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An optical tool for quantitative assessment of phycocyanin pigment concentration in cyanobacterial blooms within inland and marine environments

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ABSTRACT

Quantitative assessment of the pigment phycocyanin (*PC*) in cyanobacterial blooms is essential to assess their abundance and distribution and consequently aid their management in many recreational waters within inland and coastal environments. In contrast to the open-ocean waters, these water bodies are very complex with a pronounced heterogeneity of their optical properties, and hence accurate retrieval of the water-leaving radiances and *PC* concentration from satellite observations is notoriously difficult with existing algorithms. In the present study, a new inversion algorithm is developed as a rapid cyanobacteria bloom assessment method and its retrievals of *PC* are compared with in-situ and satellite observations and those from a previously reported inversion algorithm. The new algorithm estimates *PC* concentration on the basis of the unique absorption feature of phycocyanin at 620 nm which is isolated from the total pigment absorption by taking advantage of the well-recognized absorption and reflectance features in the red and near-infrared (NIR) wavelengths (less impacted by the influences of the overlapping absorption signatures of the mixture constituents and pigment packaging). The by-products of this work include chl-*a* concentration and predictions from reflectance data to monitor the cyanobacterial component and non-cyanobacterial component of the phytoplankton assemblage and to evaluate *PC*:Chl-*a* pigment weight ratios for specific water types. Initial validation of the algorithm was performed using in-situ field data in turbid productive waters dominated by phycocyanin and other pigments, yielding coefficients of determination and slope close to unity and mean errors less than a few percent. These results suggest that the algorithm could be used as a rapid assessment tool for the remote-sensing assessment of the spatial distribution and relative abundance of cyanobacterial blooms in many regional water bodies.

Introduction

Blooms of cyanobacteria (commonly referred to as blue-green algae) have been increasingly reported for a number of water bodies, including lakes, rivers, coastal and ocean waters. Prolific cyanobacterial growth and subsequent development of mass populations that are often dependent on factors such as a warming climate, light availability, changing landuse practice and eutrophication (Johnk et al., 2008; Paerl and Huisman, 2008; Hunter et al., 2010) are serious concerns because they can pose significant threats to water quality (e.g., it hampers recreational use, leads to hypoxia, reduces esthetics, and causes taste and odor problems) and risks to human and animal health (Codd et al.,1999; Carmichael et al., 2001; Brient et al., 2008; Hunter et al., 2009; Kudela et al., 2015). Many genera of cyanobacteria are capable of producing various forms of toxins (cyanotoxins) including neurotoxins, hepatotoxins, cytotoxins, genotoxins and endotoxins (Codd et al., 2005; Metcalf et al., 2008; Hunter et al., 2010), thus exposure to the toxic cyanobacterial blooms can result in incidences of diseases in humans such as skin irritation, gastrointestinal illnesses, cancer and tumors (associated with powerful hepatotoxins such as microcystins) and significant environmental, ecological and economic effects (Carmichael et al., 2001; Pilotto et al., 1997). In recognition of the severity of these risks posed by cyanobacterial blooms, a greater emphasis has been placed in recent years on the prediction of the locations and timing of these algal blooms for improving various management and mitigation activities.

Detection and monitoring of cyanobacterial blooms are generally achieved through the photosynthetic bio-marker pigment phycocyanin (*PC*), which exhibits a distinct diagnostic absorption feature at ~620 nm (Glazer et al., 1973) easily detected from remote sensing reflectance data using a wavelength range of 615–630 nm (Ogashawara et al., 2013; Kudela et al., 2015). This unique optical signature of cyanobacteria can be used as a good candidate for remote-sensing based techniques for the quantification of *PC* in spatially and temporally variable water bodies, wherein conventional in-situ point scale sampling can be less effective for describing pronounced patchiness in the distribution of cyanobacterial

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blooms (Ruiz-Verdú et al., 2008; Wheeler et al., 2012). Further complications with in-situ sampling are in its inability to elucidate the nature of processes controlling a bloom's spatial and temporal distribution (Hunter et al., 2008b). Remote-sensing-based techniques for detecting and monitoring the distribution of algal blooms have proven effective (Shanmugam et al., 2008, 2011, 2013), however some potential issues are associated with these techniques including the necessity to achieve sufficient spatial and spectral resolution to resolve fine-scale patchiness of cyanobacterial blooms and detect their *PC* absorption feature in remote sensed data (Kudela et al., 2015), to separate *PC* from the chlorophyll-*a* (chl-*a*) absorption feature (Ruiz-Verdú et al., 2008 and references therein), and to improve the atmospheric compensation and bio-optical algorithms in turbid productive waters (Kudela et al., 2015; Singh and Shanmugam, 2014; Varunan and Shanmugam, 2015).

Current approaches to detect and describe cyanobacterial blooms from remote sensing data are based on the reflectance spectral curvatures or optical relationships between the reflectance band ratios and the *PC* absorption or pigment. In particular, they rely on (*i*) semi-empirical (Simis et al., 2005, 2007; Randolph et al., 2008) or nested semi-empirical algorithm approaches (Dekker, 1993), (*ii*) relationships of single or multiple reflectance/radiance band ratios having the phycocyanin information with the measured *PC* concentration (Schalles and Yacobi., 2000; Vincent et al., 2004; Hunter et al., 2009; Li et al., 2010; Mishra et al., 2009; Sun et al., 2011, 2013, 2015), (*iii*) three-band reflectance algorithms (Hunter et al., 2010; Mishra et al., 2014) originally designed for the estimation of chl-*a* concentration (Gitelson et al., 2003), (*iv*) decomposition of phytoplankton absorption at 620 nm (Mishra et al., 2013b; Matthews et al., 2013), and (*v*) new techniques formulated on the basis of the reflectance band architecture (Kudela et al., 2015, Qi et al., 2014; Song et al., 2014).

Semi-empirical algorithms

Dekker (1993) developed a nested semi-empirical algorithm that uses the relative magnitude of the reflectance at 620 nm extracted through a reference baseline between 600 nm and 648 nm. This approach is susceptible to poor predictions because of its sensitivity to other confounding photo-pigments (e.g., chl-*a*) other than *PC* concentration (Mishra et al., 2009). Simis et al. (2005) proposed a semi-empirical inversion algorithm which estimates the *PC* and chl-*a* absorption values at 620 nm based on some assumptions (to avoid the complexities in modeling), reflectance band ratios and inherent optical properties (IOPs such as backscattering and absorption). This algorithm has been widely used for the estimation of *PC* as it provides some physical meaning and achieves good accuracy. However, inappropriate assumptions and simple band ratios with this algorithm cause an overestimation of *PC* at low concentrations and the error was more pronounced when *PC*:Chl-*a* ratio increased for samples with elevated accessory pigments (Simis et al., 2007). To minimize the overestimation of PC, a correction factor for the absorption by accessory pigments in the 620 nm band was introduced by Simis et al. (2005, 2007). Randolph et al. (2008) validated the Simis et al. (2005) algorithm using a data set that consisted of *PC* pigment concentrations and *PC* absorption coefficients (a_{PC}) derived from the power law instead of the mean *PC* specific-absorption coefficients (a_{PC}^*). Because the a_{PC}^*values vary with season and locations, some of the model's coefficients needed to be optimized for yielding accurate estimates of *PC*.

Empirical algorithms

Several empirical algorithms were developed based on the reflectance band ratio(s) to estimate *PC* concentration in inland and near-coastal water bodies (Schalles and Yacobi, 2000; Vincent et al., 2004; Mishra et al., 2009; Hunter et al., 2009; Li et al., 2010; Sun et al., 2011, 2013, 2015). A simple model was developed by Schalles and Yacobi (2000) which uses the relationship of reflectance band ratio (considering peak and trough around 650 nm and 625 nm) and measured *PC* concentrations. Though this model has the advantage of its simplicity, the influence of chl-*a* absorption was not corrected and thus it greatly affected the model results in turbid productive inland waters (Simis et al., 2007). Vincent et al. (2004) designed a model that directly relates the reflectance band ratio (using all the bands except the 6th band in Landsat 7 ETM+) with the *PC* concentration for remotely detecting and monitoring the cyanobacterial blooms. However, the sensitivity of this model was weak because the chosen reflectance or radiance signal beyond 750 nm contains less information regarding the phycocyanin signal (Kutser et al., 2006).

Multi-band algorithms

In other studies (Hunter et al., 2009; Mishra et al., 2009; Li et al., 2010; Sun et al., 2015), empirical algorithms were proposed which experimented with the relationships of single or multi-band reflectance ratios and *PC* concentrations. These methods are dependent on a set coefficients that are restricted to certain specific water bodies or inadequate for describing the cyanobacterial bloom seasonal variability. Ogashawara et al. (2013) evaluated the performance of several existing reflectance-based models (Dekker, 1993; Schalles and Yacobi, 2000; Simis et al. 2005; Mishra et al., 2009; Hunter et al., 2010) with samples collected from two different locations and demonstrated that the reflectance-based algorithm employing $R_{rs}(724)/R_{rs}(600)$ gave better estimates of *PC* concentration. Many of the above reflectance band-ratio algorithms are limited in application to the location and acquisition date of the data from which they are derived (Matthews et al., 2010), which imply that they need to be tuned using local data. Moreover, conventional band ratio algorithms do not employ a correction for minimizing the influence of accessory pigments on the retrieval of *PC* which makes them less robust and transferrable to water bodies with low *PC* concentrations.

Absorption decomposition

To overcome some of these issues with simple band-ratio approaches, recent studies have focused on decomposing the phytoplankton absorption at 620 nm and incorporating a correction for chl-*a* absorption for improving the *PC* retrieval (Mishra et al., 2013b; Matthews et al., 2013). In Mishra et al. (2013b), the *PC* absorption at 620 nm was estimated by solving the two algebraic equations that describe the phytoplankton absorption at 665 nm and 620 nm (on the basis of two coefficients ψ_1 and ψ_2) with the assumption of negligible accessory pigments at these wavelengths. In Matthews et al. (2013), the chl-*a* absorption at 620 nm ($a_{Chl\text{-}a}(620)$) was derived from the phytoplankton absorption ($a_{\varphi}(665)$) using the (ε) values. The estimated $a_{Chl\text{-}a}(620)$) values were then subtracted from $a_{ph}(620)$ in order to derive $a_{PC}(620)$ and subsequently estimate *PC* concentration using $a_{PC}^*(620)$ values. These methods gave fairly good *PC* retrievals although being constrained to rely on the fixed coefficients (ε) (Matthews et al., 2013) and optimized mean values (ψ_1, ψ_2 and $a_{PC}^*(620)$ (Mishra et al., 2013b).

Reflectance band architecture

More recently, Qi et al. (2014) proposed a new algorithm for the quantification of *PC* concentration using a baseline approach that uses two wavelengths (560 and 665) to determine a reference baseline, and relates *PC* concentration to the reflectance at 620 nm measured from the midpoint of the baseline. This algorithm based on field reflectance was applied to MERIS Rayleigh-corrected (aerosol + water signal) reflectance with adjustment of the empirical coefficients because of known atmospheric compensation problems in turbid productive and phytoplankton-dominated waters. In remote sensing of less turbid, optically shallow near-shore and inland waters, the bottom effect can be a