



Suitability of multisensory satellites for long-term chlorophyll assessment in coastal waters: A case study in optically-complex waters of the temperate region

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ABSTRACT

We investigated the use of multisensory satellite data to determine long-term changes in surface chlorophyll concentrations using a 19-year (1998–2016) time series of chlorophyll data in the Danish Kattegat region of the Baltic Sea. Merged satellite estimates (SeaWiFS-MODIS/Aqua-MERIS-VIIRS) were compared with *in situ* ship based time series from four monitoring stations situated with increasing distance from land and nutrient sources. *In situ* and satellite derived estimates showed similar trend in chlorophyll with several fold higher values closer to land. Satellites aligned very well with *in situ* estimates in the open water stations but showed significant differences in magnitude and inter-annual variability, in particular in shallow coastal waters. Some systematic deviation was observed with satellite underestimating the growing season average for the earlier periods (1998–2002) and overestimating for the later period (2012–2016) compared to *in situ* estimates. Comparing growing season chlorophyll means over the 19 year period showed increasing magnitude and variability in nearshore and shallower areas, most pronounced for the satellite derived chlorophyll. Satellites overestimated chlorophyll in nearshore areas 2–4 fold, despite excluding shallow nearshore areas with possible benthic interferences from the analyses. This bias needs further validation and requires correction to improve the overall applicability of satellites for long-term monitoring of chlorophyll in the Kattegat region. From analysis of normalized data, we developed a simple correction model, which reduced deviations considerably between methods, underlying the importance of *in situ* data for application of satellite observations. While significant deviations were observed from *in situ* data, satellites are clearly advantageous in the much higher temporal and high spatial coverage they provide. Multisensory satellites can, however, not be used currently as a standalone technique for long-term assessment of chlorophyll. They require validation with *in situ* measurements, which provide essential data for calibration, validation and correction of satellite based estimates. A complementary use of multisensory satellite and *in situ* measurements therefore remains essential to assess trends in the ecological status of optically complex waters such as the Kattegat region of the Baltic Sea.

1. Introduction

Eutrophication from nutrient enrichment has deteriorated coastal ecosystem worldwide (Boesch, 2002; Cloern, 2001; Kemp et al., 2005), typically manifested as increased primary production in the mixed surface layer (Krause-Jensen et al., 2012; Lyngsgaard et al., 2014) leading to increased phytoplankton biomass (Cloern, 2001). The concentration of chlorophyll is an indicator of phytoplankton biomass in natural waters (Cullen, 1982; Harvey, 1934; Lehman, 1981), and used as an ecological indicator to assess changes in water quality in response to

eutrophication (Hooper, 1969; Karydis et al., 2009; Vollenweider, 1992). The effects of eutrophication in both the open sea and coastal areas are considered undesirable, and several national as well as international agreements to combat the adverse effects on the ecosystems have been developed (Carstensen et al., 2013; Directive, 2008; Directive, 2000; OSPAR, 2017; Vollenweider and Kerekes, 1982). The need for an effective monitoring of eutrophication increased considerably as EU launched the Marine Strategy Framework Directive (MSFD) with the aim of achieving ‘good environmental status’ (GES) in all European marine waters by 2021.

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Traditionally, chlorophyll has been monitored by determining concentration from discrete *in situ* water samples collected from different depths at fixed positions. While these ship based sampling provides information about the vertical distribution of algal biomass, these measurements provide limited information on the horizontal and temporal distribution of chlorophyll. A point sample taken during one day may not represent the following day, week, month or season and not the nearby areas (Carstensen and Lindegarth, 2016). Moreover, the water samples taken represent only a small percentage of the total waterbody, and with a large spatial and temporal heterogeneity in the parameters such as abundance of phytoplankton in the sea, it is challenging to have a full assessment by measuring chlorophyll based on field measurements (Platt and Denman, 1980).

Remote sensing using satellites allows ocean observation at larger spatio-temporal scales making it possible to cover larger areas more frequently (Strong and Elliott, 2017). Satellite ocean color estimates of chlorophyll has been an effective tool to monitor the spatiotemporal distribution and variations of phytoplankton and primary productivity in open ocean and coastal waters (Legaard and Thomas, 2006; D'SA et al., 2011). Monitoring coastal waters using satellites provides easily available and cost-effective data without the spatio-temporal limitations possessed by ship based discrete *in situ* monitoring (Strong and Elliott, 2017; Stæhr et al., 2019). Satellites enable quantitative assessments of algal biomass (Harvey et al., 2015) that can be used as an ecological indicator (Platt and Sathyendranath, 2008) to understand the eutrophication effects. Recent studies indicate the potential of remote sensing to supplement and optimize marine monitoring programs (Harvey et al., 2015; Hossain et al., 2015; Kratzer et al., 2014; Markager et al., 2019). However, while there are some clear advantage of using satellites for obtaining high temporal and spatial resolution data, studies have also shed light towards strong needs to improve the accuracy and precision of the applied algorithms to obtain more reliable estimate of parameters such as chlorophyll (O'Reilly et al., 2000; Pitarch et al., 2016).

A major factor adding to the complexity of the use of a robust chlorophyll algorithm, especially in the optically complex region such as the Baltic region, relates to the presence of high concentrations of CDOM caused by humic rich freshwater inflow (Kowalczyk et al., 2006; Mélin and Vantrepotte, 2015; Pitarch et al., 2016). For optically complex water bodies with high CDOM concentrations, whose properties change significantly throughout the seasons, it is challenging to obtain accurate values of chlorophyll concentrations from satellites (Sathyendranath, 2000), leading often to an overestimation of chlorophyll concentrations through the use of standard algorithm (Attila et al., 2013; Darecki and Stramski, 2004).

An additional complicating factor while assessing a long-term change in an important water quality parameter such as chlorophyll is the use of different satellites over years. Environmental monitoring is primarily conducted through the assessment of changes in indicator values over time, as this provides essential information about the environmental state and possible effects of abatement measures. However, as the configuration of bands have changed between satellites over years, it becomes critical to evaluate the effects of this change on the environmental monitoring and decision making process through the close assessment of the available long-term satellite data.

In this study, we evaluated the use of multisensory satellite data, derived using Baltic Sea specific algorithms, for monitoring of chlorophyll in the optically complex Baltic Sea transition zone, the Kattegat region of Danish marine waters. We analyzed 19 year time series of satellite and ship based *in situ* measurements from open water and coastal stations within the Kattegat region. This enabled us to investigate and compare seasonal, inter-annual and spatial variability of chlorophyll as assessed by satellites and *in situ* sampling.

2. Materials and methods

A 19-year (1998–2016) time series of chlorophyll estimated through

both multisensory satellites and ship based *in situ* sampling were analyzed and compared for the Kattegat region of the Baltic Sea. The Baltic Sea is a large estuary (412,000 km²) connected to the North Sea through the Danish Straits and the Kattegat forming the Baltic Sea transition zone. Our data set comprise four water quality monitoring stations, including three Danish stations (Aarhus Bight (AB-St170006), Great Belt (GB-St6700053) and Griben (St 925) in the Southern Kattegat) and one Swedish station (Anholt East; AE-St32002) (Fig. 1). Aarhus Bight and Great Belt are considered coastal stations within a proximity of about 4–5 km to land, and water depth of 16 and 32 m, respectively. Griben and Anholt East are both placed in the open parts Kattegat at depth of 39 and 30 m, respectively. The four stations were sampled every 2 to 3 weeks during the growing season period from March to October and monthly during the winter.

The Kattegat has an almost permanent pycnocline at 11–12 m depths due to an annual outflow of about 500 km³ low saline waters from the Baltic Sea (Jørgensen et al., 2014). Salinity range from 10 to 28 at the surface and about 33 in bottom waters.

2.1. *In situ* and satellite data processing

Data on *in situ* sampling were extracted from the database for the Danish National Aquatic Monitoring and Assessment Program

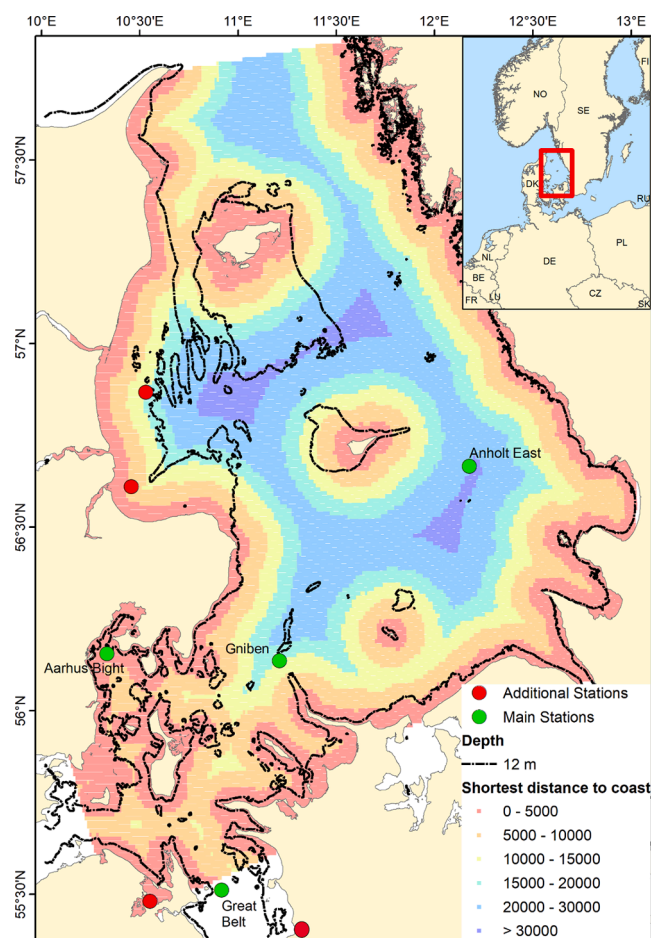


Fig. 1. Map of Kattegat showing the four main *in situ* stations (green circles) used for time series comparison with satellite data. Four additional *in situ* stations used for the depth gradient analyses is also shown in the map (red circles). The black line designates the 12 m depth contour. Colors in the Kattegat waters show areas with increasing distances to the coast. Some of the shallow areas (<12 m) to the north extend far into the central part of Kattegat. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

(DNAMAP) (Conley et al., 2002), maintained by the Department of Ecoscience, Aarhus University, Denmark. *In situ* sampling at each station was done at several depths about 20 to 40 times per year from 1998 to 2016. Chlorophyll concentrations were determined from filtered water samples, extraction with ethanol, and measured spectrophotometrically in the laboratory according to the Danish standard methods (Kaas and Markager, 1998; Markager and Fossing, 2014). Satellite chlorophyll measurements were tested and compared with *in situ* measurements from several other depths (2 m and 5 m). The best relationship was found with surface (≤ 1 m) *in situ* values and hence these were used in this study.

The chlorophyll concentrations from satellite sensors were derived from merging of SeaWiFS, MODIS/AQUA-MERIS-VIIRS remote-sensing reflectance similar to Gohin et al. (2019), processed by the combination of Copernicus Marine Environment Monitoring Services (CMEMS) Baltic Sea-Specific algorithm (BalAlg) (Pitarch et al., 2016), and the Free University Berlin (FUB) neural network (v4.01, (Schroeder et al., 2007)) algorithm. BalAlg is an adaptation of the OC4v6 algorithm for the Baltic Sea, modified by applying the coefficients of the linear regression between *in situ* and OC4v6-derived chlorophyll data to reduce the biasness between satellite observations and *in situ* measurements. BalAlg was applied to the remote-sensing reflectance (Rrs) spectra provided by the ESA-CCI processor from CMEMS, which merges data from SeaWiFS-MODIS, Aqua, MERIS, and VIIRS. FUB neural network algorithm was applied to acquire products optimized for complex case 2 waters, as is the case in the CDOM rich Kattegat region (Stedmon et al., 2000). The FUB includes both atmospheric correction and conversion to water constituents, and is especially adapted to European coastal and optically complex waters (Schroeder et al., 2007). FUB uses four separate neural networks to derive the level-2 products from top-of-atmosphere radiances; Total Suspended Matter (TSM), chlorophyll concentrations, and the absorption of Colored Dissolved Organic Matter (CDOM) at 443 nm. The fourth neural network is used to derive level-2 reflectance. FUB has been trained with an ocean-atmospheric model with simulated optical data covering chlorophyll values between 0.05 and 50 $\mu\text{g/L}$ (Schroeder et al., 2007). The BalAlg and FUB products were merged together with a priority given to FUB resulting in a time series of satellite derived chlorophyll data for the period 1998–2016. The additional quality control was applied to the BalAlg product by excluding pixels which were contaminated by high CDOM and SPM concentrations, as the adapted OC4V6 algorithms performs bad in those optically complex situations. The FUB neural network is trained to perform better under these complex situations, which results in more available pixels with data.

More details about the satellite data processing steps are available in Van der Zande et al. (2019).

The total period from 1998 to 2016 were classified into three groups based on the satellite sensors in service: 1998–2002 (SeaWiFS), 2003–2011 (MODIS-MERIS) and 2012–2016 (MODIS-VIIRS).

For satellites data, standard 1x1 km grid cell was considered in this study. We used a homogeneity criteria that at least five of the nine pixels in the defined box (3x3 pixels centered over the location of the *in situ* measurements) must be valid/quality assured to ensure statistical confidence in the mean values. The arithmetic mean and standard deviation (STDEV) of the valid/quality assured pixels were determined. To minimize the effect of outliers on the calculated mean value, especially in the case of coastal sites, a filtered mean value was also calculated following the approach of Bailey and Werdell (2006).

Considering the temporal coverage achieved through these satellites, we obtained chlorophyll data corresponding to the four monitoring stations 1 to 2 times per week using the available sensors during the 1998 to 2016 period. Coverage was, however, lower during periods of cloud cover. To reduce the influence of satellite observations poor temporal coverage caused by cloud cover, which hampers satellite observations in the Northern part of Europe, we interpolated satellite data between sampling dates using a linear interpolation approach. The effect

of the interpolation on the growing season average was tested with pairwise comparison using *t*-test. For this, we chose data from the station with highest data availability, which was the year 2004 for station GB (St6700053). To assess if the interpolated growing season mean was sensitive to the number of observations, we randomly removed 4, 10 and 20 % of the total available dataset and performed interpolation on these. While this did not change the growing season means, the interpolated dataset provided higher temporal resolution enabling more thorough analysis of variability in the seasonality in comparison with non-interpolated dataset.

Growing season averages estimated by satellites throughout the entire Kattegat were compared with the *in situ* estimates. The growing season period was considered from 1 March to 30 September following the OSPAR commission (Commission, 2005) for both *in situ* and satellite data. The start of the growing season in the studied area is well defined with a start in March whereas production in the fall is gradually fading from August but often with the largest decline from September to October (Lyngsgaard et al., 2014; Lyngsgaard et al., 2017). While this period does not capture the full extent of the spring and autumn blooms, it covers the part of the growing season where nutrient limitation is most pronounced and hence be affected by nutrients loadings from land. Moreover, it make our results directly relevant for the management practice in OSPAR. Satellite estimates above the average values from *in situ* sampling for the 19 years + 1 times STDEV were considered unrealistic and most likely a result of influence from nearby land, shallow areas or resuspension, and were therefore removed. This resulted in omitting 14 chlorophyll values from the two coastal water stations (Aarhus Bight and Great Belt) only.

Assessment of changes in the environmental status requires analysis of long-term trends in an ecological indicator such as the chlorophyll concentration. Therefore, in this study, we tested the correspondence between the *in situ* and satellite methods with respect to time. First, values were normalized for each method to zero mean and a STDEV of one by subtracting the mean values for the station across years for each type (satellite and *in situ* observation) and dividing by STDEV ($\hat{x} = (x - \bar{x}) / \text{stdev}$). Then a linear regression model (geometric mean regression) with an additive bias term was used (Eq. (1)).

$$Chl_{in\ situ} = int + slope * Chl_{sat} + bias_{SeaWiFS} * k1 + bias_{MODIS-VIIRS} * k2 \quad (1)$$

where *int* is the intercept (expectation = 0), *slope* is the overall relationship (expectation = 1) and *k1* and *k2* are dummy variable having values of 1 for the periods with SeaWiFS in service (1998–2002, *k1* = 1 otherwise *k1* = 0) or MODIS-VIIRS in service (2012–2016, *k2* = 1 otherwise *k2* = 0). In this way, the parameters *bias*_{SeaWiFS} and *bias*_{MODIS-VIIRS} express any systematic bias for the two sensors/periods compared to the central period 2003 to 2011 with the sensors MODIS-MERIS in service. The parameters *int*, *slope*, *bias*_{SeaWiFS} and *bias*_{MODIS-VIIRS} were estimated with Proc NLIN in SAS 9.4.

Since the four *in situ* stations chosen for this study were deeper than 12 m depth, which corresponds to the pycnocline (Jørgensen et al., 2014), four more *in situ* stations from depths shallower than 12 m were included (refer Fig. 1) to investigate the influence of water depth on growing season average chlorophyll values. This enabled us to explore gradients in magnitude and variability in chlorophyll from shallow to deeper waters obtained through use of satellite and *in situ* monitoring. Gradients with depth were explored using a generalized additive model (GAM). All analysis was carried out in R Studio (version 1.3.959) using the “mgcv” package (version 1.8.31) (R Core Team, (Team, 2018)).

3. Results

3.1. Changes in chlorophyll seasonality

Composite maps of satellite estimated chlorophyll concentrations for the three periods 1998–2002, 2003–2011 and 2012–2016, showed

changes over years, especially in the near shore regions. The maps show high concentrations ranging $2\text{--}20\ \mu\text{g L}^{-1}$ of chlorophyll in the near shore areas all three periods compared to the open water areas where chlorophyll levels ranged around $1\text{--}4\ \mu\text{g L}^{-1}$ for all periods (Fig. 2). However, for some nearshore areas, elevated values, i.e. above $15\ \mu\text{g L}^{-1}$ follow the isolines of shallow water (refer Fig. 1), and this might be due to reflection from the sandy seafloor or resuspension of sediment.

Comparing *in situ* chlorophyll concentrations for the open part of Kattegat (Anholt East station) with corresponding satellite data, provided a detailed insight into the seasonal variation in chlorophyll for the three periods (Fig. 3). Please refer to [supplementary material](#) for other stations.

The *in situ* based values show a similar pattern for the three periods but with declining average values as expected due to the long-term reduction in annual nitrogen loadings to the area (Lyngsgaard et al., 2014; Riemann et al., 2016), with all four stations showing the lowest average *in situ* values for the last period (Table 1). Particularly the amplitude of the spring bloom tends to decline. The most prominent result is, however, that the satellites were unable to detect the spring bloom, particular for the two first periods. For the period 1998–2003 there is no sign of a spring bloom and hardly any of the autumn bloom that is clearly visible with the *in situ* data. For the second period, a spring bloom is visible but less than half of the magnitude observed through *in situ* sampling. However, there is an improved match between two methods throughout the summer and autumn periods. Only during the third period from 2012 to 2016, the spring bloom as depicted from satellites matches well with *in situ* values. In particular after DOY 65 where we observed a very good match up observed during the summer to the autumn period. Note that satellite values were not available before DOY 50. Similar patterns were observed for three other stations in the Kattegat (Figure S1, S2 and S3 – supplementary figures). We attribute the lack of satellite data before DOY 50 and the systematic underestimation of the spring bloom to the low sun angle in the Northern Europe at this time of the year, which reduces the water leaving irradiance to such low levels increasing the noise/signal ratio at all channels.

3.2. Long-term changes in growing season mean chlorophyll concentrations

Comparing the long-term changes showed a common pattern in the annual variability for both *in situ* and satellite estimates (Fig. 4). However, some extreme satellite values were observed at the two coastal stations (AB (St170006) and GB (St6700053)), with satellites values sometimes several fold higher than the highest observed *in situ* value, represented by dashed grey lines in Fig. 4. Applying a filter of mean + 1 STDEV greatly reduced these deviations.

Growing season mean values were overall higher for the two coastal stations, which also had higher within and between year variability (Table 1). Both the time series for *in situ* and satellite estimates showed high values in 2007, 2011 and 2015 for all four stations, with much higher values for the satellite estimates. The years 2007 and 2015 correspond to the years with highest run off over the 19 years period and the run off in 2011 was also above average. Nutrient inputs, particularly for nitrogen, closely correlate with freshwater run off, so the annual peaks in chlorophyll concentrations reflect the input of nutrients to the area and with the highest impact for coastal stations. The lower chlorophyll in open water compared to coastal waters indicates that open water conditions are dominated by long-distance nutrient loading, eg. from the outflow from the Baltic Sea, whereas the coastal zone is mostly affected by local run off of nutrients (Maar et al., 2016). Overall, the growing season average from two methods showed similar patterns and compared really well in the two open water stations (Fig. 4).

In situ and satellite values were both higher for the coastal stations. However, a decreasing trend over time observed by *in situ* data was not clear from satellites and the two methods provided significantly

different estimates in 4 out of 12 periods (Table 1). Satellite values were generally lower than *in situ* values for the period 1998–2002, and higher for the period from 2012 to 2016 for the coastal stations, in particular for the shallow AB station. This was the case even after some very higher values, considered as outliers (chlorophyll $> 36\ \mu\text{g L}^{-1}$) were removed from the time series of the coastal stations. For the two open water stations, satellite estimates were significantly lower than *in situ* values, especially during the first period (1998–2002). However, unlike coastal stations, the values from *in situ* and satellites were not significantly different during the latter period (2012–2016). The overall deviation between *in situ* and satellite estimates (mean of all stations and all years) was small (8%) and insignificant (Table 1). The variability (STDEV of means) for satellites estimates were up to 2–3 times higher for the coastal stations compared to open water stations, whereas *in situ* sampling showed a uniform variability for the four stations (Table 1). Nonetheless, a systematic deviation between methods was observed, with satellite estimates being lower than *in situ* from 1998 to 2002 and higher from 2012 and onwards for the four stations in the Kattegat region (Fig. 4).

3.3. Correction of deviations in satellite chlorophyll estimates

The observed deviation of satellite observations compared to *in situ* concentrations reduces the usefulness of satellites for the assessment of long-term changes in chlorophyll concentrations. To understand the systematic behavior of this deviation, we compared satellites and *in situ* data using normalized values (Fig. 5).

While differences between methods were smaller and more evenly distributed around the 1:1 line during the 2003–2011 period (int = 0.05 and slope = 0.99), satellites systematically provided significantly lower chlorophyll values during the 1998–2002 ($\text{bias}_{\text{SeaWiFS}} = 1.17 \pm 0.23$ (mean \pm STDEV)) and significantly higher values during 2012–2016 ($\text{bias}_{\text{MODIS-VIIRS}} = -0.98 \pm 0.23$).

The corrected satellite values using Eq. (1) is shown in Fig. 5b and Fig. 6b.

The average changes in the growing season mean values for four stations over the 19 years period were analyzed (Fig. 6). For the normalized values, the expectation is zero mean throughout the period. The *in situ* observations showed positive values from the year 1998 to 2008, with year 2003 as an exception, and negative values from 2009 with the wet year 2011 as an exception and an overall negative trend of -0.06 STDEV per year ($p = 0.006$). The raw satellites observations showed an opposite pattern during this period with negative values when the *in situ* was positive and vice versa (Fig. 6A). Correcting the satellite estimates using the derived equation improved the relationship pattern between two methods (Fig. 6B).

3.4. Importance of depth and distance to shore on chlorophyll concentrations

One of the obvious advantages of satellites is the better spatial coverage compared to *in situ* sampling. The availability of the long-term satellite data throughout the Kattegat provided the opportunity to investigate growing season means at multiple sites representing depth gradients for the entire Kattegat region (Fig. 7). Comparing the satellite data with data from eight *in situ* monitoring stations (note the addition of the four more *in situ* stations within shallower depth area), both showed higher levels and variability in the chlorophyll concentration at shallow depths (Fig. 7), which mostly occurred close to the shore line (refer Fig. 1). Fitting a GAM model to explore relationship between satellite growing season average value with depth explained 39% of the variance and a significant exponential relationship between seasonal averages with depth ($p < 0.01$). Although the satellite estimates showed much higher variability in waters shallower than approximately 30 m (up to 4 fold higher than *in situ* at 2 m depth), the modeled values lied within the variation of the *in situ* data (Fig. 7). This suggests that the detailed depth

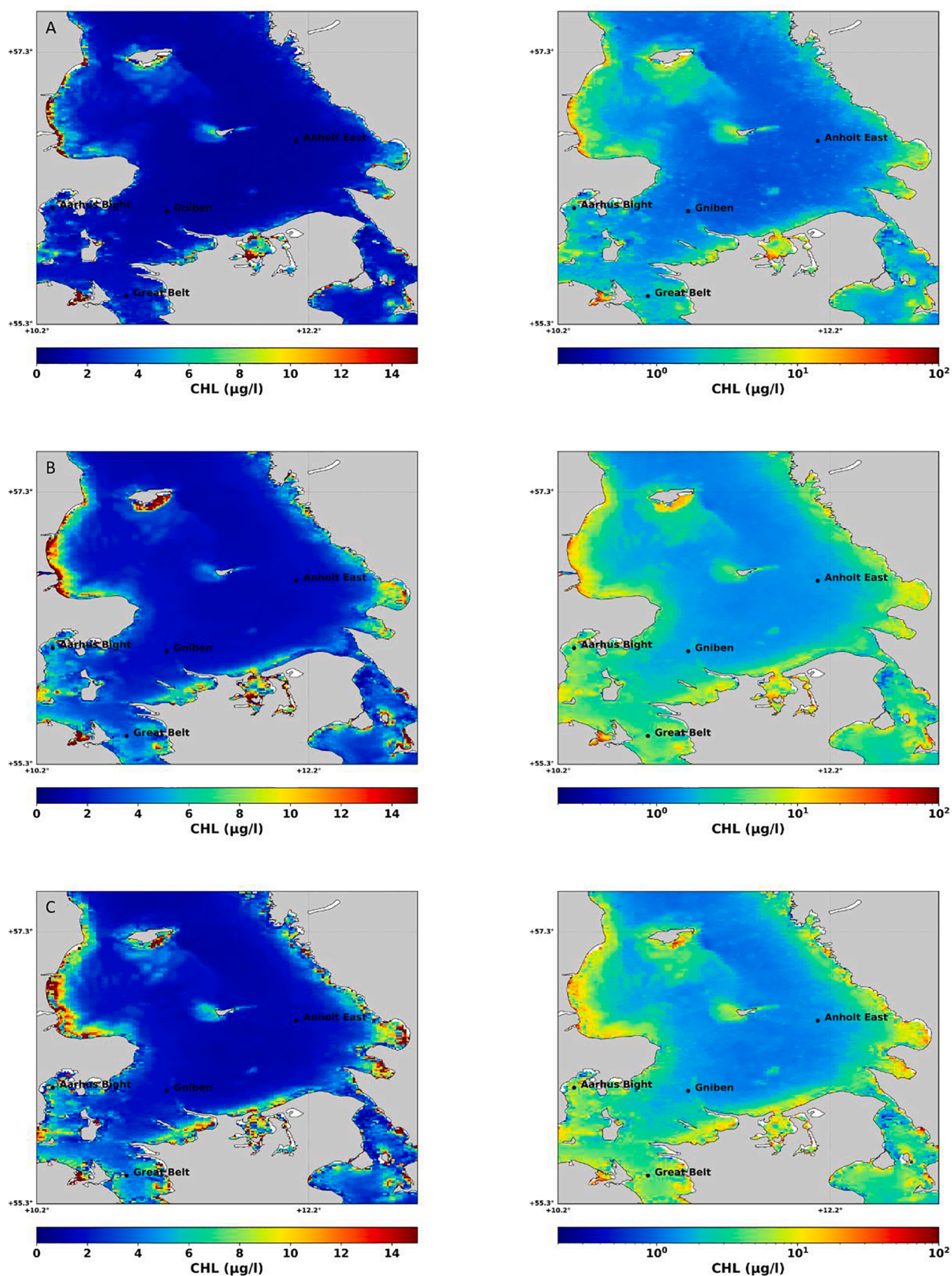


Fig. 2. Satellite estimates of chlorophyll ($\mu\text{g L}^{-1}$) for three periods (Left: absolute values, right: log-transformed values; A) 1998–2002, B) 2003–2011, and C) 2012–2016) covering the Kattegat region. Chlorophyll concentration were calculated from satellite data using 1×1 km grid sized cells. Four monitoring stations from which we have long-term *in situ* data are shown.

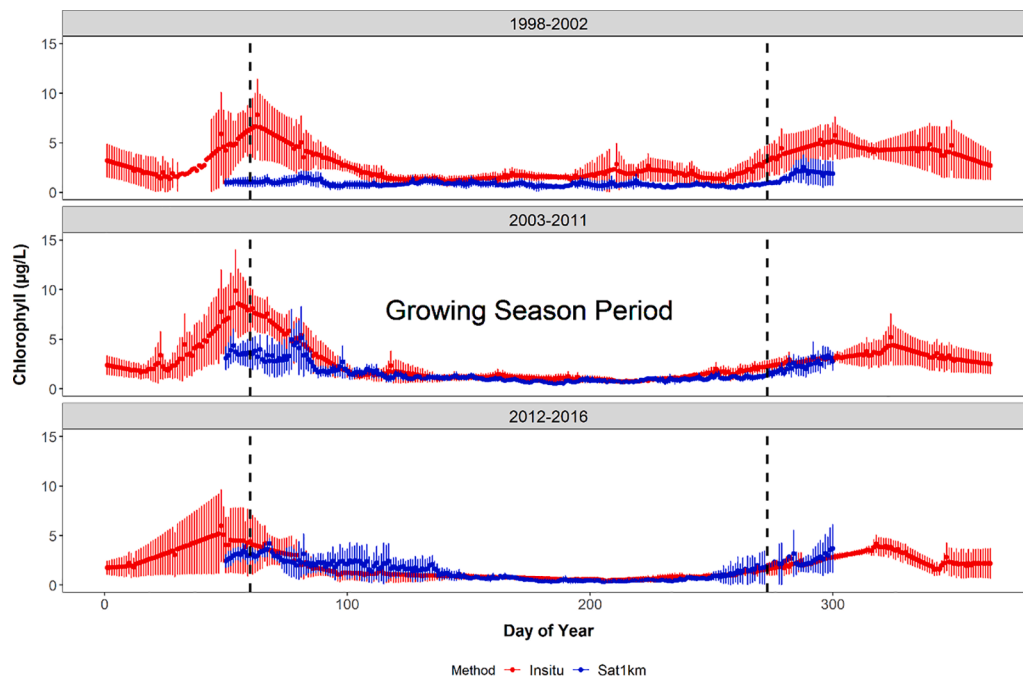


Fig. 3. Time series of daily chlorophyll concentrations from ship based (*in situ*) and satellite derived observations averaged over three periods (1998–2002, 2003–2011, and 2012–2016) for Anholt East station (AE-St32002) in the open part of Kattegat. The growing season period (1 March to 30 September) is indicated. Error bars are 95 % confidence interval of the mean.

Table 1

Growing season mean chlorophyll values ($\mu\text{g L}^{-1} \pm \text{STDEV}$) for four stations in the Kattegat region estimated from *in situ* and satellite data. Data are shown for three successive periods and for the entire data set (1998–2016). Differences in mean values are shown in absolute (Diff; $\mu\text{g chlorophyll L}^{-1}$) and relative (Deviation; %) values. Significant differences (p-values in bold) between *in situ* and satellite values were tested using Students *t*-test. The shown satellite estimates for the coastal stations (AB-St170006 and GB-St6700053) were corrected for extreme high values (see text).

Station	Area	Station type	Depth (m)	Period	<i>In situ</i> estimates	Satellite estimates	Diff	Deviation (%)	P value
AB-ST170006	Aarhus Bight	Coastal	16	1998–2002	2.83 ± 0.59	1.49 ± 0.94	−1.33	−47%	0.032
				2003–2011	2.55 ± 0.69	4.34 ± 2.64	1.78	70%	0.080
				2012–2016	1.90 ± 0.76	4.52 ± 1.68	2.63	139%	0.021
				All years	2.45 ± 0.74	3.64 ± 2.38	1.18	48%	0.050
GB-ST6700053	Great Belt	Coastal	32	1998–2002	2.50 ± 0.18	1.62 ± 0.81	−0.88	−35%	0.069
				2003–2011	2.92 ± 1.04	3.41 ± 1.03	0.49	17%	0.328
				2012–2016	1.99 ± 0.45	3.64 ± 1.40	1.65	83%	0.055
				All years	2.56 ± 0.83	3.00 ± 1.33	0.44	17%	0.235
Gniben-ST925	Gniben	Open water	39	1998–2002	1.79 ± 0.25	1.04 ± 0.26	−0.76	−42%	0.001
				2003–2011	2.05 ± 1.01	1.68 ± 0.81	−0.37	−18%	0.400
				2012–2016	1.21 ± 0.52	1.45 ± 0.82	0.23	19%	0.609
				All years	1.76 ± 0.81	1.45 ± 0.73	−0.31	−18%	0.216
AE-ST32002	Anholt East	Open water	30	1998–2002	2.27 ± 0.33	0.83 ± 0.24	−1.44	−63%	<0.001
				2003–2011	1.92 ± 0.62	1.38 ± 0.50	−0.54	−28%	0.059
				2012–2016	1.19 ± 0.32	1.27 ± 0.47	0.08	7%	0.765
				All years	1.82 ± 0.62	1.21 ± 0.48	−0.61	−34%	0.001
	All stations			1998–2002	2.35 ± 0.52	1.25 ± 0.68	−1.1	−47%	<0.001
				2003–2011	2.36 ± 0.92	2.70 ± 1.89	0.34	14%	0.335
				2012–2016	1.57 ± 0.62	2.72 ± 1.80	1.15	73%	0.013
				All years	2.15 ± 0.82	2.32 ± 1.74	0.17	8%	0.435

gradient observed from satellites delineates a tendency which is also observed using much coarser ship based monitoring of chlorophyll.

4. Discussion

Marine ecosystems provide a range of important ecological and economical services to societies, and monitoring the state of these ecosystems is an essential component of proper management of the sea (De Jonge et al., 2006; Markager et al., 2019). The necessity to obtain reliable data on status and changes in key environmental conditions has increased over time as the anthropogenic pressure exerted on the marine ecosystem services has intensified (Carstensen, 2014; Halpern et al.,

2008). While satellites provide many data points at relevant temporal and spatial scales, implementation of satellite methods for assessment of long-term changes in water quality properties still requires thorough evaluation (Markager et al., 2019; Staehr et al., 2019).

In this study, we evaluated the performance of multisensory satellites, which are expected to provide cost-efficient additional data by increasing the number of temporal observations and a greater spatial coverage for the monitoring of seasonal and long-term changes in surface chlorophyll concentrations in the optically complex Kattegat region. The use of satellite data from different sensors was required to compare the long-term trend in chlorophyll. Therefore, 19 years of merged satellite data (1998–2016) were compared with ship based *in*

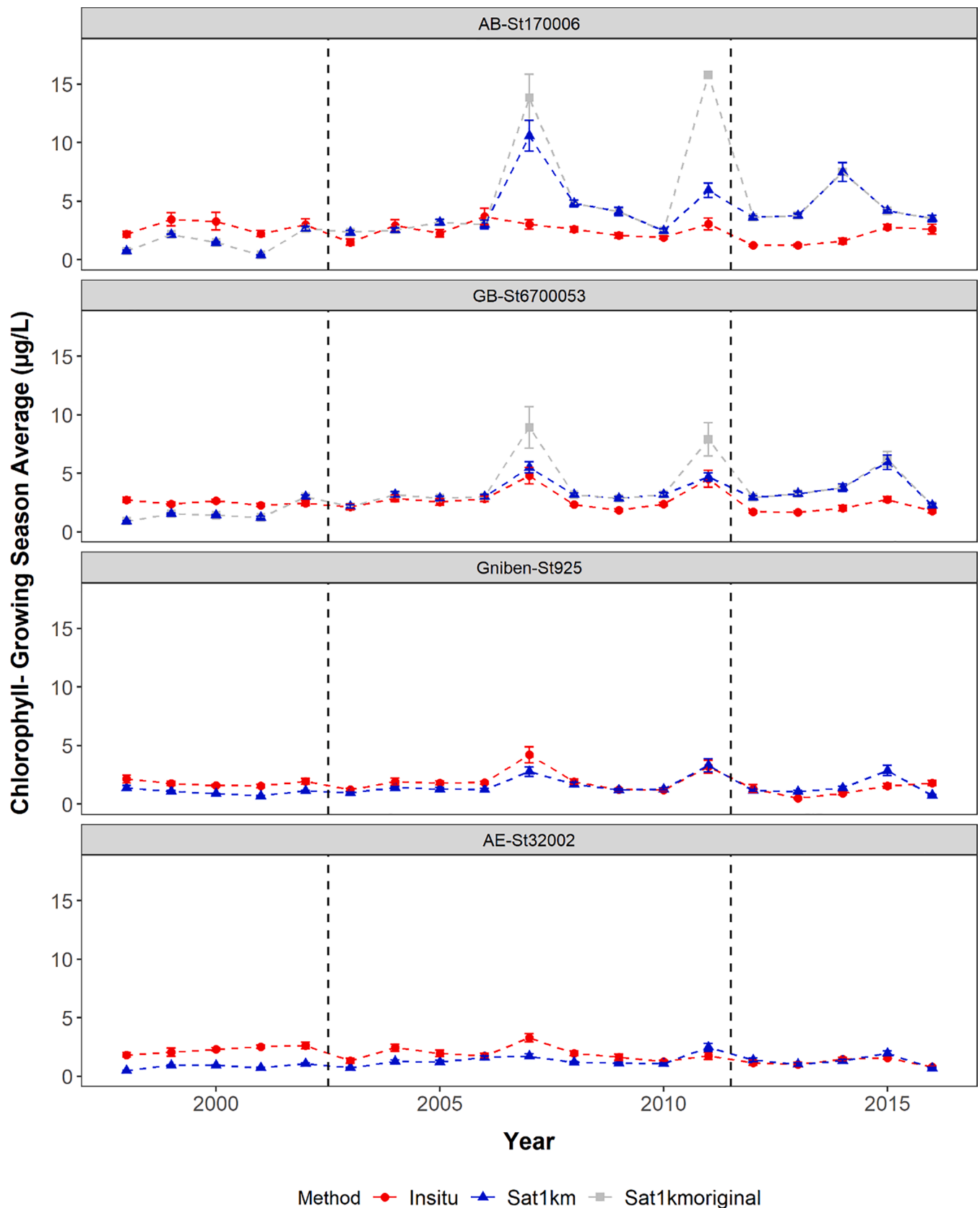


Fig. 4. Growing season mean chlorophyll concentrations ($\mu\text{g L}^{-1}$) for four stations in the Kattegat region. Red lines represent *in situ* values sampled from ship. Grey lines are raw satellite estimates based on 1x1 km grid sized cells. The blue line indicates satellite estimates where outliers with values above one time the standard error of *in situ* values were removed from the two coastal stations. Stations are shown in order of increasing distance from the coast. Vertical dashed lines separate periods of different satellite sensors. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

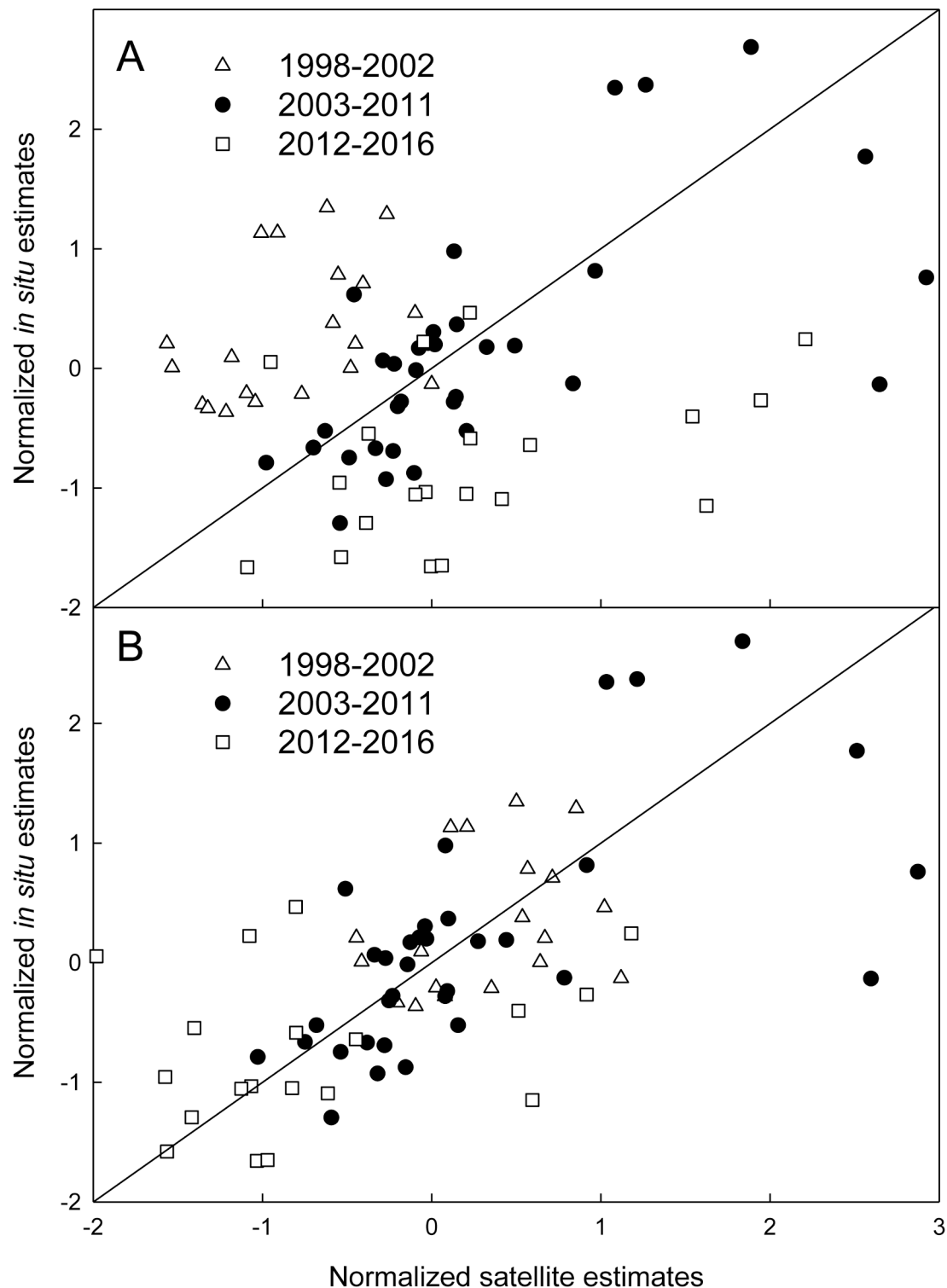


Fig. 5. Normalized *in situ* versus satellite chlorophyll values for all years and stations. A) Values before correction. B) Values after correction with Eq. (1). The 1:1 line is shown.

situ estimates at stations covering a decreasing chlorophyll gradient from near shore coastal to the open part of the Kattegat.

Although *in situ* and satellite data showed similar seasonal patterns in chlorophyll value, the satellites greatly underestimated the spring blooms for most years, especially prominent in the year 1998–2002, as compared to *in situ* data. This underestimation by satellites was evident when comparing both seasonal trends and long-term time series of the growing season average values.

Water-leaving reflectance measured by satellite sensors depends on the amount and angle of the solar radiation. When the angle of the incoming light is low, as during the winter months in Northern Europe, the major part of the light is absorbed and scattered in the atmosphere, and the signal/noise ratio of the radiance used to calculate the reflectance from the satellite sensor is low

(Sathyendranath, 2000). This not only limits the period for satellite observations between late March and October, but also affects the

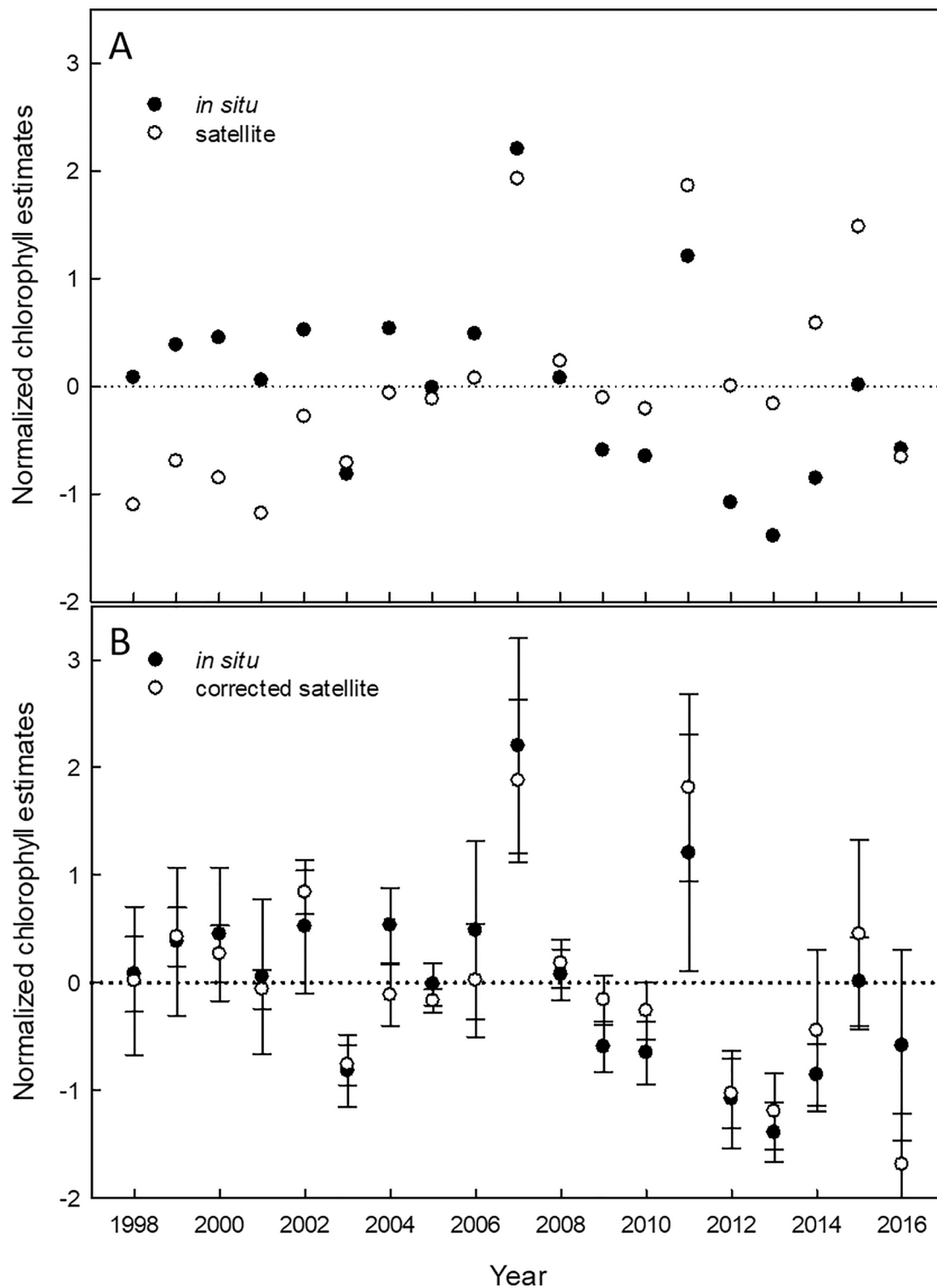


Fig. 6. Time series of normalized (mean = zero, STDEV = 1) chlorophyll concentration estimated with two methods for four stations in the Kattegat region from 1998 to 2016. A) Non-corrected data where error bars are omitted for clarity. B) Values where satellites estimates are corrected using Eq. (1) and error bars (\pm STDEV) are shown.

possibility of capturing the real extent of early spring and a part of autumn bloom leading to larger offset between estimates from satellite and *in situ* techniques, as observed in this study. This limitation of satellite to capture early spring and autumn bloom has also been highlighted in a study in the Baltic Sea which warranted caution on interpretation of satellite data during this period (Harvey et al., 2015). This combination of the lack of data due to cloud cover and the low sun

angle affecting the reflectance restricts and challenges the usefulness of satellites, especially during the early spring and autumn bloom period.

Comparing trends in long-term growing season averages of chlorophyll at four different sampling stations, satellite and *in situ* both showed a similar pattern over years. However, a systematic overestimation of chlorophyll by satellites compared to *in situ* estimates was observed in the coastal areas. Satellite performance was better in open water areas

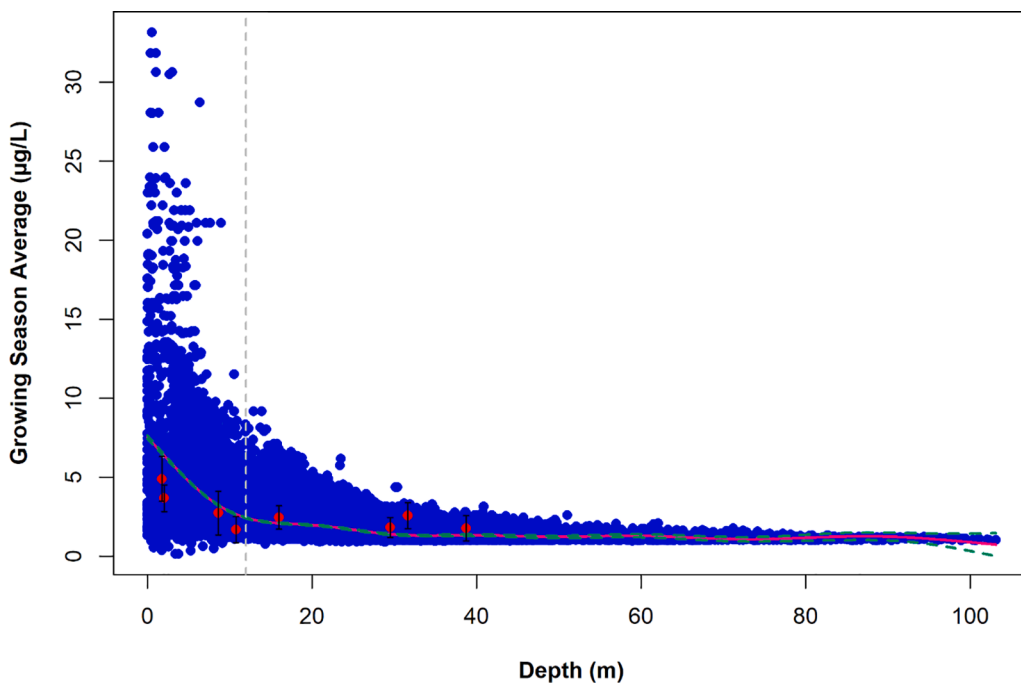


Fig. 7. Satellite derived growing season average chlorophyll (blue circle) throughout the entire Kattegat plotted for sites across the depth gradients. 12 m depth which is the depth of the permanent pycnocline is marked with a dashed grey line. *In situ* estimates from eight stations (including four additional stations) are shown with red diamonds. Error bars for *in situ* are STDEV of the growing season average estimates. Pink line represents the GAM model estimated from satellite values with 95 % confidence interval as green striped lines. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

further away from the shore where interferences from land or the sea floor was lower. While the deviation between *in situ* and satellite estimates were very small and insignificant for the open water stations, the variability in chlorophyll estimates through satellites were up to 2–4 times higher for the coastal stations, whereas the variability was uniform for the four stations for *in situ* sampling. The extreme and unrealistic high chlorophyll values reported by satellites closer to the coast is not uncommon, and suggest interferences from benthic vegetation or the sea floor reflectance (Gohin et al., 2008; Staehr et al., 2019). In addition, the interference from high levels of CDOM and suspended material may also be an important issue in the studied region (Kowalczyk et al., 2006; Pitarch et al., 2016). However, the issue is complicated further by the fact that chlorophyll values are generally higher in shallow water, due to inflow from nearby freshwater sources and efflux of nutrients from the sediment into the photic zone, both stimulating algal growth, as observed also through *in situ* observations (Fig. 7). Hence, it is difficult to distinguish high values caused artifacts such as reflection from the sea floor, resuspension of sediment and in some cases outflow of CDOM from rivers and streams from correctly elevated chlorophyll values closer to the coast.

The studied Baltic region is widely recognized as a challenging area for ocean color remote sensing due to not only high concentrations of CDOM but also of suspended materials (Kowalczyk et al., 2006; Mélin and Vantrepotte, 2015; Pitarch et al., 2016). Overestimation of chlorophyll through satellites in the Baltic Sea with Case 2 waters are therefore not uncommon (Attila et al., 2013; Darecki and Stramski, 2004). Our findings of overestimation of chlorophyll by satellites is supported by a recent study by Pitarch et al. (2016) in the Kattegat region, that observed up to 45% overestimation despite using a Baltic Sea-Specific chlorophyll algorithm. This indicates that it is technically challenging to utilize ocean color signals in the Kattegat region, and highlights the importance to apply sensors and algorithms, which adequately accounts for the CDOM effect on chlorophyll estimates to reduce this potential bias (Tassan, 1988). We hope that these shortcomings can be solved in the future, particular with the Sentinel program, which is expected to aid in the separation of the CDOM contribution with the addition of 400 nm band, given the proper atmospheric correction is applied (Pitarch et al., 2016).

Furthermore, satellites showed significant systematic deviations

from *in situ* measurements, when comparing long-term changes in growing season means, providing uncertainty in detection of trends in chlorophyll levels. Given that the environmental status is monitored and the management decision is made based on the long-term time series trends, this also has implications on the usefulness of satellites for management of water quality. While new satellites like Sentinel 3 are likely to perform better, analysis of long-term trends from satellites requires ways of correcting and reducing deviations from ship based *in situ* data. In this study, we showed that application of a simple correction factor to the satellite using the *in situ* observations improved the alignment between two methods greatly.

Looking beyond uncertainties associated with satellite observations, these were found advantageous in terms of providing a much better temporal and spatial coverage of chlorophyll observations, in particular during the mid-summer period. Despite issues with cloud cover reducing the number of useful satellite images, there were on average 44 satellite observations each year during the growing season period for the station in the Anholt East (St 32002), as compared to 15 observations by ship based *in situ* monitoring. Analyzing the frequency and variability, the satellites generally provided chlorophyll at higher frequency and with a smaller time lap and less variability than *in situ* samples. For example, Anholt East (St 32002) was sampled on average every fifth day with satellites compared to 14 days sampling interval for ship based *in situ* monitoring. Clearly satellites provided much more information on chlorophyll concentrations compared to *in situ* measurements during the growing season period. In this respect, satellites provide higher confidence to estimate growing season averages as compared to the patchily available *in situ* measurements.

In conclusion, despite several spatial and temporal advantages over *in situ*, we find that multisensory satellites currently cannot be used as a standalone technique to determine the chlorophyll based long-term trends in Good Ecological Status in the Kattegat region without validation with *in situ* observations. As also highlighted by Gohin et al. (2019), we conclude from our study that a detailed analysis of the correspondence between satellite and *in situ* data is crucial, not just to assess the performance of the satellite, but to enable correction and insure the optimal use of satellite data in monitoring and assessment of environmental status. Although multisensory satellites provide a promising supplement to contemporary monitoring of environmental status of the

Kattegat, they are strongly reliant on *in situ* data for validation and assessment of uncertainties related to proximity to land, water depth and seasonal coverage, thereby limiting their overall applicability. We hope that these shortcomings will be solved in the future, particular with the Sentinel program which are designed for environmental monitoring, with Sentinel-3 specifically for aquatic systems applications. Currently, multisensory satellite observations should be viewed as complementary and valuable supplement rather than exclusive of ship based observations of chlorophyll.

CRedit authorship contribution statement

Sanjina Upadhyay Staehr: Conceptualization, Methodology, Investigation, Formal analysis, Writing – original draft, Writing – review & editing. **Dimitry Van der Zande:** Formal analysis, Methodology, Writing – review & editing, Resources. **Peter A.U. Staehr:** Conceptualization, Methodology, Writing – review & editing. **Stiig Markager:** Conceptualization, Formal analysis, Methodology, Writing – review & editing, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ecolind.2021.108479>.

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