplankton play a significant role in aquatic ecosystems. They provide organic compounds for aquatic organisms to sustain food webs and maintain essential ecological functions (Falkowski & Raven, 2013). In coastal and inland waters, on the other hand, the role of phytoplankton can be associated with the adverse effects of surface blooms that taint water resources, disrupt recreation and tourism activities. As one of the largest brackish water bodies located in the northern Europe, the Baltic Sea is known to have annual occurrence of summer phytoplankton blooms. Over the last few decades, the extensive nuisance algal blooms with a surface coverage of up to 100,000 km² have been more frequently observed in this region (Kahru et al., 2007).

Satellite remote sensing has been shown to be one of the most effective means to derive phytoplankton information from various water bodies (Kutser, 2004; Martin, 2004; Kahru et al., 2007; Stumpf et al., 2008; Hu et al., 2010; Hunter et al., 2010). It provides synoptic views, with spatially and temporally cohesive coverage of global waters from open oceans to inland lakes at a near daily frequency. Chlorophyll-a (Chl-a), acting as the primary photosynthetic pigment of phytoplankton, has been widely used as a proxy to indicate phytoplankton

20 abundances (Vos et al., 2003; Gons et al., 2008; Ruiz-Verdu et al., 2008; Nair
 21 et al., 2008; Moses et al., 2009; Brewin et al., 2013; Al-Naimi et al., 2017).
 22 To derive phytoplankton abundances in productive inland and coastal waters
 23 through Chl-a concentrations, the recently developed bio-optical algorithms are
 24 primarily focused on the use of the spectral features observed in the red and
 25 NIR regions (Gons, 2005; Dall’Olmo & Gitelson, 2005; Duan et al., 2010; Le
 26 et al., 2013; Kutser et al., 2016). A number of studies have demonstrated their
 27 performances and applicability to ocean colour data (Dall’Olmo & Gitelson,
 28 2006; Gons et al., 2008; Moses et al., 2012). Yet these studies were either
 29 based on *in situ* radiometric observations or subject to atmospheric correction
 30 procedures.

31 Another type of approach developed for estimating Chl-a concentrations and
 32 bloom distributions is ocean colour indices. These indices were established on
 33 the basis of baseline subtraction methods, and are characterised by the calcula-
 34 tion of the reflectance peak heights at a few Chl-a related red and NIR signals
 35 measured at the top-of-atmosphere (TOA). Because of the simplicity and the
 36 lack of needs for fully atmospheric corrected spectral data, ocean colour indices,
 37 such as Fluorescence Line Height (FLH, Gower et al. 1999), Maximum Chloro-
 38 phyll Index (MCI, Gower et al. 2005), Floating Algae Index (FAI, Hu 2009) and
 39 Maximum Peak Height (MPH, Matthews et al. 2012) have been widely used.
 40 During bloom seasons, however, phytoplankton biomass varies significantly in
 41 time, location and scale. Only considering the spectral variation observed in
 42 a single band, such as SICF or particulate backscattering, the derived index
 43 may not be sufficient to reveal all over changes in phytoplankton abundances
 44 within the water considered (Hu et al., 2012). This especially true for the case
 45 in the Baltic Sea, where the surface phytoplankton species composition shifts
 46 from eukaryotes to cyanobacteria through summer. A number of studies have

demonstrated that the index derived from the FLH approach has a great potential to retrieve Chl-a concentrations from low-medium biomass waters (Gower et al., 1999; Gower & King, 2007; Gons et al., 2008; Palmer et al., 2014; Hu & Feng, 2017), and the magnitudes of NIR reflectance peak heights are more suitable for determining phytoplankton abundances and bloom distributions in high biomass waters (Gower et al., 2006, 2008; Alikas et al., 2010; Hu et al., 2010; Binding et al., 2011; Palmer et al., 2014; Qi et al., 2015). In order to obtain all over information on phytoplankton community, it is necessary to simultaneously consider all Chl-a related reflectance features measured within the red and NIR bands.

Being a heritage satellite sensor, Medium Resolution Imaging Spectrometer (MERIS) had been providing higher spectral ocean colour data over the first decade of the 21st century. The continued exploitation of the MERIS data archive will significantly informs the algorithm development and allows new applications for the Sentinel-3 Ocean and Land Colour Instrument (OLCI) launched in February 2016.

In this paper, we present a new approach for determining phytoplankton abundance or Chl-a in the optically complex Baltic Sea using MERIS Rayleigh corrected surface reflectance or Bottom of Rayleigh Reflectance (BRR). The proposed algorithm, named the Summed Positive Peaks (SPP), calculates the magnitudes of three Chl-a related MERIS TOA signals, and considers the summation of the positive line heights to define the SPP variables. The objectives here are to (1) evaluate the accuracy of the established SPP algorithm and its performance under various environmental conditions over the study site; (2) assess the reliability of standard satellite Chl-a products in comparison with the SPP Chl-a estimates; (3) discuss the advantages and limitations of the SPP approach in estimating phytoplankton abundances in the Baltic Sea.

74 2. Data and methods

75 2.1. Description of study area

76 Covering a surface area of $\sim 410,000 \text{ km}^2$, and with an average depth of 52
77 m (Wasmund & Uhlig, 2003), the Baltic Sea is one of the largest semi-enclosed
78 shallow brackish inland seas in Europe. It consists of several major sub-basins
79 including the Gulf of Bothnia, Gulf of Finland, Gulf of Riga, Baltic Proper
80 and Kattegat (see Figure 1) that are separated by shallow sills. The extensive
81 catchment, with an area of over $1,700,000 \text{ km}^2$, is comprised of nine surrounding
82 coastal countries (HELCOM, 2003, 2006). Compared with open ocean waters,
83 the restricted saline water inflow from the North Sea has made the salinity
84 of the Baltic Sea relatively low (Kratzer et al., 2008). Generally, the salinity
85 level is characterised by a horizontal gradient with the higher values observed
86 in the southwest Danish straits decreasing towards the northernmost region in
87 the Bothnian Bay. In addition, the salinity also exhibits a vertical gradient with
88 the lowest values in the surface layer.

89 This vertical stratification is associated with the formation of a halocline
90 that isolates the surface water from the dense deep waters, and restricts vertical
91 mixing of the water column. With respect to the vertical temperature stratifi-
92 cation, the thermocline develops in spring and becomes prevalent at a depth of
93 between 15 m and 20 m in most Baltic basins during the summer (Reissmann
94 et al., 2009). Substantial nutrients, organic and inorganic substances together
95 with suspended sediments have been retained in its coastal lagoons (e.g. Vistula
96 and the Curonian Lagoon), the Gulf of Riga and Gulf of Finland. These sub-
97 stantial nutrient concentration have led the coastal regions of the Sea becoming
98 eutrophicated (HELCOM, 2003; UNECE, 2007). The transition of organic ma-
99 terials and suspended sediments from the coastal areas to the central region has
100 also resulted in the entire sea being optically dominated by CDOM (Kowalczyk

Figure 1: Baltic Sea map showing the locations of the near-concurrent *in situ* data used in this study. The coloured lines show the ship transects of *in situ* observations where near-concurrent satellite images are available. The red filled dots show the locations of the reference stations where water samples were collected for the *in situ* data validation. The legend shows the dates of *in situ* measurements, and *in situ* data used for the algorithm calibration and validation are indicated with C and V in superscripts, respectively.

et al., 2005, 2006).

In terms of phytoplankton communities, annually occurring algal blooms are observable in both spring and summer seasons. In particular, the spring blooms usually start in the southern Baltic Sea during early March, progress through the central part of the sea in April and then reach the Gulf of Finland during May. The composition of the spring bloom assemblages includes large-celled diatoms such as *Thalassiosira levanderi* and chain-forming single-celled, and sometimes toxin-producing, dinoflagellates such as *Peridiniella catenata* and

109 *Dinophysis acuminata* (Wasmund et al., 1998; Hållfors et al., 2011). During
 110 the summer months, when persistent solar irradiance and little wind mixing
 111 are present, cyanobacteria dominate the phytoplankton assemblages and form
 112 dense surface accumulations. The proliferation of cyanobacteria usually starts
 113 in the Baltic Proper in early summer and extends into the Gulf of Finland
 114 by the end of August. Compared with spring blooms, summer phytoplankton
 115 blooms primarily consist of toxic *Nodularia spumigena*, *Dolichospermum spp.*
 116 and *Aphanizomenon flos-aquae* (Sellner, 1997), and the biomass is generally
 117 low with a Chl-a concentration of less than 2 mg m⁻³ typically observed in
 118 the Bothnian Bay and Kattegat. An increased biomass is measurable in the
 119 Bothnian Sea, Baltic Proper and Gulf of Finland; whereas higher concentrations
 120 of more than 20 mg m⁻³ are common in the coastal lagoons of Vistula and Oder
 121 (Håkanson & Bryhn, 2008). With respect to a subsurface chlorophyll maximum,
 122 this is normally observed in the Kattegat and the Skagerrak (Karlson et al.,
 123 1996).

124 2.2. *In situ* data

125 The *in situ* dataset was collected using an automated flow-through system by
 126 the Swedish Meteorological and Hydrological Institute (SMHI) during its routine
 127 water quality monitoring programme. A series of physical and biochemical
 128 variables, including water temperature and salinity, were measured along the
 129 pre-defined pathway between Kattegat and the Bothnian Bay at a depth of 3
 130 m. Meanwhile, the geo-locations of *in situ* measurements were recorded by a
 131 Global Positioning System (GPS) onboard the research ferry at a frequency of
 132 20 seconds that provides a traverse sampling resolution of ~200 m. *In situ*
 133 Chl-a fluorescence was measured simultaneously with water turbidity by the
 134 integrated fluorometer and turbidity sensor (ECO FLNTU, WET Labs, Inc.).

135 To control the quality of the collected datasets, only when all variables at

136 a sampling point were within the acceptable range, the measurements were
 137 considered valid. For instance, if the difference between the water temperature
 138 measured at the inlet and inside of the system was larger than 1 °C, then, an
 139 inappropriate water flow was considered to pass through the system and all
 140 other variables recorded at this time are excluded.

141 To calibrate the Chl-a concentrations measured *in situ*, an automated sam-
 142 pler (6712FR, ISCO, Inc.) pre-configured with the geo-locations of 6 reference
 143 stations between Lübeck (Germany) and Gothenburg (Sweden) (see [Figure 1](#))
 144 was carried onboard to collect water samples every two weeks when the flow-
 145 through system was in operation. The collected water samples were kept re-
 146 frigerated, at a fixed temperature of 4 °C in a dark environment, before be-
 147 ing transferred to the laboratory. They were then filtered through Whatman
 148 GF/F filters, then the pigment extraction was performed immediately using
 149 96% ethanol ([Arvola, 1981](#)) in a subdued light environment. After the extrac-
 150 tion, Chl-a fluorescence of each water sample was determined through a fluo-
 151 rescence spectrophotometer (Hitachi F-2500, Inc.) at excitation and emission
 152 wavelengths of 430 nm and 665 nm, respectively. The measured fluorescence
 153 was then converted to Chl-a concentrations using the following equation:

$$[\text{Chl-a}] \text{ (} mgm^{-3} \text{)} = R \times f \times s \times e \times V^{-1} \quad (1)$$

154 where R is the fluorescence intensity from the direct fluorometer reading; f
 155 is the calibration factor determined using certified reference material, see ([HEL-
 156 COM, 2005](#)); s is the slit factor, from the slit width settings of the instrument;
 157 e is the volume of ethanol used for the pigment extraction, in a unit of cm^3 ; V
 158 is the volume of filtered sample water, in litres.

159 Then, the obtained Chl-a data were used to calibrate the *in situ* measured
 160 Chl-a concentrations. Note that water samples were only collected between

161 Lübeck and Gothenburg to minimise the Chl-a pigment degradation. The cali-
 162 bration of the Ferrybox system is performed at the Finnish Environment Insti-
 163 tute (SYKE) on an annual basis, with a culture of microalgae *Monoraphidium*
 164 *contortum* used to create a set of standardised Chl-a concentrations.

165 2.3. Satellite data

166 The 3rd re-processed collection of Reduced Resolution (RR) MERIS im-
 167 agery is used in this paper. The datasets were acquired from the European
 168 Space Agency Earthnet FTP site (ftp://eo-a-up.eo.esa.int), and processed with
 169 the Basic ENVISAT AATSR and MERIS (BEAM Ver. 4.10.3.) Toolbox. The
 170 L1b Radiometry Processor (Ver. 1.1.1) was first applied to the RR L1b datasets
 171 for the radiometric recalibration and for the "smile" effect and the detector-to-
 172 detector systematic radiometric difference corrections. Then, the Cloud Prob-
 173 ability Processor (Ver. 1.5.203) was used to produce a cloud probability product.
 174 To minimise potential errors related to the atmospheric correction, only atmo-
 175 spheric effects of gaseous absorption, ozone and molecular Rayleigh scattering
 176 were removed using the bottom-of-Rayleigh reflectance processor (Ver.2.3). The
 177 output reflectance product, known as the Rayleigh corrected surface reflectance
 178 or Bottom of Rayleigh Reflectance (BRR), can be described as follows:

$$\rho_{BRR} = \rho_{TOA}^* - \rho_R \quad (2)$$

179 where ρ_{TOA}^* is the top-of-atmosphere (TOA) reflectance after removing ozone
 180 and gaseous absorption effects, and ρ_R is the reflectance from the Rayleigh scat-
 181 tering. ρ_R was calculated using the 6S radiative transfer code (Vermote et al.,
 182 1997) within the bottom-of-Rayleigh reflectance processor.

183 To evaluate the performance of the proposed method in retrieving Chl-a

184 concentrations, the MERIS C2R_Ch1-a product generated by the MERIS Case-
 185 2 Regional processor (C2R, Ver. 1.5.8) (Doerffer & Schiller, 2008) alongside
 186 the standard MERIS Level 2 (L2) Algal-2 product from the Earthnet FTP site
 187 are used for this investigation. In addition, MODIS-Aqua datasets, provided by
 188 the U.S. NASA Goddard Space Flight Center (GSFC) ([http://oceancolor.
 189 gsfc.nasa.gov/](http://oceancolor.gsfc.nasa.gov/)), are also included. The datasets were processed with the
 190 default atmospheric correction algorithm (2-band model selection and iterative
 191 NIR correction) in the SeaWiFS Data Analysis System (SeaDAS, version 6.4)
 192 to generate the MODIS Ocean Colour 4 (OC4) Ch1-a product. The invalid
 193 Ch1-a retrievals and no data pixels within the above three satellite products are
 194 excluded based on the indication of 'invalid' flag within each product. Table 1
 195 lists the satellite datasets used in this study.

Table 1: Description of the satellite datasets used in this study.

Data Name	Data Type	Application	Source
BRR	TOA reflectance	calibration and validation	BEAM, BRR processor
MERIS C2R Ch1-a	Ch1-a product	algorithm evaluation	BEAM, C2R processor
MERIS Algal-2	Ch1-a product	algorithm evaluation	ESA Earthnet
MODIS OC4	Ch1-a product	algorithm evaluation	SeaDAS, GSFC

196 2.3.1. Match-up data selection

197 During the match-up data selection procedure, the cloud masks from the
 198 cloud probability product together with the L1b 'bright' pixel available in the
 199 Rayleigh corrected surface reflectance datasets were used to exclude cloud pix-
 200 els. To minimise the mismatch of the sampling time between satellite and *in*
 201 *situ* measurements, a strict time window of ± 2 hours (Bailey & Werdell, 2006)
 202 was used for the satellite pixel extraction. Additionally, to minimise the error
 203 associated with satellite sensor noise, a 3×3 median filter was applied, where

only the satellite pixels ($1.2 \text{ km} \times 1.2 \text{ km}$) containing more than three *in situ* records were considered and used for the algorithm development; otherwise, the satellite pixels were discarded (Hu et al., 2001). Under these strict criteria, only seven of the datasets were matched up. These datasets were collected during the summer 2010, covering an area from the south west to the north east of the Baltic Sea with *in situ* Chl-a concentrations spanning a range from 0.5 to 4 mg m^{-3} , see Figure 1 for the location of the ship transects of the *in situ* observations used for the algorithm calibration and validation. In particular, to calibrate the algorithm, four match-up datasets were used, two of which were collected from the Gulf of Bothnia and the other two match-ups from the Baltic Proper. The remaining three match-ups, collected from the central and northern parts of the sea, were used for the algorithm validation.

3. Algorithm Development

3.1. Observed Rayleigh corrected surface reflectance

Figure 2 shows the Rayleigh corrected surface reflectances observed over the Baltic Sea. In particular, the reflectance spectra in Panel A show noticeable peaks of chlorophyll fluorescence at 681 nm, whereas troughs are readily observable at the same wavelength in Panel C and D. Panel B contains reflectance spectra that have less distinct fluorescence peaks and observable reflectance peaks at 709 nm, with the reflectance line heights calculated using MERIS bands 8 and 9 both being positive. Panel C shows the case where the 709 nm reflectance overwhelms the 681 nm SICF, and the positive line height is only obtainable from MERIS band 9. The reflectance spectra shown in Panel D possess terrestrial vegetation-like reflectance shapes that are characterised by strong reflectance signals in the NIR region, and have marked reflectance peaks at 754 nm (MERIS band 10). In this case, two positive reflectance line heights

are encountered at 709 and 754 nm when separate baselines are used, see Panel D.

Figure 2: Rayleigh corrected surface reflectance for four different water types encountered in the Baltic Sea. The filled black dots on each spectrum are the positions of MERIS bands 6, 7, 8, 9, 10, 12 and 13 centred at 620, 664, 681, 709, 754, 779 and 865 nm, respectively. (A) represents the reflectance spectra of eukaryote dominated waters, where the peak of the sun-induced chlorophyll fluorescence is observable in MERIS band 8 at 681 nm; (B) shows the reflectance spectra of water that has an increased biomass in the surface layer; (C) presents the spectral reflectances where surface accumulations occur, with a distinct reflectance peak at 709 nm; (D) shows the reflectances that possess land vegetation-like spectral shapes and have the marked reflectance signal at 754 nm. The dotted lines on each panel show two baselines used by the SPP algorithm.

The presence of the Chl-a fluorescence peak at 681 nm is usually related to sufficient phytoplankton biomass (Gower et al., 1999; Gower & King, 2007), and the emergence of the 709 nm reflectance peak is known from the increased Chl-a concentrations of phytoplankton assemblages comprised of either eukaryotes or cyanobacteria (Gower et al., 2003; Ruiz-Verdu et al., 2008). However, in the case where eukaryotes and cyanobacteria coexist, the 709 nm peak is unlikely to

238 result from the eukaryotes, as most cyanobacteria species have competitive ad-
 239 vantages over eukaryotic phytoplankton during summertime (Paerl & Huisman,
 240 2009).

241 3.2. The Summed Positive Peaks algorithm

242 Based on the reflectance spectra observed over the Baltic Sea and the chang-
 243 ing species composition of phytoplankton assemblages during the growing sea-
 244 sons, a modified baseline subtraction algorithm termed the Summed Positive
 245 Peak height (SPP) algorithm is proposed. This algorithm has a similar form to
 246 other baseline approaches established for detecting phytoplankton blooms, such
 247 as FLH (Gower et al., 1999), MCI (Gower et al., 2005) and FAI (Hu, 2009).
 248 Instead of measuring a single line height at a fixed wavelength, the SPP ap-
 249 proach considers three Chl-a related reflectance features in MERIS bands 8, 9
 250 and 10 (681, 709 and 754 nm) simultaneously. It calculates the line heights for
 251 the 681 nm SICF and 709 nm particulate backscattering and sums the positive
 252 magnitudes to define the SPP variables. To avoid artifacts that might appear
 253 in band 10 when the variable is derived from low biomass waters, separate base-
 254 lines are utilised during the algorithm development process. The mathematical
 255 definition of the SPP algorithm can be described using the following equations:

$$SPP = \sum_{i=1}^3 Peak_i(\lambda_i), \text{ if } Peak_i > 0, \quad (3)$$

$$Peak_{1,2}(\lambda_{1,2}) = \rho_{BRR,\lambda_{1,2}} - \rho_{BRR,664} - ((\rho_{BRR,754} - \rho_{BRR,664}) * (\lambda_{1,2} - 664) / (754 - 664)) \quad (4)$$

$$Peak_3(\lambda_3) = \rho_{BRR,\lambda_3} - \rho_{BRR,709} - ((\rho_{BRR,779} - \rho_{BRR,709}) * (\lambda_3 - 709) / (779 - 709)) \quad (5)$$

256 where λ_i is the wavelength of MERIS bands at 681, 709 and 754 nm, respectively.

257 The succession of species dominance in phytoplankton assemblages from
258 early to late summers in the Baltic Sea can be generally separated into three
259 stages:

- 260 1. In early summer, before the thermocline develops and the water column
261 is well mixed, eukaryotic species such as diatoms and dinoflagellates are
262 homogeneous distributed in the upper layer with low to medium cyanobac-
263 teria biomass;
- 264 2. When the thermocline develops and the water column is gradually sepa-
265 rated, cyanobacteria start growing and gradually become abundant in the
266 surface layer;
- 267 3. When the thermocline is well developed in late summer, high biomass
268 cyanobacteria-dominated phytoplankton assemblages are prevalent in the
269 surface water;
- 270 4. When solar irradiance and calm weather conditions persist for a few days
271 (or weeks), surface scums appear at the water surface.

272 The variation of species dominance in the surface layer phytoplankton assem-
273 blages alters the MERIS reflectance shapes. For each stage, it can be considered
274 separately.

275 3.2.1. *Eukaryote dominant waters*

276 Prior to cyanobacteria assemblages becoming abundant in the surface layer,
277 eukaryotes make up most of the total phytoplankton biomass and coexist with
278 cyanobacteria in the upper layer (Stal et al., 2003). Under this condition, the
279 Chl-a concentration in the surface water is relatively low (generally less than 2
280 mg m⁻³ in the Baltic Sea), and SICF produced by the eukaryotic phytoplankton

281 is readily detectable. To utilise SICF for retrieving chlorophyll from phytoplank-
 282 ton assemblages, a baseline subtraction approach measuring the 681 nm peak
 283 height of the SICF has been established. A number of studies have investigated
 284 the relationship between measured FLH and Chl-a concentrations (Hoge et al.,
 285 2003; Hu et al., 2005), and the impacts of non-algal materials and CDOM on
 286 the observed water-leaving SICF signal (McKee et al., 2007). Validation studies
 287 have further demonstrated the significant potential of using FLH for deriving
 288 Chl-a concentrations from phytoplankton dominated inland and coastal waters
 289 (Gower et al., 1999; Gower & King, 2007; Gons et al., 2008; Palmer et al., 2014).
 290 In this case, the SPP approach calculates the line height of the 681 nm SICF
 291 peak above the baseline.

292 *3.2.2. Eukaryotes and cyanobacteria coexist in phytoplankton assemblages in* 293 *the surface mixed layer*

294 The second stage is that cyanobacteria start growing and their biomass grad-
 295 ually becomes abundant within phytoplankton assemblages in the surface mixed
 296 layer. During this period, slightly decreased eukaryote biomass together with
 297 increased dominance of cyanobacteria typically account for a total Chl-a con-
 298 centration of 2-4 mg m⁻³. The enhanced cyanobacteria biomass in the surface
 299 mixed layer enlarges the backscattering between 700 and 705 nm rather than
 300 elevating the SICF signal at 681 nm (Metsamaa et al., 2006). This enhanced
 301 reflectance causes the 709 nm reflectance peak to emerge. This is the case in the
 302 Baltic Sea where cyanobacteria gradually dominate phytoplankton assemblages
 303 in early and middle summer. Despite the fact that the MERIS sensor does
 304 not have the band configuration between 700 and 705 nm, the signal measured
 305 in the band 9 (709 nm) is still able to provide sufficient information for Chl-a
 306 retrievals. For example, a number of red to NIR band ratio algorithms have
 307 been developed to estimate Chl-a concentrations in inland and coastal waters

(Dall’Olmo & Gitelson, 2005; Gons et al., 2008; Gitelson et al., 2009; Moses et al., 2009; Gilerson et al., 2010; Moses et al., 2012). For the mixed eukaryote and cyanobacteria water, the SPP approach summates the positive line heights of the 681 nm reflectance and 709 backscattering to account for the decreased eukaryotes and increased cyanobacteria.

3.2.3. *Cyanobacteria are dominant in the surface mixed layer*

When optimal weather conditions of persistent irradiance and little wind mixing appear, the subsurface cyanobacteria-dominated phytoplankton assemblages tend to float up towards the water surface to optimise their photosynthetic needs, and consequently form dense surface aggregations. The occurrence of surface cyanobacterial accumulations leads to the reflectance troughs and peaks at 681 nm and 709 nm, respectively.

In high biomass phytoplankton dominated waters, the 709 nm peak height has been suggested as having a significant correlation with Chl-a concentration (Yacobi et al., 1995; Gitelson, 1992). Validation studies on inland lakes and coastal waters have further confirmed the potential of using the 709 nm reflectance for retrieving Chl-a concentrations from surface phytoplankton blooms (Gower et al., 2006, 2008; Alikas et al., 2010; Binding et al., 2011; Palmer et al., 2014; Qi et al., 2015). In this case, the SPP approach resembles the form of MCI, calculating the peak height of the 709 nm reflectance for estimating Chl-a concentrations.

When the optimal weather conditions persist for several days, or weeks, some of the surface blooms can further develop as surface scums. The appearance of surface scums is thought to be the effect of photoinhibition, photo-oxidation and dehydration that causes physical damage to cyanobacteria cells and results in the loss of buoyancy regulation (Abeliovich & Shilo, 1972; Zohary & Madeira, 1990). Assessing Chl-a concentrations for the water that contains cyanobacte-

rial surface scums is difficult. The surface scums restrict the light availability
 in the water column and make the optical properties beneath the scum areas
 undetectable by satellite sensors. Quantitatively estimating Chl-a for the sur-
 face scums themselves is also not a trivial task (Kutser, 2004; Reinart & Kutser,
 2006; Hu et al., 2010). Optical properties of surface scums or dry floating al-
 gae resemble land vegetation, and Chl-a may vary with the health status as
 well as the age of cyanobacteria species. In addition, excessive heating and
 photo-oxidation can cause pigment decomposition, resulting in pigment bleach-
 ing (Sellner, 1997). Although an attempt was made to derive Chl-a from the
 surface scums (Kutser, 2004), using a bio-optical model, the result showed that
 the detailed bio-optical properties are needed for the further quantitative esti-
 mation. Therefore, the floating algae index (FAI) was proposed by Hu (2009) for
 deriving the spatial distribution. It calculates the peak height of the 859 nm re-
 flectance observed in a MODIS land-band, and application examples have been
 demonstrated for detecting surface cyanobacteria scums in Lake Taihu, China
 (Hu et al., 2010). However, in temperate coastal waters such as the Baltic Sea,
 the occurrence of surface scums may not be as frequent as in hypertrophic lakes,
 which makes the distinct reflectance peak undetectable in the region beyond 800
 nm. Therefore, the line height of the 754 nm reflectance is calculated for distin-
 guishing cyanobacteria-dominated phytoplankton assemblages alongside surface
 scums from the background water, and is described in the following section.

3.3. A flag for cyanobacteria dominant waters

By considering the sign of the measured SICF line heights, and comparing
 the reflectance difference between MERIS bands 9 and 10 at wavelengths of
 709 and 754 nm respectively, a *CyanoBloom_flag* is proposed to distinguish
 cyanobacteria dominated waters (i.e. surface blooms and surface scums) from
 the background water. This flag can be defined as follows:

$$CyanoBloom_flag = \begin{cases} 2, & \text{if } \rho_{BRR,865} < \rho_{BRR,754}, Peak_1 < 0, \rho_{BRR,754} > \rho_{BRR,709} \\ 1, & \text{if } \rho_{BRR,865} < \rho_{BRR,754}, Peak_1 < 0, \rho_{BRR,754} < \rho_{BRR,709} \\ 0, & \text{if } \rho_{BRR,865} > \rho_{BRR,754}, (mask_out_as_land); \end{cases} \quad (6)$$

where $Peak_1$ is the SICF peak height calculated using Equation 4. $\rho_{BRR,681}$, $\rho_{BRR,754}$, $\rho_{BRR,865}$ are Rayleigh corrected surface reflectances measured at wavelengths of 681, 754 and 865 nm. $\rho_{BRR,754}$, $\rho_{BRR,865}$ are used to exclude land pixels when the reflectance difference is positive.

Based on the observed reflectance spectra over the Baltic Sea, see Figure 2, eukaryote dominant waters can be distinguished from cyanobacteria dominant waters using the observed 681 nm reflectance trough (Wynne et al., 2008). In particular, when cyanobacteria-dominated phytoplankton assemblages prevail in the surface mixed layer, strong backscattering overcomes water absorption and produces a distinct reflectance peak discernible in MERIS band 9 (709 nm), see Panel C in Figure 2; As surface blooms develop, the 709 nm reflectance peak shifts toward the longer wavelength, and consequently produces the distinct reflectance peak (terrestrial-type spectral reflectance) readily observable in MERIS 10 when surface scums appear, see Panel D in Figure 2; and for both cases, the reflectance trough is presented in MERIS band 8.

Finally, to associate the derived SPP variables with Chl-a concentrations, three models were tested: a linear model of $y = a + bx$; an exponential function of $y = a \exp(bx)$; and a power-law function $y = (a + bx)^c$. The function that has the highest correlation coefficient (R) is used for tuning the coefficients of the SPP algorithm. The root mean square error (RMSE) was used to judge the goodness of fit, and the mean absolute percentage error (MAPE) was calculated

383 to estimate the systematic errors, the mathematical equations are as follows:

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (Y_i - \hat{Y}_i)^2}{N}} \quad (7)$$

$$MAPE = \frac{1}{N} \sum_{i=1}^N \left| \frac{Y_i - \hat{Y}_i}{Y_i} \right| * 100 \quad (8)$$

384 Where N is the number of observations, Y is the observed value and $\hat{Y}$ is
385 the predicted value.

386 3.4. Algorithm calibration and validation

387 In order to obtain a single algorithm for estimating Chl-a concentrations in
388 the Baltic Sea, four match-up datasets are chosen for the algorithm calibration.
389 The criteria applied to the selection of calibration match-up datasets are as
390 follows:

- 391 1. *In situ* observations should cover as much of the Baltic Sea as possible;
- 392 2. *In situ* measurements should span as long a time period as possible;
- 393 3. *In situ* data should cover as wide a range of Chl-a concentrations as pos-
394 sible;
- 395 4. Area surrounding *in situ* measurements should contain as little cloud cov-
396 erage as possible.

397 Based on these criteria, four match-up datasets collected on 20th June, 1st
398 July, 8th July and 15th August 2010 were selected. In the algorithm calibration
399 procedure, the SPP variables are regressed against the near-concurrent *in situ*
400 Chl-a using a non-linear power-law model $y = (a + bx)^c$ that gave the highest
401 correlation values, with the best fit given in Panel A [Figure 3](#) with [Equation 9](#)
402 showing the calibration result.

Figure 3: Scatter plots showing the calibration and validation results of the SPP algorithm. Panel A shows the SPP variable versus *in situ* chlorophyll. Panel B shows the SPP chlorophyll concentrations versus Chl-a measured *in situ*.

$$\text{Chl-a} = [1.79 \times (\text{SPP} \times 10^3) + 0.28]^{1.32} \quad (9)$$

403 The calibration result shows that the coefficient of determination (R^2) is
 404 equal to 0.79 and RMSE is 0.23 mg.m^{-3} ($\text{MAPE} = 16.9\%$, $p = 0.00$, $N = 379$) for
 405 a Chl-a range from 0.5 to 4 mg.m^{-3} , indicating that 79% of the variance within
 406 the *in situ* data is explained by the SPP variables with a minimum Chl-a con-
 407 centration of 0.19 mg.m^{-3} detectable.

408 To assess the accuracy of the calibrated equation, the remaining match-up
 409 datasets collected on 28th June, 1st August and 20 August 2010 were used (see
 410 [Figure 1](#) for the ship transects). The result is shown in Panel B [Figure 3](#). In
 411 particular, for the water where Chl-a ranges from 0.5 to 3 mg.m^{-3} , 69% of
 412 the variance within the *in situ* data can be interpreted by the derived equation
 413 ($R^2 = 0.69$, $p = 0.00$, $N = 264$) and the RMSE of Chl-a estimates is 0.24 mg.m^{-3}
 414 that is equivalent to a MAPE of 16.5%. The validation demonstrates the accu-
 415 racy of the SPP algorithm in estimating Chl-a concentrations for phytoplankton
 416 assemblages.

4. Results

4.1. Assessment of satellite chlorophyll products

The previous section showed the result of the algorithm calibration and validation. It is necessary to evaluate the accuracy of the SPP Chl-a retrievals in the comparison with the standard Chl-a products generated for the Baltic Sea. Therefore, the satellite Chl-a obtained from the MERIS Algal-2, MERIS C2R processor and MODIS OC4 algorithm together with the SPP Chl-a estimates are compared against *in situ* observations. To avoid dependence on the calibration dataset, only the validation datasets are used. The dataset is comprised of the concurrent measurements taken from two Baltic regions: the Baltic Proper and the Gulf of Bothnia.

To better demonstrate the performance of each algorithm, the match-up dataset is separated into two subsets based on the region where it was taken. The first dataset contains the data collected in the Gulf of Bothnia, which is known to have higher CDOM concentrations (Kowalczyk et al., 2005, 2006), the second dataset was collected from the Baltic Proper. The comparison results are presented in Figure 4

Figure 4: The comparison of the MERIS Algal-2, MERIS C2R, MODIS OC4 and SPP Chl-a estimates derived from the Baltic Sea. Panels A shows the results using the data collected from the Bothnian Sea, and Panel B present the results for the Baltic Proper.

434 It can be seen from Panel A [Figure 4](#) that MODIS OC4 Chl-a concen-
 435 trations show no correlation with the near-concurrent *in situ* observations in
 436 the CDOM dominated Gulf of Bothnia, and have the highest error ($R^2=0.03$,
 437 $N=148$, $RMSE=3.08 \text{ mg m}^{-3}$, $MAPE=174.2\%$). The MERIS Algal-2 and the
 438 Case II regional chlorophylls show a similar performance, both have R^2 values
 439 of 0.32. However, the error in the C2R Chl-a retrievals is higher ($RMSE=1.88$,
 440 $MAPE=152.7\%$) than that of Algal-2, which has an $RMSE$ and $MAPE$ of 1.5
 441 and 121.5%, respectively. An improved Chl-a estimation is made by the SPP
 442 algorithm. It has a R^2 value of 0.66 ($N=164$), and the error in the Chl-a es-
 443 timation is the lowest ($RMSE=0.29$, $MAPE=20.2\%$). Note that the difference
 444 in sample numbers is due to the exclusion of invalid Chl-a estimates from the
 445 MODIS OC4 and MERIS Algal-2 products.

446 In Panel B [Figure 4](#), the three Chl-a retrievals show good agreement with
 447 the *in situ* observations, except the MODIS OC4 that has a R^2 value of 0.34
 448 ($N=100$) with a $RMSE$ of 6.61 mg m^{-3} and a $MAPE$ of more than 400%. As for
 449 the MERIS Chl-a estimates, both of the Algal-2 ($R^2=0.71$, $N=100$) and C2R
 450 algorithm ($R^2=0.56$, $N=100$) have good correlations with the *in situ* measure-
 451 ments, especially Algal-2 that has a $RMSE$ of 0.25 mg m^{-3} that is equivalent to
 452 a $MAPE$ of 26%. In this case, the R^2 and $RMSE$ of the SPP Chl-a retrievals are
 453 0.64 and 0.14 mg m^{-3} , which is equal to a $MAPE$ of 10.3%. [Table 2](#) presents
 454 the statistical comparison between the three Chl-a retrievals predicted for the
 455 Bothnian Sea and Baltic Proper.

456 4.2. *CyanoBloom_flag testing*

457 In order to demonstrate the performance of the flagging method for detect-
 458 ing the spatial distributions of surface blooms and scums, a cloud free MERIS
 459 image collected on 3rd August 2011 was used to produce the corresponding
 460 *CyanoBloom_flag* image. Ideally, the extent of surface blooms and scums should

Table 2: Statistical comparison between different Chl-a products generated for the Bothnian Sea and Baltic Proper.

Region	Product Name	RMSE (mg.m ⁻³)	MAPE (%)	R ²	N
Bothnian Sea	MODIS OC4	3.08	174.2	0.03	148
Bothnian Sea	MERIS Algal-2	1.5	121.5	0.32	163
Bothnian Sea	MERIS C2R	1.88	152.7	0.32	164
Bothnian Sea	SPP Chl-a	0.29	20.2	0.66	164
Baltic Proper	MODIS OC4	6.61	467.6	0.34	100
Baltic Proper	MERIS Algal-2	0.25	26	0.71	100
Baltic Proper	MERIS C2R	0.89	91	0.56	100
Baltic Proper	SPP Chl-a	0.14	10.3	0.64	100

be validated using concurrent *in situ* data. Unfortunately, this is not practical in the Baltic Sea as field survey platforms such as research vessels can significantly disturb natural distributions of surface blooms and/or scums, resulting in bloom and scum samples being uncollectable, hence the false representation of the sampled areas (Kutser, 2009). Due to this difficulty, the MERIS Full Resolution (FR) image (spatial resolution of 300×300 m) is used to create a TC composite for the visual validation.

It can be seen from Panel A Figure 5 that dense surface blooms appeared in the north-west part of the Baltic Proper and extended into the Gulf of Finland. The visual examination for the reflectance spectra of these waters showed that they are characterised by distinct reflectance troughs at 681 nm, with a reflectance peak either at 709 nm or 754 nm; whereas for the rest water, they either possess the 681 nm reflectance peaks or have relative constant reflectance shapes in the red and NIR regions.

Furthermore, the bright-green pixels of the bloom waters presented in Panel A have the higher reflectance magnitudes at 754 nm than that at 709 nm, and the surrounding green pixels have clearly discernible 709 nm reflectance peaks,

Figure 5: The performance of the CyanoBloom_flag in mapping surface blooms and scums in the Baltic Sea. Panel A shows a MERIS full resolution TC composite derived from MERIS bands 7 (red), 5 (green) and 2 (blue). Panel B presents the corresponding CyanoBloom_flag image, where the background water, surface bloom and scum pixels are shown in blue, green and red respectively.

478 with reduced 754 nm reflectance magnitudes. As for the bright-green pixels,
 479 they are all identified as surface scums, shown in red in Panel B; as for the
 480 green pixels, they are identified as surface blooms, presented in green colour
 481 in Panel B. Interestingly, most of the identified bloom and scum pixels also
 482 have the 665 nm reflectance peaks, which is thought to be due to the sun-induced PC
 483 fluorescence (Kutser et al., 2006; Qi et al., 2014). Note that the identified scum
 484 pixels aligned with the shoreline are the actual coastlines according to the L1B
 485 coastline flag identification. Thus, these pixels should be neglected.

4.3. SPP variables from low-to-medium phytoplankton biomass waters

To demonstrate the algorithm's performance in retrieving Chl-a concentrations from low-to-medium phytoplankton biomass waters, an alternative baseline subtraction approach termed MPH (Matthews et al., 2012) is selected for the comparison. The *in situ* dataset collected on 8th July 2010 spanning a Chl-a range from 0.5 to 1.5 mg m⁻³ was used to represent the case of low-to-medium biomass waters. As the MPH algorithm was not parameterised for the Baltic Sea, the original variables derived from the two approaches are used to compare against the *in situ* measurements. As can be seen from Figure 6, the correlation between the MPH variables and *in situ* Chl-a is negligibly small ($R^2=0.0$, $N=114$); whereas for the SPP variables, 72% of the variance of the *in situ* data is interpreted ($R^2=0.72$, $N=114$). Despite that there is no overall correlation between the MPH variables and *in situ* data, the derived variables are covariant with *in situ* Chl-a when the concentration is below 0.7 mg m⁻³. This is because that the chlorophyll fluorescence band is the only channel that produces an observable peak, and the other bands have negative reflectance line heights. This means that the two algorithms essentially calculate the same reflectance line height at 681 nm. When Chl-a concentration becoming higher than 0.7 mg m⁻³ and the 709 nm backscattering overcomes water absorption, two positive reflectance line heights are measurable in MERIS bands 8 (681 nm) and 9 (709 nm), see Panel B Figure 2 for example.

4.4. SPP Chl-a retrievals from cyanobacteria dominant waters

Due to the limited range of *in situ* Chl-a data used for the algorithm calibration and validation, it is also necessary to assess the algorithm's accuracy in retrieving Chl-a from high biomass phytoplankton assemblages such as surface blooms and scums. Therefore, the MERIS image acquired on 20th July 2010 that includes surface blooms and scums (according to the identification of the

Figure 6: Comparison between the SPP and the MPH with the *in situ* Chl-a collected on 8th July 2010. The horizontal dashed line on the figure shows $Y=0$.

513 CyanoBloom_flag) is selected to extract SPP Chl-a retrievals from an artificial
 514 defined ship transect. The artificially defined transect crosses surface bloom
 515 and scums in the south Baltic Proper, see Panel A Figure 7, where the SPP
 516 Chl-a estimates span a range of ~ 1 to 50 mg m^{-3} . In the assessment, the op-
 517 erational MERIS-based NIR/red ratio algorithm, also known as the advanced
 518 two-band MERIS NIR-red algorithm (Moses et al., 2012), is used to produce
 519 the corresponding Chl-a estimates along the ship transect. This algorithm was
 520 chosen for the comparison as it has been parameterised for highly productive
 521 waters, with the ability to retrieve Chl-a concentrations up to 110 mg m^{-3} .
 522 As MERIS L2 reflectance data are generally invalid for the Baltic Sea and the
 523 two-band NIR-red algorithm needs R_{rs} as the input parameter, therefore, the
 524 simple atmospheric normalisation procedure of subtracting BRR14 from BRR7
 525 and BRR9 is used to roughly obtain $R_{rs}(665)$ and $R_{rs}(709)$. Note that this pro-
 526 cedure also produces a number of invalid reflectance values that are excluded
 527 from the analysis.

528 It can be seen from Panel B Figure 7 that the Chl-a retrievals from the two
 529 algorithms are highly covariant ($R^2=0.5$, $N=173$) and within the Chl-a range

Figure 7: MERIS SPP Chl-a image acquired on 20th July 2010 (Panel A) and the comparison result between SPP and the two-band NIR/ratio algorithm. The overlaid blackline on Panel A defines the artificial ship transect.

from approx. 1 to 60 mg m^{-3} . However, the two-band NIR-red algorithm has consistently higher Chl-a estimates than the SPP algorithm, and the maximum bias factor between the two algorithms is around 10-fold. This is probably due to the poor atmospheric correction applied. Also, the coefficients of the advanced two-band MERIS NIR-red algorithm tuned for turbid productive waters may not be suitable for the Baltic Sea. Indeed, a number of studies have shown that the specific absorption coefficient of phytoplankton varies significantly with the composition of phytoplankton assemblages as well as the trophic status of water bodies (Bricaud et al., 1995, 2004). Such variation in the phytoplankton specific absorption coefficient directly affects the algorithm coefficient tuning for specific regions, hence resulting in the bias in Chl-a estimates. However, being an operational algorithm, the advanced two-band MERIS NIR-red algorithm is potentially useful for providing Chl-a estimates for turbid regions within the Baltic Sea, such as coastal lagoons where concentrations of suspended particles are known to be high. These preliminary results suggest that the SPP algorithm may still have the ability to provide Chl-a estimates for cyanobacteria dominant waters with the upper detection limit of 50 mg m^{-3} , but *in situ* datasets with wider Chl-a ranges are needed for the conclusion.

548 4.5. Application examples in the study site

549 It has been reported that dense surface blooms reached an unprecedented
550 extent in the central Baltic Sea during the summer of 2005 (Kahru et al., 2007).
551 The field campaign undertaken by SYKE reported that toxic *Nodularia spumi-*
552 *gena* blooms were observed in the central Bothnian Sea in late July of the same
553 year. Although dense cyanobacterial blooms are known to occur less frequently
554 in the Gulf of Bothnia, compared with the central region, it is still necessary to
555 test the algorithm’s performance for this region. Therefore, a series of MERIS
556 images taken from the Baltic Proper and Gulf of Bothnia in July 2005 were
557 acquired. As shown in the first four panels in Figure 8, dense surface blooms
558 are observed in the central Baltic Sea, with the estimated Chl-a values being
559 above $\sim 50 \text{ mg m}^{-3}$. The retrieved bloom distribution shows good agreements
560 with the TC composites, although a large proportion of MERIS imagery was
561 contaminated by sun glint.

562 The final case is made for *Nodularia spumigena* blooms in the Gulf of Both-
563 nia on 30th and 31st July 2005 (see Panels E and F). SPP Chl-a estimates
564 correctly identified the less intense blooms in the central Bothnian Sea, which
565 has been confirmed by *in situ* observations¹. However, the Chl-a estimates from
566 MERIS Algal-2 products (see Panels G and H) show inconsistent surface bloom
567 distributions, having completely different bloom patterns to that shown in the
568 corresponding TC composites and SPP Chl-a images.

¹See the report of field campaign http://www.itameriportaali.fi/en/ajankohtaista/uutisia_muualta/2005/en_GB/843/

Figure 8: Application of the SPP algorithm to the Baltic Sea in determining phytoplankton abundances under various atmospheric conditions. The inset image on each panel shows the corresponding TC composite derived from MERIS bands 7 (red), 5 (green), 2 (blue). Panels A-D show the examples in the central Baltic Sea. Panels E and F represent examples from the Gulf of Bothnia. Panels G and H show Chl-a retrievals from the MERIS Algal-2 algorithm. The overlaid lines on panels F and H are the artificial transects showing inconsistent bloom distributions.

569 5. Discussion

570 5.1. Reliability of satellite chlorophyll products

571 5.1.1. MODIS blue-green band ratio algorithm

572 Results from the comparison of satellite Chl-a with *in situ* observations
573 (Figure 4) showed that the operational MODIS OC4 algorithm had very poor
574 performance in retrieving Chl-a concentrations, suggesting the MODIS Chl-a
575 product is not directly usable in the Baltic Sea.

576 The MODIS OC4 algorithm (O'Reilly et al., 2000), developed on the basis of
577 the absorption and backscattering features in the blue and green regions, was
578 originally designed for assessing Chl-a in open oceans where phytoplankton is
579 optically dominant. The reason to include the MODIS OC4 chlorophyll product
580 in the inter-comparison was to test the degree to which the known issues of
581 CDOM affect the performance of a standard algorithm designed for open oceans.
582 Indeed, in the central Baltic Sea where the terrestrial inputs are less dramatic
583 compared with the coastal gulfs, the MODIS OC4 Chl-a had good covariance
584 with *in situ* observations, having the overestimation up to 20-fold. This result
585 implies that the blue-green band ratio type approach is potentially applicable
586 to the open region of the Baltic Sea in the conditions that the water is relatively
587 clear with no surface blooms occurring and the coefficients are localised.

588 However, the covariance disappeared when the algorithm was applied to the
589 Gulf of Bothnia where yellow substances are known to be high. The absorption
590 spectra of yellow substances (or CDOM) is characterised by an exponential
591 shape decreasing from the blue (~ 400 nm) to NIR region. In the spectral region
592 between ~ 440 and 600 nm, phytoplankton indicated by Chl-a also possesses a
593 quasi exponential decreasing trend in the absorption coefficient that is similar
594 to CDOM. In optically CDOM dominant waters, increasing concentrations in
595 either CDOM or Chl-a would lead to the blue-green reflectance peak to shift

from the blue region towards the green region. The MODIS OC4 algorithm, using the ratio of the maximum reflectance measured at wavelengths of 443, 490 and 510 nm to the reflectance measured at 555 nm, is not able to separate water-leaving signals resulted from Chl-a and CDOM, as no inversion model is available. Thus, a general outcome of the application of the blue-green band ratio algorithm to CDOM dominant waters would result in overestimated Chl-a concentrations.

5.1.2. MERIS chlorophyll products

The operational scheme applied by the MERIS sensor for producing the Algal-2 and C2R products was developed on the basis of a Neural Network (NN) approach (Doerffer & Schiller, 2007). The algorithm derives inherent optical properties (IOPs) from a trained NN for three optically active water constituents, including absorption coefficients of phytoplankton pigments, yellow substance and bleached particulate matter. All these IOPs are defined at the wavelength of 442 nm for MERIS band 2, and subsequent satellite products such as water constituent concentrations are derived from several pre-defined empirical relationships with the IOPs.

As shown in Figure 4, Chl-a concentrations derived from the Algal-2 and C2R products were well correlated with *in situ* data, especially the estimation made in the Baltic Proper, see Panel B Figure 4. Whereas for the north Baltic basin: the Gulf of Bothnia, Chl-a from the two products generally had higher Chl-a estimates than the near concurrent *in situ* observations, see Panel A Figure 4. This is probably because bio-optical properties of the Gulf of Bothnia are out of the scope of the training sets, resulting in inappropriate IOPs being applied to estimate Chl-a. As stated by (Doerffer & Schiller, 2007), the training sets applied to the NN training were primarily collected from the North Sea and some other European waters, and only a few of the sets were collected from the

623 south Baltic Sea.

624 Another factor that can cause the overestimation of the two chlorophyll
625 products in the comparison may result from the *in situ* data collected at a depth
626 of 3 m. However, [Alikas et al. \(2015\)](#) and [Alikas & Kratzer \(2017\)](#) demonstrated
627 that monthly means of the first optical depth of the north-west Baltic region and
628 Bothnian Sea (i.e. the region where the *in situ* data were obtained) are generally
629 deeper than 3 m except the month July. Therefore, the discrepancy between
630 the datasets is unlikely to be the key factor resulting in the overestimation, if
631 the water samples were collected from the well mixed water column with no
632 surface blooms occurring during sampling days in July. It is worth noting that
633 the comparison results shown in [Figure 4](#) were based on the data collected in
634 June and August.

635 In addition to the effect of training sets, insufficient atmospheric correction
636 and the occurrence of algal blooms can also cause bias and exceptions in Chl-a in
637 the Algal-2 products. Indeed, in late July 2005 when surface blooms and cloudy
638 atmosphere occurred in the Gulf of Bothnia, the chlorophyll map of the Algal-2
639 product falsely represented the spatial distributions of bloom areas (Panel G and
640 H in [Figure 8](#)) and Chl-a estimated along the artificially defined ship track was
641 inversely correlated with the SPP Chl-a. Therefore, caution needs to be applied
642 to MERIS Algal-2 product when using it to study phytoplankton abundances
643 in the Gulf of Bothnia.

644 5.2. *Phytoplankton abundance from ocean colour indices*

645 Being an empirical TOA type method, various baseline subtraction algo-
646 rithms have been developed for estimating Chl-a concentrations in optically
647 complex inland and coastal waters. These algorithms usually take advantage
648 of Chl-a related spectral features observed in the red and NIR regions to es-
649 tablish empirical relationships between the measured reflectance peak height

650 and Chl-a concentrations. Despite the fact that these algorithms avoids the
 651 need for fully atmospheric corrected spectral data and can be simply applied to
 652 various waters, the limitation is evident when using it to study phytoplankton
 653 dynamics on the basis of the single reflectance peak height measured. This is
 654 because the shift of distinct reflectance peak from the red to NIR region when
 655 phytoplankton biomass becomes abundant, shown in [Figure 2](#). To overcome the
 656 weakness of single-band based subtraction algorithms, the recently developed
 657 MPH approach considers multi-spectral signals observed in red and NIR regions
 658 and utilises the maximum reflectance peak height to determine Chl-a concentra-
 659 tions. The approach works very well in eutrophic and/or hypertrophic waters.
 660 However, in low-medium biomass waters where the maximum reflectance peak
 661 located in the SICF band, phytoplankton abundances may not be accurately
 662 retrievable due to the weak signal observed, see [Figure 6](#).

663 Instead of measuring a single red and NIR reflectance peak height, the cur-
 664 rently proposed SPP algorithm takes advantage of the sum of all the positive
 665 signal line heights for estimating phytoplankton abundance. The comparison
 666 results demonstrated that the SPP approach performed better over the standard
 667 satellite chlorophyll products ([Figure 4](#)) and sensitive to phytoplankton abun-
 668 dance changes in low-medium biomass waters in the Baltic Sea, see [Figure 6](#),
 669 suggesting that the algorithm is potentially suitable for studying phytoplankton
 670 bloom initiation.

671 As for the case where surface cyanobacterial blooms and/or scums formed,
 672 the currently proposed SPP approach may not able to provide accurate Chl-a
 673 estimates. This is not only due to the limited in situ data available for the
 674 algorithm calibration and validation, but also the challenge to collect and ex-
 675 tract chlorophyll pigments from cyanobacteria dominant phytoplankton assem-
 676 bages ([Kutser, 2009](#); [Simis et al., 2007](#)). Therefore, an alternative method of

677 CyanoBloom_flag is proposed for qualitatively detecting spatial distributions of
 678 surface blooms and/or scums based on the appearance of the reflectance trough
 679 in SICF band. Such a spectral shape of the SICF trough is considered as the
 680 result of cyanobacterial bloom occurring (Wynne et al., 2008). The negative
 681 spectral feature has been used to determine bloom intensities in inland lakes
 682 (Wynne et al., 2010; Stumpf et al., 2012).

683 Considering the observed reflectance from surface scums resembles land veg-
 684 etation spectral shapes, and the water-leaving signal from surface blooms is neg-
 685 ligibly small beyond the wavelength of 750 nm, thus, the two types of blooms
 686 can be roughly differentiate from one of the other. As can be seen from Fig-
 687 ure 5 that the detected surface scums are usually surrounded by surface blooms,
 688 which is coherent with the natural situation that surface scums and/or floating
 689 algae are the extreme case of surface blooms

690 Compared with MERIS, the recently launched OLCI is optimised for better
 691 ocean colour measurements over optically complex inland and coastal waters.
 692 The SPP algorithm should be directly transferable to OLCI imagery, and the
 693 new band configured at 674 nm for the improved SICF measurement shall pro-
 694 vide an insight into TOA type algorithm development.

695 5.2.1. Impacts of the physiological state and environmental factors on SICF

696 As a byproduct of photosynthesis, SICF produced by phytoplankton has long
 697 been used for estimating primary production and Chl-a concentrations (Neville
 698 & Gower, 1977; Booth, 1989; Falkowski & Kolber, 1995; Chamberlin et al.,
 699 1990; Chamberlin & Marra, 1992; Kiefer & Reynolds, 1992; Letelier & Abbott,
 700 1996). For instance, it is known that the rate of photosynthesis varies with
 701 the rate of natural fluorescence, and the fluorescence quantum yield efficiency
 702 is inversely correlated with photosynthetic quantum efficiency. However, the
 703 prediction of the photosynthetic quantum efficiency is not a trivial task. Geo-

704 physical processes (such as the availability of nutrients) and diurnal variations in
705 the fluorescence quantum yield make the application of natural fluorescence to
706 primary production estimation less effective in global waters (Stegmann et al.,
707 1992; Falkowski & Kolber, 1995).

708 In addition, it has also been suggested that the natural fluorescence may not
709 be useful for the detection of spatial and temporal variations in phytoplankton
710 abundances, even in oligotrophic marine environments. In particular, the rate
711 of Chl-a fluorescence is dependent on two factors: the light flux absorbed by the
712 photosystem (primarily by PS II) and the fluorescence quantum yield (the frac-
713 tion of photons fluoresced by Chl-a to photons absorbed by all pigments). Under
714 light saturated conditions, the absorbed light flux is assumed to be constant,
715 thus, the fluorescence signal per unit Chl-a is proportional to the fluorescence
716 quantum yield ². From a satellite remote sensing perspective, Chl-a concentra-
717 tions derived from the natural fluorescence or the FLH algorithm are under an
718 assumption that the fluorescence quantum yield is constant, in other words, the
719 ratio of fluorescence to Chl-a is assumed to be invariant. In most cases, how-
720 ever, fluorescence quantum yield is highly variable. For instance, Borstad et al.
721 (1985); Babin et al. (1996) have stated that changes in phytoplankton species
722 composition, nutrient concentrations and the availability of ambient light can
723 cause significant variations to the fluorescence quantum yield. In addition, the
724 physiological state of phytoplankton assemblages is another source causing the
725 variability to the fluorescence quantum yield (Suggett et al., 2009).

726 Clearly, the variability in fluorescence quantum yield related to phytoplank-
727 ton physiology and environmental conditions results in difficulties in the inter-
728 pretation of the observed fluorescence signal, and introduces complications in
729 using natural fluorescence for retrieving Chl-a. However, a recent study (Giler-

²SICF per Chl-a concentration=const.× fluorescence quantum yield

son et al., 2007) of the HYDROLIGHT simulation has shown that the variability of the fluorescence quantum yield is relatively stable in coastal waters, having a value of around 0.01. The study also indicates that the variation in fluorescence quantum yield is less significant to cause changes to the natural fluorescence compared to the signal attenuation in the water column. Although McKee et al. (2007) has suggested that increased concentrations of yellow substances and non-algal particles can cause the natural fluorescence per Chl-a to decrease by more than 50%, their study shows that the FLH is less prone to variations in CDOM concentrations. These results imply that the assumption of the constant ratio of fluorescence to Chl-a is applicable to the retrieval of Chl-a concentrations. The results from the algorithm calibration and validation indicate that using peak height of fluorescence provides good Chl-a estimates in the Baltic Sea, given that *in situ* datasets were collected from different regions.

5.2.2. Impact of suspended particles on the 709 nm signal in the Chl-a retrievals

In the Baltic Sea, riverine inflow from the southern catchment areas persistently brings in inorganic materials and detrital particles to the coastal and shallow zones and causes re-suspension of bottom sediments in the water column. Such substantial amounts of suspended particles, resulting in the increase of water turbidity, could give rise to inaccurate SPP Chl-a estimates.

As shown in Figure 8, the two lagoons located in the southeast of the Baltic Sea had consistently high SPP Chl-a concentrations during summer. Therefore, Chl-a concentrations derived in these turbid productive waters may not be accurate, because of the interference of suspended materials to the observed signal. It is acknowledged that suspended matter is related to the primary production, sediment transport and water clarity, and can be used as an indicator of water quality (Dekker et al., 2002). However, using the empirical baseline subtraction approach such as the SPP and MCI algorithm for deriving Chl-a concentrations

757 from turbid waters may have issues, due to the difficulty in using the current
758 satellite data to separate the signals of phytoplankton and suspended matter.
759 In suspended particle dominant waters, the reflectance spectra are characterised
760 by a distinct peak observable at ~ 700 nm (Doxaran et al., 2003; Härmä et al.,
761 2001), resembling the backscattering from phytoplankton. The similarity in the
762 spectral shapes can cause significant ambiguity between Chl-a and suspended
763 particle retrievals, as the baseline subtraction algorithm is not able to distin-
764 guish one from the other, and miscounts the peak height as phytoplankton.

765 Not only causing ambiguity to Chl-a retrievals, strong backscattering from
766 suspended matter also make atmospheric correction over Case II waters chal-
767 lenging. The direct application of an atmospheric correction scheme designed
768 for open oceans to turbid coastal and inland waters would not yield accurate re-
769 flectance data. Furthermore, the geographical nature of turbid coastal zones and
770 inland waters (the high contrast between land and water scenes) also compli-
771 cates atmospheric correction procedures. However, the high spectral resolution
772 and the additional NIR and SWIR bands available on new satellite sensors can
773 provide an insight into improving Chl-a estimation and atmospheric correction
774 in turbid productive waters.

775 6. Conclusion

776 In conclusion, a new method termed Summed Positive Peaks is proposed
777 to retrieve Chl-a concentrations for determining phytoplankton abundances in
778 an optically complex coastal water, the Baltic Sea. The results demonstrate
779 that the red and NIR spectral features such as SICF and 709 nm backscat-
780 tering can provide reasonable Chl-a estimates for phytoplankton abundance
781 assessments using a baseline subtraction approach. The calculation of the SPP
782 variables based upon the TOA type approach is an effective means to normalise

783 atmospheric effects under the assumption that atmospheric aerosol effects are
784 relatively constant at the red and NIR wavelengths used. Thus, the Rayleigh
785 corrected TOA dataset is efficient for the phytoplankton abundance estimation,
786 and it can be employed as an alternative dataset that avoids complicated and
787 error-prone atmospheric aerosol corrections for phytoplankton-oriented water
788 quality monitoring programmes in Baltic regions.

789 Additionally, the red and NIR spectral reflectance features observed by
790 MERIS during the period studied enabled Chl-a concentrations to be esti-
791 mated for eukaryote dominated, cyanobacteria dominated and mixed eukary-
792 ote and cyanobacteria waters. This is achieved through the calculation of the
793 reflectance magnitude differences over the predefined baseline, and the sum-
794 mation of the positive line heights. Based on the sign of the calculated SCIF
795 line height, and the reflectance difference between MERIS bands 9 and 10, the
796 CyanoBloom_flag is proposed to deal with intensive surface blooms and scums
797 and/or floating algae. The results from the algorithm calibration and validation,
798 with the near-coincident *in situ* observations, suggest that the algorithms Chl-a
799 retrieval range is from 0.5 to 4 mg m⁻³ with an RMSE of 0.24 mg m⁻³. Due to
800 limited *in situ* measurements being available, the advanced two-band MERIS
801 NIR-red approach is further used to confirm that the practical Chl-a retrieval
802 limit of the SPP algorithm is up to 50 mg m⁻³. As for the extreme case, the
803 proposed CyanoBloom flag provides the spatial distribution of surface blooms,
804 and discriminates bloom and scum waters from the background. The compari-
805 son with standard satellite chlorophyll products and MPH approach reveals the
806 algorithms robustness and sensitivity to phytoplankton abundance changes in
807 low-to-medium biomass waters. These results indicate that the SPP approach is
808 potentially suitable for detecting the initiation of phytoplankton blooms. Fur-
809 thermore, the Baltic Sea examples demonstrate the algorithms performance in

810 estimating phytoplankton abundances under various atmospheric conditions in
811 different time periods. Therefore, it is proposed that this approach is also po-
812 tentially suited for phytoplankton related real-time water quality monitoring.

813 Overall, the SPP approach is demonstrated as a novel empirical algorithm for
814 determining phytoplankton abundance in an optically complex coastal water,
815 the Baltic Sea. This is one of a few studies showing the significant correla-
816 tion between the empirical derived Chl-a concentration and the TOA variable
817 determined through the red and NIR signals from MERIS observations. The
818 advantages of this TOA type approach are not only evident in processing time,
819 but it also avoids the errors potentially introduced during atmospheric correc-
820 tion procedures. The findings from this research have significant implications
821 for the study of long-term phytoplankton bloom dynamics in the Baltic water
822 based on historical MERIS observations and for the development of phytoplank-
823 ton oriented near-realtime water quality monitoring programmes and warning
824 systems using the Copernicus Sentinel-3 OLCI.

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