Remote Sensing of Environment 159 (2015) 134–151

Contents lists available at ScienceDirect

Remote Sensing of Environment

journal homepage: www.elsevier.com/locate/rse

# Hyperspectral optical discrimination of phytoplankton community structure in Funka Bay and its implications for ocean color remote sensing of diatoms

Tomonori Isada [a,*], Toru Hirawake [a], Tsukuru Kobayashi [a], Yuichi Nosaka [b], Masafumi Natsuike [a], Ichiro Imai [a], Koji Suzuki [b,c], Sei-Ichi Saitoh [a]

[a] *Faculty of Fisheries Sciences, Hokkaido University, 3-1-1 Minato-cho, Hakodate, Hokkaido 041-0821, Japan*
[b] *Graduate School of Environmental Science, Hokkaido University, North 10 West 5, Kita-ku, Sapporo, Hokkaido 060-0810, Japan*
[c] *Faculty of Environmental Earth Science, Hokkaido University, North 10 West 5, Kita-ku, Sapporo, Hokkaido 060-0810, Japan*

## ARTICLE INFO

*Article history:*
Received 26 December 2013
Received in revised form 8 December 2014
Accepted 8 December 2014
Available online 29 December 2014

*Keywords:*
Phytoplankton pigments
Light absorption
Derivative spectroscopy/similarity index
CHEMTAX
Hyperspectral remote sensing

## ABSTRACT

Identification of phytoplankton functional groups is key to understanding marine biogeochemical cycles. For more accurate understanding of phytoplankton community structure and its implications for ocean color remote sensing applications, we investigated seasonal changes in phytoplankton pigments with high-performance liquid chromatography (HPLC), hyperspectral absorption coefficients of detritus ($a_d(\lambda)$), phytoplankton ($a_{ph}(\lambda)$), and colored dissolved organic matter ($a_{CDOM}(\lambda)$), and hyperspectral $a_{ph}(\lambda)$ derived from remote sensing reflectance ($a_{ph\_Rrs\text{-derived}}(\lambda)$) in the coastal waters of Funka Bay from 2010 to 2012. Chlorophyll *a* (Chl *a*) concentrations measured by HPLC ranged from 0.29 to 8.6 mg $m^{-3}$. Phytoplankton community compositions, as estimated by chemotaxonomic analysis (CHEMTAX) based on HPLC phytoplankton pigments, showed a seasonal succession of diatoms, chlorophyll *b*-containing phytoplankton (chlorophytes and prasinophytes), and cyanobacteria. Additionally, to identify the dominant type of phytoplankton with an alternative technique to CHEMTAX analysis, we employed a derivative spectroscopy/similarity index (SI) approach for $a_{ph}(\lambda)$ as an optical detection technique for discriminating between different types of phytoplankton. In particular for diatom-dominated stations, SI values relative to the second derivative spectra of $a_{ph}(\lambda)$ of diatom cultures, isolated from our study region, were significantly higher than those for chlorophyll *b*-containing phytoplankton- and cyanobacteria-dominated stations. Furthermore, we found a strong relationship between the SI values calculated from the second derivative spectra and the composition of diatoms as estimated by CHEMTAX. These results suggest that the two different methods validated each other's performance and precision in estimating relative diatom abundance from bulk samples and that it is possible to optically discriminate the dominance of diatoms using derivative spectra of $a_{ph}(\lambda)$. We extended this combination approach to hyperspectral $a_{ph\_Rrs\text{-derived}}(\lambda)$, using a quasi-analytical algorithm within 400–546 nm range. We found a significant correlation between SI values obtained from the second derivative spectra of $a_{ph\_Rrs\text{-derived}}(\lambda)/a_{ph\_Rrs\text{-derived}}(443)$ and the composition of diatoms derived by CHEMTAX, but it was not as high as for $a_{ph}(\lambda)$ measured by filter-pad analysis. These results indicate that using hyperspectral optical data of $a_{ph}(\lambda)$ and $R_{rs}(\lambda)$ with derivative spectroscopy is potentially a promising approach to identify seasonal variability in the composition of diatoms in coastal waters. Furthermore, a hyperspectral approach in combination with CHEMTAX analysis as a reference for phytoplankton community structure has proven useful in improving our understanding of phytoplankton community structure in the coastal waters of Funka Bay.

## 1. Introduction

Phytoplankton play a central role as carbon fixers in aquatic ecosystems. Although all phytoplankton utilize $CO_2$ to produce organic matter, some different taxonomic groups have unique physiological processes, which in turn affect marine biogeochemical cycles. For example, diatoms utilize silicates and are important bloom-forming phytoplankton, contributing ~40% of global ocean productivity (Armbrust, 2009; Falkowski, Barber, & Smetcek, 1998). In contrast, small cells such as cyanobacteria contribute to phytoplankton biomass and both primary and export production in oligotrophic waters (Richardson & Jackson, 2007). In coastal waters, phytoplankton contribute largely not only to the aquatic carbon cycle but also to aquaculture. It is well known that

---

[*] Corresponding author at: Akkeshi Marine Station, Field Science Center for Northern Biosphere, Hokkaido University, Aikappu 1, Akkeshi-cyo, Akkeshi-gun, Hokkaido 088-1113, Japan.
*E-mail address:* t-isada@fsc.hokudai.ac.jp (T. Isada).

http://dx.doi.org/10.1016/j.rse.2014.12.006
0034-4257/

diatoms (e.g., *Pseudo-nitzschia* spp.), as well as harmful algae such as raphidophytes and dinoflagellates, influence cultured aquatic organisms, leading to concerns for both fishery markets and human health (Babin et al., 2005; Imai, Yamaguchi, & Hori, 2006). Therefore, it is essential to quantify and monitor phytoplankton community structure to understand the contribution of each phytoplankton group to marine biogeochemical cycles and their influence on cultured aquatic organisms.

Although several methods exist for identifying phytoplankton groups (e.g., microscopy, flow cytometry, and genetic analysis), phytoplankton pigment chemotaxonomy with high performance liquid chromatography (HPLC) is the most widely adopted method for estimating phytoplankton biomass and community structure (Kozlowski, Deutschman, Garibotti, Trees, & Vernet, 2011; Llewellyn, Fishwick, & Blackford, 2005). Phytoplankton pigments are also increasingly essential for recognizing phytoplankton functional types through satellite ocean color remote sensing (e.g., Alvain, Moulin, Dandonneau, & Bréon, 2005; Hirata et al., 2011; Pan, Mannino, Russ, Hooker, & Harding, 2010). For estimating phytoplankton community structure, the CHEMTAX program based on matrix factorization (Mackey, Mackey, Higgins, & Wright, 1996) is recognized as a useful and reliable tool. This program has been applied to various geographic domains, including the open ocean (e.g., Veldhuis & Kraay, 2004), iron fertilization experiments (e.g., Suzuki et al., 2005), and coastal waters (e.g., Isada et al., 2009). CHEMTAX has also been applied to satellite ocean color remote sensing (Pan, Mannino, Marshall, Filippino, & Mulholland, 2011). The program uses factor analysis and a steepest-descent algorithm to optimize the relative ratios of pigment:chlorophyll *a* (Chl *a*) used in calculating the abundance of each phytoplankton group contributing to Chl *a* concentration (Mackey et al., 1996). Therefore, the initial ratio matrix of pigment:Chl *a* influences the program's output of phytoplankton abundances. However, one of the major difficulties of the CHEMTAX program is the choice of an initial ratio matrix of pigment:Chl *a*, which is required to find the optimal ratio (Latasa, 2007; Wright et al., 2009).

Change in pigment composition is one of the major factors influencing the light absorption coefficient of phytoplankton, $a_{ph}(\lambda)$ (Bricaud, Claustre, Ras, & Oubelkheir, 2004; Hoepffner & Sathyendranath, 1991). Variations in $a_{ph}(\lambda)$ also depend on variations in the package effect (Morel & Bricaud, 1981), the size structures of phytoplankton (Ciotti, Lewis, & Cullen, 2002), light (Fujiki & Taguchi, 2002), and nutrients (Matsuoka, Larouche, Poulin, Vincent, & Hattori, 2009). Therefore, currently, $a_{ph}(\lambda)$ is used as an indicator of phytoplankton physiology and primary productivity (Hirawake, Shinmyo, Fujiwara, & Saitoh, 2012; Isada et al., 2013; Marra, Trees, & O'Reilly, 2007). Variations in $a_{ph}(\lambda)$ influence the light in the water column and, in turn, affect reflectance. Therefore, optical observations, including observations from in situ moored systems and ocean color remote sensing, are an effective tool for monitoring variability in phytoplankton dynamics in aquatic ecosystems (Cullen, Ciotti, Davis, & Lewis, 1997; Schofield et al., 1999). Derivative spectroscopy provides more detailed information on the spectral shape of $a_{ph}(\lambda)$ (Bidigare, Morrow, & Kiefer, 1989; Butler & Hopkins, 1970a,b; Faust & Norris, 1985; Millie, Kirkpatrick, & Vinyard, 1995; Smith & Alberte, 1994). This analysis amplifies minor inflections in the absorption spectrum and separates closely related pigments features. In this sense, several studies have investigated the relationship between photosynthetic pigments or species-specific pigments and the derivative spectra of $a_{ph}(\lambda)$ at a given wavelength in order to develop algorithms for retrieving phytoplankton pigments (Aguirre-gómez, Weeks, & Boxall, 2001; Astoreca et al., 2009). Based on derivative analysis, Millie et al. (1997) showed a method for detecting the toxic dinoflagellate *Karenia brevis* (formerly known as *Gymnodinium breve*) using the similarity index (SI), calculated by comparing the fourth derivative absorption spectra of an unknown sample with those of a reference monospecific *K. brevis* culture in laboratory experiments. Subsequently, Kirkpatrick, Millie, Moline, and Schofield (2000) demonstrated a linear relationship between *K. brevis* biomass and SI values in natural mixed populations. Thus, the derivative spectroscopy/similarity index (SI) approach for $a_{ph}(\lambda)$ would provide useful information to distinguish among phytoplankton groups, and potentially among species.

Recently, improvements have led to bio-optical hyperspectral sensors that become powerful tools for investigating phytoplankton dynamics in more detail (Chang et al., 2004; Devred et al., 2013; Ryan, Davis, Tufillaro, Kudela, & Gao, 2014). Highly resolved spectra of reflectance allow the discrimination of several distinguishing features related to the pigments and fluorescence of phytoplankton. Therefore, hyperspectral measurements of phytoplankton absorption ($a_{ph}(\lambda)$) and remote sensing reflectance ($R_{rs}(\lambda)$) with derivative spectroscopy have been exploited for use in various estimations such as seafloor types in carbonate sediments with microbial pigments (e.g., Louchard et al., 2002), seagrass and benthic algae (Dierssen, Zimmerman, Drake, & Burdige, 2010), phytoplankton pigment assemblages in open ocean (Torrecilla, Stramski, Reynolds, Millán-Núñez, & Piera, 2011), bio-optical provinces (Taylor et al., 2011), and phytoplankton size structure (Organelli, Bricaud, Antoine, & Uitz, 2013). Craig et al. (2006) developed a method for detecting *Karenia brevis* using hyperspectral $R_{rs}(\lambda)$ with a quasi-analytical algorithm (QAA, Lee & Carder, 2004), which is the inversion method for estimating $a_{ph}(\lambda)$. In this study, a derivative spectroscopy/SI approach for $a_{ph}(\lambda)$ was employed. Similarly, Lubac et al. (2008) assessed the suitability of multispectral and hyperspectral approaches for identifying *Phaeocystis globosa* blooms using field measurements of $R_{rs}(\lambda)$. They showed the advantage of a hyperspectral approach based on a derivative spectroscopy/SI analysis over a multispectral approach to detect different phytoplankton taxonomic groups with remote sensing.

The hyperspectral $a_{ph}(\lambda)$ data with the derivative spectroscopy/SI approach has been proven appropriate for discriminating among phytoplankton groups. However, extracting information on specific phytoplankton groups from $a_{ph}(\lambda)$ still remains a challenging task. In this sense, the use of CHEMTAX analysis based on HPLC phytoplankton pigments in natural waters can contribute to the investigation of the relationship between phytoplankton community structure and bulk optical absorption properties. An assessment of phytoplankton community structure and its relation to the light absorption of phytoplankton could improve our ability to use ocean optics and ocean color remote sensing to predict primary productivity and biogeochemical cycling.

The objective of this study is to investigate the utility of hyperspectral optical data for assessing the variability of phytoplankton groups using CHEMTAX analysis as a reference for phytoplankton community structure and also improve our ability to obtain more accurate estimations of phytoplankton community composition via ocean color remote sensing. To achieve this goal, an in situ seasonal dataset of phytoplankton pigments, cell densities of diatoms, hyperspectral absorption coefficients of detritus, phytoplankton, and colored dissolved organic matter ($a_d(\lambda)$, $a_{ph}(\lambda)$, and $a_{CDOM}(\lambda)$), and hyperspectral $R_{rs}(\lambda)$ was collected in the coastal waters of Funka Bay, which is located off the southwest of Hokkaido Island, Japan. Funka Bay is known to be one of the most important aquaculture regions for scallops, which depend on phytoplankton biomass and composition as a food source (Baba, Sugawara, Nitta, Endou, & Miyazono, 2009). The growth of hanging cultured scallops in Funka Bay is influenced by the diatom blooms (Hashimoto, Ueno, Takahashi, Suzuki, & Itabashi, 2010). In particularly, a method for discriminating diatoms from other phytoplankton taxa using hyperspectral optical measurements is described.

## 2. Methods

### 2.1. In situ samples and data collection

Seawater sampling and radiometric measurements were conducted from onboard the T/S *Ushio* Maru and T/S *Oshoro* Maru from April 2010 to January 2012 in Funka Bay and the Tsugaru Strait, in the coastal waters off southwestern of Hokkaido, Japan (Fig. 1 and Table 1). Water