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Applicability of Earth Observation chlorophyll-*a* data in assessment of water status via MERIS — With implications for the use of OLCI sensors

Jenni Attila*, Pirkko Kauppila, Kari Y. Kallio, Hanna Alasalmi, Vesa Keto, Eeva Bruun, Sampsa Koponen

Finnish Environment Institute, P.O. Box 140, FI-00251 Helsinki, Finland

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ABSTRACT

Earth Observation (EO) offers spatially and temporally unique data for generating information required under various environmental regulations for assessing the status of surface waters. These requirements, which are laid down in, for example, European Union directives and the Clean Water Act in the United States, share two core elements with respect to status assessments: 1) the status assessment is done using discrete classes, typically for water bodies, sub-areas or critical sites representative for certain area of interest, and 2) phytoplankton chlorophyll *a* (chl-a) is one of the main variables considered. We analysed the benefits of using chl-a concentrations derived from EO data for the status assessments specified in the EU Water Framework Directive (WFD). Our study focused especially on EO observations' ability to capture extreme and transient events (such as instances of cyanobacteria blooms) more frequently than the monitoring-station data conventionally employs. The accuracy of EO-based chl-a assessment was studied for, in all, 129 Finnish water bodies in the area of the Baltic Sea, in Northern Europe. Natural conditions in this coastal area – particularly its multitude of small bays, numerous estuaries, and mosaic of islands – impose exceptionally strict requirements for an EO instrument's spatial resolution. The analysis revealed that an instrument with a 300 m resolution, such as the MEdium Resolution Imaging Spectrometer (MERIS) or Ocean and Land Colour Instrument (OLCI), can be used to estimate the water quality in 62% of these water bodies. Processing of MERIS data into chl-a concentrations by means of a FUB inversion model demonstrated good accuracy relative to monitoring stations' measurements for the open-water season in 2003–2011. This extensive dataset showed a 23% difference in modal values between EO- and station-sampling-based chl-a concentrations. The bias in EO chl-a estimates was found to increase with low Secchi disk depth, elevated turbidity, and the presence of intensive phytoplankton blooms. The monitoring-station and EO data showed similar distributions of chl-a observations for a given day and location, a finding that supports the comprehensive use of EO-derived chl-a concentrations in assessment. For determination of a water body's status, the EO data required but also allowed for statistical analysis that differs from what has typically been utilised with sparse measurements from monitoring-station data. The geometric mean or the mode of the EO observations was found to represent the main bulk of the chl-a concentrations well statistically. In contrast, the arithmetic mean of EO observations yields chl-a concentrations that are roughly 1.1–1.6 μg/l higher and hence can lead to over-estimation in the associated status assessment. This paper also presents a new approach applicable for evaluating the validity of EO-based algorithms for any coastal water area requiring assessment. With this quality-grade (QG) method, the EO chl-a estimation accuracy is rated in terms of three grades, with water bodies taken as the evaluation units. For this, the method utilises statistical differences between EO and station-sampling chl-a concentrations and applies background information on optical properties obtained from measurements at routine-monitoring stations. The QG method showed the EO-based chl-a accuracy to suffice for assessing the status of 65% of the coastal water bodies examined. At concentrations representing the threshold for the target of "good status" under the WFD, the EO approach produced 0.6 μg/l higher chl-a values than the stations' sampling did. The MERIS results point to clear benefits of using OLCI-based status assessment throughout the Sentinel-3 era.

* Corresponding author.
E-mail address: jenni.attila@ymparisto.fi (J. Attila).

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1. Introduction

Requirements for comprehensive water-quality monitoring for purposes of assessing coastal marine waters' ecological and environmental status have been set by various regulations, among them the European Union's Water Framework Directive, or WFD (Ferreira et al., 2007), and Marine Strategy Framework Directive, MSFD (Zampoukas et al., 2013), and the Clean Water Act, or CWA, in the USA. The stricter demands imposed by these regulations call for efficient implementation and full use of sophisticated automatic monitoring methods and advanced approaches to utilising them. Clearly, it is impractical to base the status assessments on data derived from conventional station-based monitoring alone. The benefits of using Earth Observation (EO) data for the status assessments required in coastal areas under the WFD have been analysed by, for example, Domingues et al. (2008), Gohin et al. (2008), Novoa et al. (2012), Kratzer et al. (2014) and Harvey et al. (2015), and the advantages for inland waters have been considered by Bresciani et al. (2011) and Alikas et al. (2015). With respect to MSFD specifications, EO data have been found beneficial likewise in relation to Portuguese marine waters (Cristina et al., 2015). Beyond the EU, similar needs for EO's application in status assessment were studied in the coastal waters of Florida (Hu et al., 2004). The US Environmental Protection Agency (EPA) has identified 450 target sites for collection of water-quality data, such as chlorophyll-*a* levels, for work in the "Estuary" portion of the Environmental Monitoring and Assessment Program (EMAP-E). As every state carries out its own monitoring, employing various sampling designs and indicators (EPA, 2000), the future use of EO data should ensure consistency across the status assessment (Hu et al., 2004). Furthermore, studies examining the utility of EO data for meeting national assessment needs have already been carried out, with specific reference to the coastal waters of Vietnam (Loisel et al., 2017) and the needs of South Africa (Matthews et al., 2010) in respect of national environmental legislation (van Ginkel, 2003). In general, not only national monitoring programmes, such as EPA, EMAP, and DWAF work, but also international schemes cover phytoplankton chlorophyll-*a* (chl-a). For instance, marine-environment protection conventions such as the North-East Atlantic's OSPAR efforts, HELCOM's for the Baltic Sea, and the Black-Sea-focused Bucharest Convention all entail implementing the associated provisions of the MSFD. At any rate, the potential to improve and extend monitoring and assessment through the aid of EO data has been acknowledged world-wide.

However, algorithms for calculating chl-a concentrations from EO data can be especially sensitive to error sources in coastal waters. The area we chose for study, in the northern Baltic Sea, is an optically specific absorption- and pigment-scattering-dominated marine coastal area that represents an extreme among Case II waters (Gordon and Morel, 1983; Morel, 1988; Morel and Prieur, 1977), with especially high absorption of coloured dissolved organic matter, or CDOM (a_{CDOM}). For deriving water-quality information for a water body of this type, the capabilities of medium-resolution imaging spectrometer (MERIS) Envisat instrumentation and the Ocean Land Colour Instrument (OLCI) on-board the Sentinel-3 satellites offer particular advantages (Donlon et al., 2012), thanks to their spectral characteristics but also with 300 m spatial resolution (Härmä et al., 2001; Kallio et al., 2001; Kratzer et al., 2008). Several studies have examined the accuracy of various algorithms' determination of chl-a from MERIS data for Case II waters (Attila et al., 2013; Beltrán-Abaunza et al., 2014; Harvey et al., 2015; Kallio et al., 2015; Kratzer et al., 2008; Loisel et al., 2017; Matthews, 2011; Odermatt et al., 2012; Reinart and Kutser, 2006; Tilstone et al., 2017). The overall conclusion from this research is that the capability of an inversion model, empirical algorithm, or semi-empirical band algorithm to interpret chl-a is related to the optical properties of the water area and depends greatly on the water region of interest. Among the influential properties are the concentration ranges of the optically important water constituents, their relative contributions, and the specific inherent optical properties (SIOPs) of the water body. Therefore, an algorithm that is suitable for highly turbid Case II environments may produce results that do not suffice for other, CDOM- and phytoplankton-absorption-dominated Case II waters. Furthermore, the optical properties of coastal waters can vary greatly within small spatial scale. The water entering river estuaries from drainage basins influences the optical characteristics of coastal waters mainly by increasing the concentrations of total suspended matter (TSM) and the absorption of CDOM (e.g., Alexandridis et al., 2016; Cherukuru et al., 2016; Corbari et al., 2015; Saldías et al., 2016). In addition, the sunlight reflected from the bottom of the sea in shallow coastal areas can influence interpretations of chl-a concentrations from EO data (Baban, 1993; Hellweger et al., 2004). During the season chosen for the WFD-specified ecological classification in our study – the middle of summer in Finnish coastal waters – the level of suspended matter and humus may temporarily increase in response to runoff after heavy rains. Therefore, in estuaries and in waters shallower than their transparency level (Baban, 1993; Höjerslev, 1977), EO-derived chl-a estimates may be biased.

A useful starting point for our work was provided by Kratzer et al. (2008), Kratzer and Vinterhav, 2010 and Beltrán-Abaunza et al. (2014), who used the coastal estuaries of the Baltic Sea as a context for cross-comparing several algorithms for chl-a estimation using MERIS data. These studies indicated that the inversion model developed at the Free University of Berlin, the "FUB model" (Schroeder et al., 2007a, 2007b), estimated chl-a concentrations better than the other examined processors, such as MERIS ground segment processor (MEGS) and the Case-2 regional processor (C2R) (Doerffer and Schiller, 2007). The assessment of coastal water bodies is not feasible with the Baltic Sea chl-a products generated by the Copernicus Marine Environment Monitoring Service (CMEMS) (Pitarch et al., 2016; CMEMS Quality Information Document, 2016) due to its 1-4 km spatial resolution and its limited accuracy in comparison to in situ data over the Baltic Sea ($r^2 = 0.2$ and $r^2 = 0.46$ for 1 km product and reprocessed time series (4 km, REP), respectively, Pitarch et al., 2016).

In this paper, we examine the benefits of EO chl-a for meeting status-assessment requirements and demonstrate ways to ascertain the approach's accuracy with regard to a given water body. We demonstrated it by the EU WFD's requirement of assessing the status of Finnish coastal waters with respect to chl-a. The overall objective behind the directive is to achieve a good ecological status for surface waters by 2021 (Ferreira et al., 2007). The status assessment for the water bodies under the WFD is performed in line with an ecological classification that has five classes (excellent, good, moderate, poor, and bad). The boundary that is most relevant with regard to the target of the WFD – reaching "good" status – is that between "good" and "moderate": if a water body does not meet the target, the WFD requires that the Member State initiate water-protection measures to improve its condition. Accordingly, highly reliable ways of determining chl-a concentrations near this class boundary are needed.

EO is able to produce much higher volumes of data than traditional measurements from monitoring stations can. In the Baltic Sea, during intensive and small-scaled surface-floating cyanobacteria blooms of mid-summer season, the EO-derived estimates of chl-a may vary between one and several hundred μg/l over small distances, and the concentrations estimated by EO chl-a can be one to two orders of magnitude higher than the concentrations measured from mixed water layer with bottle samples at monitoring stations (Reinart and Kutser, 2006). For status assessments, the monitoring at station locations have been targeted to determine the average level of chl-a concentration and to identify inter-annual variation, whereas the coastal sampling has not been organized to catch the most extreme concentrations occurring during the cyanobacteria bloom situations. Ideally, the locations of the sampling sites should be spatially and temporally representative to meet the monitoring and assessment obligations set, among others, by the EU directives, but, in practice, this is not always the case especially as regards to the water bodies in the outer archipelago. During the

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