Satellite monitoring of algal blooms in Norwegian coastal waters

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The degree philosophiae doctor (PhD)

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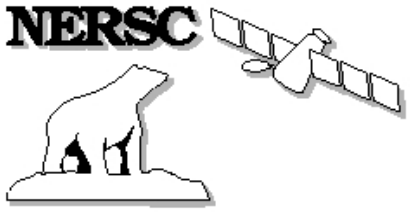

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Are Folkestad

Contents

1. Introduction

During the last decades, an increasing number of harmful algal blooms (HABs) have been reported worldwide, and received a lot of attention due to their negative impact on the marine environment in which they occur (Hallegraeff *et al.* 2003). HAB events are characterised by two main features; they are caused by microalgae and they have a negative impact on human health and/or activities such as fisheries, aquaculture, and tourism. Despite these common features, HABs are very diverse in terms of harmfulness, causative organisms, dynamics of blooms and types of impact.

Also in Norwegian coastal waters, an increasing amount of HAB events have been reported during the last 25 years. Some of these events have resulted in significant mortality of farmed salmon and economic losses to fish farmers. These occasions have been associated with high biomass blooms of phytoplankton species such as the dinoflagellate *Gyrodinium aureolum* (Dahl and Tangen, 1993) and the flagellates *Chrysochromulina polylepis* in 1988 and 1991 (Dundas *et al.* 1989, Johannessen *et al.* 1989) and *Chattonella* spp. in 1998, 2000 and 2001 (Horstmann *et al.* 1998, Durand *et al.* 2002, Pettersson *et al.* 2005).

Substantial efforts have been provided to understand and monitor HABs, as reviewed by Hallegraeff *et al.* (2003). Optical detection for assessment of harmful algal blooms has been demonstrated (Cullen *et al.* 1997) including the use of satellite ocean colour (Zeichen and Robinson 2004, Bernard *et al.* 2005, Gower *et al.* 2005). The ocean colour refers to spectral characteristics of the ocean reflectance, which is the ratio of solar radiation propagating upwards from beneath the surface to the solar radiation entering the sea surface from above. Variations in the spectral distribution of the reflectance in the visible part of the electromagnetic spectrum can be detected by ocean colour sensors mounted on satellites orbiting the earth. This is demonstrated in Fig. 1 for an algal bloom along the coast of south-western Norway. The quantitative reflectance measurements can be interpreted to provide information about the phytoplankton biomass, through estimations of the phytoplankton pigment Chlorophyll-a (Chl-a, Fig. 2).

As a part of investigating the concept and challenges of ocean colour remote sensing we need to understand the components and processes that are influencing the light field in the ocean. The ocean colour is determined by absorption and scattering of visible light by pure water

Figure 1: A phytoplankton bloom along the Norwegian west coast. This true colour composite was obtained from an image taken by the SeaWiFS sensor in June 2000. Data courtesy: NASA.

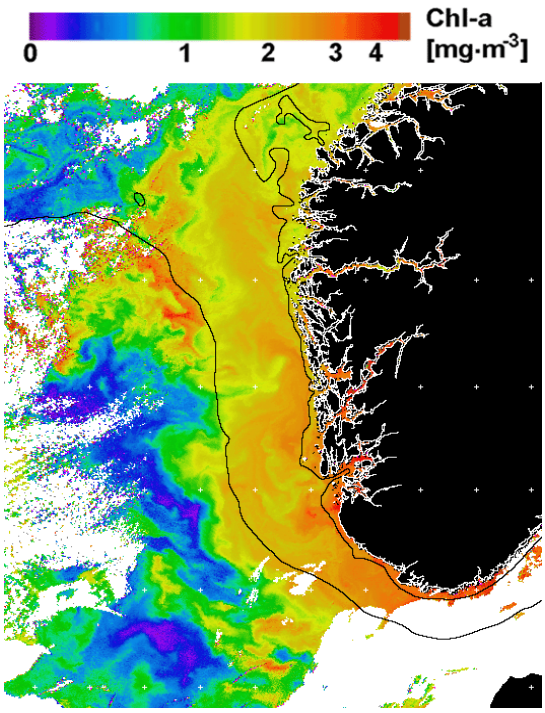

Figure 2: Concentrations of the phytoplankton pigment chlorophyll-a retrieved from the same image as Fig. 1. Black lines indicate bottom depth of 200m. Data courtesy: NASA.

itself, as well as by the inorganic and organic, particulate and dissolved, material present in the water. In order to model the aquatic light propagation it is useful to differentiate the various water constituents into components with similar absorption and scattering properties. These can be referred to as the colour producing agents (CPAs). Often three main CPAs are defined, namely phytoplankton represented by its photosynthetic pigment Chl-a, total suspended matter (TSM) including both organic and inorganic particulate matter, and Yellow Substances (YS) including fulvic and humic acids, also referred to as coloured dissolved organic matter (CDOM). The concentration of Chl-a is used as a proxy of the phytoplankton biomass. This parameter is therefore very important for mapping the biological activity at the ocean surface, including e.g. monitoring of algal blooms and estimation of primary production.

When dealing with open ocean waters, phytoplankton (and its co-varying retinue of material of organic origin) is the dominant component influencing the light regime, apart from the pure water itself. In these waters, referred to as Case I (Morel and Prieur, 1977), the optical contribution from YS and TSM are either assumed to be small compared to Chl-a, or they can

be quantified as functions of Chl-a. In contrast, Case II waters are defined to contain TSM and/or YS varying independently of Chl-a, and in such amounts that they significantly influence the optical properties in the water. Case II waters are generally found in inland and coastal water bodies, carrying YS and TSM from terrestrial sources by e.g. river runoff. Re-suspensions of bottom sediments can also occur in shallow waters, increasing the TSM concentration in the water column.

A commonly used parameter in the field of ocean colour is the remote sensing reflectance, R_{rs}, which is defined as the ratio between the upwelling radiance, L_w, just above the water surface to the downwelling irradiance, E_d, at the same level. R_{rs} is a function of wavelength, λ, as well as the viewing angle. Several studies have shown that R_{rs} can be expressed in terms of the absorption coefficient, $a(\lambda)$ and the backscattering coefficient, $b_b(\lambda)$ in the water (IOCCG 2000). In Case I waters variations in $a(\lambda)$ and $b_b(\lambda)$ are due to phytoplankton only. Consequently, simple empirical relationships can be established between Chl-a and variations in R_{rs}, when a large number of concurrent *in situ* measurements of these two parameters are undertaken (O'Reilly 1998, 2000, Morel and Antoine 2000). On the other hand, in Case II waters TSM, YS, and phytoplankton contribute to $a(\lambda)$ and $b_b(\lambda)$ independently and in a non-linear manner. However, the contribution to $a(\lambda)$ and $b_b(\lambda)$ from each CPA are additive, and can for each CPA be expressed as the product between the concentration of the constituent and its concentration specific absorption and backscattering coefficient, respectively. These coefficients are collectively termed specific inherent optical properties (SIOP). The SIOP are functions of the wavelength, and can vary substantially between different water bodies containing various types of constituents (IOCCG 2000). Thus, even though expressions relating the SIOP and CPA concentrations to R_{rs} in principle can be universally applicable for Case II waters, the coefficients of SIOP must be determined for each water body in question.

In the absence of clouds, satellite ocean colour sensors can be used to retrieve R_{rs} at the surface. The sensors measure the radiance at the top of the atmosphere (TOA) in distinct wavelength bands in the visible and near-infrared (NIR) domains of the electromagnetic spectrum, aiming at the surface of the earth in a narrow field of view (FOV). Due to scanning devices and the movement of the sensor data are acquired from different points on the earth, with a spatial resolution of up to 300m. Depending on the FOV and the latitude a single point on the surface is mapped every 1-3 days. Thus, ocean colour sensors provide data on a large

synoptic regional scale with relatively high temporal resolution. These are the major advantages of ocean colour sensors as compared to sea-based observation systems. Under cloud free conditions ocean colour data is therefore a very cost-efficient way to monitor the biological status of the ocean surface layer. The regional synoptic overview enables mapping of the horizontal distribution of water constituents in the water surface, as well as detection of fronts between water masses, and their movement.

The light reaching the satellite sensor originates ultimately from the sun. However, the remotely sensed signal over the ocean can be divided into three main components: light scattered by atmospheric molecules and aerosols; specularly reflected direct sunlight at the water surface; and light upwelling from beneath the sea surface after being backscattered in the water. As mentioned above, the latter component is the only one carrying useful information about the water constituents. In this context the other two components of the detected signal constitute noise, and must be corrected for. In fact, atmospheric contribution may account for more than 80% of the TOA signal (Morel 1980). Due to temporal and spatial variability of the types and amount of aerosol, quantifying the atmospheric contribution is a difficult task. The situation is further complicated over coastal waters, where the mixing of various types of aerosols frequently occur. A lot of scientific efforts have therefore been invested in modelling the optical properties of the aerosols, as well as in the development of algorithms for atmospheric correction (Gordon and Wang 1994, Antoine and Morel 1999, Moore *et al*. 1999, Ruddick *et al*. 2000, Siegel *et al*. 2000).

Even if R_{rs} is perfectly retrieved after atmospheric correction, several factors limit or complicate the use of ocean colour data for HAB detection and monitoring. Even though methods are being developed for discrimination between different algae groups, the ocean colour data is not able to determine the harmfulness of a detected bloom. Furthermore, R_{rs} is representing the optical status in the upper few metres of the water column. Bloom formations below this depth can therefore not be detected by the ocean colour sensor. The presence of some algae species can also cause large negative impact even in low concentrations, and may consequently not be detected as a possible harmful event.

The optical complexity of coastal waters calls for sophisticated algorithms for interpreting the ocean colour data. Several approaches have been developed to obtain quantitative information of optical properties and CPA concentrations from R_{rs} measured by the satellite sensors.

These approaches range from simple empirical to complex analytical model-based algorithms, as reviewed by IOCCG (2000). However, common to all approaches is that they need a certain degree of local tuning to the optical properties of the water constituents for the water body in question. As addressed above the SIOP of the CPA in these waters can provide a quantitative relationship between the CPA concentrations and the remotely sensed R_{rs}. Even within a defined region SIOP can exhibit large spatial and temporal variability, due to e.g. fluctuations in the algae community composition, varying impact from terrestrial sources, as well as variations in vertical mixing of water masses and in ocean circulation patterns. The natural SIOP variability clearly complicates the task of interpreting ocean colour data in these areas. Case II water algorithms should therefore be developed to take this variability into account. Another difficulty arises in shallow waters. If not properly corrected for, the contribution to R_{rs} from reflectance at the sea bed may significantly influence the CPA concentration retrievals.

The water masses present along the Norwegian coast originate from mixing between warm, saline and nutrient-rich Atlantic water and brackish water from the Baltic Sea. Inorganic particulate matter is often brought into suspension in the shallow waters close to the Danish coast. The mixing of the water masses occurs in the inner part of the Skagerrak. Freshwater containing yellow substances is also entering the area from adjacent rivers. The flow of the mixed water masses continues along the Norwegian coast as the Norwegian Coastal Current (NCC) (Sætre and Mork 1981). Consequently, the Skagerrak and NCC waters must be treated as Case II waters in ocean colour remote sensing. The problem with atmospheric correction over coastal waters as described above is also persistent in this area.

Several ocean colour sensors have been operating during the last decade. Among these are the Sea-Viewing Wide Field-of-View sensor (SeaWiFS), launched in 1997 (Hooker *et al.* 1992), the Medium Resolution Imaging Spectrometer Instrument (MERIS) launched in 2002 (Rast *et al.* 2000), and the Moderate Resolution Imaging Spectroradiometer (MODIS) onboard the Terra and Aqua satellites launched in 1999 and 2002, respectively (Esaias et al. 1998). All of these sensors measure R_{rs} in the visible. However, the sensors differ in terms of their technical specifications, including the number and position of wavelength bands. A great challenge is therefore to ensure consistency between equivalent data products obtained from the various sensors.

2. Objectives

The main objectives of the thesis have been to implement and validate a new analytical inverse algorithm for improved processing of ocean colour data in Norwegian coastal waters, and to investigate the capabilities of various operational ocean colour sensors for algal bloom monitoring. Several specific tasks were accordingly formulated.

The first task was to quantify the differences between the SeaWiFS, MODIS, and MERIS sensors with respect to their standard Chl-a products. Moreover, the capabilities of the various sensors for algal bloom monitoring were examined regarding their respective available standard data products. These tasks were dealt with in Paper I.

Three specific tasks were carried out in Paper II. Firstly, SIOP were retrieved from ship borne data collected in Norwegian coastal waters. Second, the SIOP and *in situ* CPA concentrations were fed into a hydro-bio-optical model (HBOM) that was used to estimate the subsurface remote sensing reflectance, R_{rsw}. Third, an inverse method was introduced to retrieve CPA concentrations from measured R_{rsw}. An operational algorithm applying this integrated approach was also tested for sensitivity to SIOP variability.

The inverse algorithm introduced in Paper II was also applied to real satellite data over Norwegian waters and thoroughly validated against synoptic ship borne observations. Subsequent quality testing and evaluation of the algorithm performance was performed. These tasks were undertaken in Paper III.

3. Data and Methods

The ocean colour data processed and analyzed in this thesis were obtained from the SeaWiFS, MODIS and MERIS sensors. Data from SeaWiFS and MODIS were provided by the National Aeronautics and Space Administration (NASA), while MERIS data were provided by the European Space Agency (ESA).

Ship borne data were obtained from several sources. Data from a cruise in May 2002 on board R/V “Håkon Mosby“ in the Norwegian Coastal Current were used for obtaining a set of concentration specific inherent optical properties (SIOP) needed for operating the new inverse

algorithm. This cruise was a joint effort between NERSC and the Norwegian Institute for Water Research (NIVA) in Oslo. Two short cruises in the Skagerrak performed by NIVA in June and August 2002 provided data for testing the inverse algorithm. Data from the Ferrybox system operated by NIVA onboard a ship of opportunity in Skagerrak in 2003 and 2004 provided data for *in situ* validation of the ocean colour algorithms using MERIS data.

The inverse algorithm introduced in this study converts the satellite-measured R_{rsw} to CPA through the use of a forward hydro-bio-optical model and a multivariate optimization procedure. The algorithm is described in more detail in Papers I and II and was selected based on several criteria. First of all, the algorithm has previously proven to retrieve accurate estimates of CPA concentrations for other optically complex inland and coastal waters (Pozdnyakov and Grassl 2003, Pozdnyakov *et al.* 2003, 2005a). It has also shown to be adequately robust to noise in the input data (Pozdnyakov *et al.* 2005b). In contrast to empirical algorithms developed for Case 1 waters, the selected algorithm simultaneously retrieves concentrations of the major constituents that influence the water colour. This is a prerequisite for obtaining adequate results in Case 2 waters, since the various components are not co-varying with each other. The algorithm itself is not site-specific, as it reads an external tabulated set of spectral SIOP coefficients. Thus, the algorithm can readily be applied to any water body, as long as this tabulated set is available for the water body in question. Finally, the core of the algorithm is not sensor-specific. In other words, it is capable of processing input reflectance spectra from sensors with different spectral resolution and band configuration. Previous applications of the algorithm include processing of SeaWiFS and MODIS data, suggesting that processing of MERIS data could also be adequately performed.

4. Key results

Paper I: Inter-comparison of ocean colour data products during algal blooms in the Skagerrak

In this paper, concurrent images obtained by the SeaWiFS, MODIS, and MERIS sensors were compared by several methods. The data were acquired during an early algal spring bloom in Skagerrak in 2004. The study shows a high level of correlation between all sensors with regards to the Case 1 water Chl-a products. Further, the agreement between Chl-a products for each pair of sensors depends on the method of comparison. The better correlation is found for

data averaged over large areas (~100-1000km^2) pre-selected to depict homogeneous values of Chl-a, as compared to data averaged over small areas (~30km^2) that were not pre-selected as being homogeneous. The discrepancies between sensors when comparing large areas are assessed to be mostly due to inherent sensor and algorithm differences. For small areas the discrepancies can also be explained by temporal variability in observation conditions on time scales less than the difference in overpass time between the sensors (2-3 hours). Comparisons between the MERIS Case 2 water Chl-a product, all sensors' Case 1 water Chl-a products, and *in situ* Chl-a measurements were also performed. These comparisons do not give a clear conclusion as to which Chl-a product that is the most reliable. On the other hand the study demonstrates that interpreting additional available MERIS products (e.g. quality flags, and concentrations of suspended particulate matter and yellow substance) in concert with Chl-a estimation for both Case 1 and 2 waters possibly improves the overall understanding of the atmospheric and marine conditions at the time of data acquisition.

Paper II: Parameterization and sensitivity testing of a hydro-bio-optical model for Norwegian coastal waters.

In this paper, a hydro-bio-optical model (HBOM) has been parameterized for Norwegian coastal waters. The model relates in-water concentrations of colour producing agents (CPAs) and their corresponding specific inherent optical properties (SIOP) coefficients to spectral subsurface remote sensing reflectance, R_{rsw}. The CPAs are divided into Chl-a, Total Suspended Matter (TSM), and Yellow Substance (YS). The relevant SIOP coefficients were in this study obtained from ship borne data and the observed values generally fall within the ranges reported in the literature (Roesler *et al.* 1989, Bricaud *et al.* 1995, Nelson and Guarda 1995, Bowers *et al.* 1996, Høkedal 1999, Ferrari 2000, IOCCG 2000, Stedmon *et al.* 2000, Højerslev and Aas 2001, Babin *et al.* 2003, and Aas *et al.* 2005). However, the number of ship borne observations is low and the observed SIOP variability is high.

The HBOM was further used in an inverse algorithm to retrieve the CPA concentrations from R_{rsw}. When applied to ship borne data, the inverse algorithm accurately retrieved concentrations of the water constituents for the majority of the observations, even though in some cases substantial retrieval errors were observed. For practical use of the inverse algorithm on satellite ocean colour data the impact of the observed variability of the SIOP coefficients on algorithm retrieval accuracy was quantified. A sensitivity test showed that the retrieval accuracy of Chl-a and TSM is highly affected by the variability in the TSM

backscattering coefficient, $b_b{}^*_{TSM}(\lambda)$. Furthermore, the SIOP of the dominant water constituent need to be modelled accurately in order to minimize the retrieval error of Chl-a. The inverse algorithm used in this study has previously been applied to satellite ocean colour data from various inland and coastal water bodies. The results obtained in this study enable for the first time the algorithm to be applied to satellite imagery from Norwegian coastal waters (Paper III), and indicate further the expected accuracy of the algorithm retrievals.

Paper III: An analytical Case 2 water algorithm for Norwegian coastal waters.

In the study presented in this paper the algorithm introduced in Paper II was for the first time applied to satellite ocean colour data from Norwegian waters. Relevant *in situ* measured parameters obtained from the Ferrybox system in the Skagerrak were used for validation of the algorithm when applied to synoptically acquired data from the MERIS sensor. An error function, *f*, that is an output parameter of the algorithm proved to be an important tool for assessing the accuracy of the retrieved results. The agreement between *in situ* and inversely retrieved CPA concentrations increased when the comparison was confined to observations for which *f* was below a certain threshold (f <0.05). In that case 45.0% (55.0%) and 51.6% (82.6%) of the inverse algorithm Chl-a concentrations were retrieved within 35% (70%) error relative to *in situ* Chl-a determined by HPLC and fluorescence methods. For the standard MERIS Chl-a algorithm the equivalent numbers were 10.0% (15.0%) and 31.2% (53.0%). Concentrations of TSM were inversely retrieved within 70% error for 85.2% of the observations when compared to *in situ* turbidity. For the standard MERIS TSM algorithm the equivalent number was 95.5%. No validation of YS was performed due to lack of relevant *in situ* observations. However, the features observed when comparing YS retrievals with measurements of salinity along the SOOP transect were indicating a good algorithm performance regarding the YS parameter. When comparing *in situ* and satellite data several factors reduce the expected agreement. These factors include e.g. the time difference between water sampling and satellite overpass, difference in spatial resolution between *in situ* and satellite data, natural SIOP variability, and uncertainties in atmospheric correction. Taking these sources of uncertainty into account the observed retrieval accuracy is well within the expected range.

To further evaluate the algorithm performance 133 MERIS images from March to May 2005 covering the Norwegian coastal waters south of 66°N were processed by the algorithm. The

results revealed realistic patterns regarding seasonal dynamics of the water constituents, and were used to study the evolution of a phytoplankton spring bloom in the area. It was also shown that the algorithm is capable of processing reflectance spectra from waters containing a wide range of concentrations of the three CPA components.

5. Summary and future perspectives

Paper I: The agreement between the three different satellite sensors compared in this study indicates that retrievals by the Case I water Chl-a product are not significantly dependent on which of the three sensors is used. However, when using data from the MERIS sensor, additionally available products (flags, TSM, and YS) should be examined. This will improve the understanding of the atmospheric and marine conditions at the time of satellite data sampling, and can be used to evaluate the reliability of the Chl-a products for both Case 1 and Case 2 waters.

Paper II: The set of spectral SIOP coefficients established for Norwegian coastal waters generally fall within the expected range of values. A relatively high variability was, however, observed. When ingested into a new inverse algorithm, a sensitivity test revealed the relative importance of the SIOP coefficients for accurate retrievals of the various CPA concentrations. Moreover, the impact of the observed SIOP variability on the algorithm retrieval accuracy was quantified. This knowledge is important for operational use of the algorithm since the SIOP coefficients can exhibit substantial temporal and spatial variability.

Paper III: The inverse algorithm was for the first time applied to MERIS data and thoroughly validated against ship borne data. Considering the inherent uncertainties that exist when comparing *in situ* and satellite data, the observed retrieval errors of the algorithm are well below the required values. The error function given by the algorithm is moreover seen to be important for assessing the quality of the retrieved products. The realistic patterns of CPA concentrations observed when applying the algorithm to a large number of MERIS images moreover imply a good capacity of the algorithm for operational application. The new algorithm can be applied to different ocean colour satellites as long as the SIOP coefficients are tabulated at the sensor wavelengths. This means that the algorithm can easily be tuned to handle data from future sensors with possibly other band configurations.

The findings summarized above imply an improved capability of using satellite ocean colour data for algal bloom monitoring in Norwegian coastal waters. Furthermore, an improved ocean colour algorithm has implications that are not only relevant for algal bloom monitoring. A long term monitoring of the concentrations and distribution of the various water constituents can be performed by applying the new algorithm to both historical and future satellite data from the region. This enables studies of seasonal and inter-annual variability of these constituents, and may thereby improve our understanding of the dominant long term biological and physical processes in the marine environment.

In 2005 the ocean colour data source in an existing operational algal bloom monitoring system for the North Sea region (Durand *et al.* 2000) was switched from SeaWiFS to MERIS. This system has been based on standard Chl-a products valid for Case I waters. The findings in Paper I suggest that the performance of the system should not be influenced by the change in data source, as the Case I water Chl-a products from the two sensors were seen to be very similar. Routines for downloading of MERIS data from the European Space Agency's (ESA) rolling archive were established. Access to this archive enabled visualization of MERIS ocean products for the North Sea region few hours after sensor overpass. The number of biogeochemical products is furthermore being extended to include concentrations of Total Suspended Matter and Yellow Substance, in addition to Chl-a. Information from the MERIS flags is also taken into account to evaluate the product quality.

The new inverse algorithm introduced in Paper II and validated in Paper III is also implemented into the monitoring system and is used for operational processing of the MERIS data. SIOP coefficients as obtained in Paper II are applied. The new algorithm is expected to provide increased accuracy of the system's Chl-a product. Its output products can be visualized together with the standard MERIS algorithm products. Daily, weekly and monthly averaged products will be calculated and presented both as distribution maps, and as plots along selected transects of interest. This enables direct comparison with field observations and possibly numerical model output fields. The monitoring system is primarily designed for daily interpretation of the algal bloom status in Norwegian coastal waters. Additionally, it is expected that routine access to the algorithm products can be used for validation of numerical model output fields. This will, in turn, allow better considerations for data assimilation into coupled physical-biogeochemical models.

The practical implementation of the algorithm has been performed in close cooperation with the Nansen International Environmental and Remote Sensing Centre (NIERSC) in St. Petersburg, Russia. A technical report (Folkestad *et al.*, 2005) describes in detail the various components of the autonomous MERIS processing procedure. The updated version of the ocean colour component of the monitoring system is expected to be fully operational in February 2006. Products will become freely available at http://HAB.nersc.no/.

Further improvement and refinement of the algorithm should include investigations of the temporal and spatial SIOP variability in the monitoring area. These investigations may lead to the generation of several SIOP sets valid for specified seasons and/or sub-regions. The algorithm could be further developed to select between the different SIOP sets during the optimization procedure. The validity of the inverse algorithm for a specified water body is only limited to the existence of a valid set of SIOP for that region. The use of the algorithm could therefore easily be extended to include other coastal and inland water bodies of interest. If sets of relevant SIOP are not readily available for the selected regions they consequently need to be established from *in situ* observations.

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