Continental Shelf Research 55 (2013) 17–28

Contents lists available at SciVerse ScienceDirect

Continental Shelf Research

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

Research papers

Algorithm development for predicting biodiversity based on phytoplankton absorption

Tiffany A.H. Moisan [a,*], John R. Moisan [a], Matthew A. Linkswiler [b], Rachel A. Steinhardt [c]

[a] Wallops Flight Facility, NASA Goddard Space Flight Center, Wallops Island, VA 23337, United States
[b] URS Corporation, Wallops Flight Facility, NASA Goddard Space Flight Center, Wallops Island, VA 23337, United States
[c] Sigma Space Corporation, Wallops Flight Facility, NASA Goddard Space Flight Center, Wallops Island, VA 23337, United States

ARTICLE INFO

Article history:
Received 24 February 2012
Received in revised form
11 December 2012
Accepted 20 December 2012
Available online 23 January 2013

Keywords:
Phytoplankton
Oceanography
Algorithm
Phytoplankton functional type
Gulf of Maine
Mid Atlantic Bight

ABSTRACT

Ocean color remote sensing has provided the scientific community with unprecedented global coverage of chlorophyll a, an indicator of phytoplankton biomass. Together, satellite-derived chlorophyll a and knowledge of Phytoplankton Functional Types (PFTs) will improve our limited understanding of marine ecosystem responses to physiochemical climate drivers involved in carbon cycle dynamics and linkages. Using cruise data from the Gulf of Maine and the Middle Atlantic Bight (N=269 pairs of HPLC and phytoplankton absorption samples), two modeling approaches were utilized to predict phytoplankton absorption and pigments. Algorithm I predicts the chlorophyll-specific absorption coefficient (a^*_{ph} (m^2 mg chl a^{-1})) using inputs of temperature, light, and chlorophyll a. Modeled r^2 values (400–700 nm) ranged from 0.79 to 0.99 when compared to *in situ* observations with ~25% lower r^2 values in the UV region. Algorithm II-a utilizes matrix inversion analysis to predict a_{ph}(m^{-1}, 400–700 nm) and r^2 values ranged from 0.89 to 0.99. The prediction of phytoplankton pigments with Algorithm II-b produced r^2 values that ranged from 0.40 to 0.93. When used in combination, Algorithm I, and Algorithm II-a are able to use satellite products of SST, PAR, and chlorophyll a (Algorithm I) to predict pigment concentrations and ratios to describe the phytoplankton community. The results of this study demonstrate that the spatial variation in modeled pigment ratios differ significantly from the 10-year SeaWiFS average chlorophyll a data set. Contiguous observations of chlorophyll a and phytoplankton biodiversity will elucidate ecosystem responses with unprecedented complexity.

1. Introduction

Merging remote sensing variables such as ocean color chlorophyll a and phytoplankton taxonomic composition will allow for a more mechanistic understanding of past and future changes between climate and ecosystem impact (Cermeño et al., 2008; Iglesias-Rodriguez et al., 2008; Boyce et al., 2010). These goals support the Intergovernmental Panel on Climate Change (IPCC) that recognizes the feedback between climate and biodiversity (Fischlin et al., 2007). Climate Data Records such as High Performance Liquid Chromatography pigment (HPLC) and Inherent Optical Property (IOP) data sets exist, but they fall short of fully representing many ocean regions in both space and time of year. Expanding the ability to remotely sense key PFTs is a primary goal of this study. The drive for this information is not only motivated by global climate change issues, but favors novel approaches in the scientific community to formulate biogeochemical models that incorporate ecosystem function and marine productivity (Edwards, 2006; Striebel et al., 2009; Boyce et al., 2010).

There have been several reviews written on phytoplankton community structure, dynamics, and biogeochemistry as measured by ocean color (Martin, 2004; Mueller et al., 2004; Miller et al., 2005; Richardson and LeDrew, 2006 Longhurst, 2007; McClain, 2009; Robinson, 2010; Moisan et al., 2012). Approaches for the remote sensing detection of PFTs require defined optical signatures of phytoplankton that are detectable by aircraft sensors or satellite platforms and indirectly by the exploitation of relationships between chlorophyll a concentration and functional types.

New technological advances and developments in scientific knowledge have ushered in the development of several approaches for detecting phytoplankton biomass and some functional groups of phytoplankton including coccolithophores (Balch et al., 1996) and *Trichodesmium* (Subramaniam et al., 2001, Hu et al., 2010). More recently, algorithms have been developed to distinguish additional phytoplankton groups such as diatoms and size classes (Bouman et al., 2003, Sathyendranath et al., 2004).

Phytoplankton taxa are generally characterized by specific pigment complements called biomarkers and can be identified from pigment inventories and optical properties derived from *in situ* samples (Margalef, 1978; Brown and Podestá, 1997; Subramaniam et al., 2001; Bricaud et al., 2004). These characteristics allow for the

* Corresponding author. Tel./fax: +1 757 824 1046.
E-mail address: tiffany.a.moisan@nasa.gov (T.A.H. Moisan).

0278-4343/$ - see front matter Published by Elsevier Ltd.
http://dx.doi.org/10.1016/j.csr.2012.12.011

potential to separate out different sources of spectral variation using remote sensing reflectance inversion techniques, phytoplankton biomass, taxonomic composition, and possibly phytoplankton community size distribution (Hoge et al., 1993, 1995, 2001, Lee and Carder, 2004, Aiken et al., 2007, Moisan et al., 2011). While this approach is still far from classifying species composition in a classical manner, it allows for ecological forecasting between major algal groups and is a significant improvement over simply monitoring chlorophyll a biomass (Westberry and Siegel, 2006, Li et al., 2006, Hirata et al., 2008). The advantage of these approaches lies in the potential for remotely monitoring of ocean color to detect changes in the phytoplankton community that are linked to carbon sequestration and longer term climate changes.

Historically, there has been an emphasis on characterizing the development of remote sensing models to estimate the quantity of various optically active constituents in the upper ocean surface. In Case 1 waters, where optical properties are determined primarily by phytoplankton and their related dissolved organic matter and detrital products (Morel and Prieur, 1977) the spectral remote sensing reflectance, $R_{rs}(\lambda)$, defined as the ratio of upward radiance $L_u(\lambda)$ to downward irradiance $E_d(\lambda)$ (Mobley, 1994), has been shown by Gordon and Morel (1983) to be directly related to inherent optical properties of seawater such that

$$R_{rs}(\lambda)=\frac{L_u(\lambda)}{E_d(\lambda)}\approx 0.54\sum_{i=1}^{2} g_i\left[\frac{b_b(\lambda)}{b_b(\lambda)+a(\lambda)}\right]^i \ (\mathrm{sr}^{-1}), \tag{1}$$

where $g_1=0.0949$, $g_2=0.0794$, $a(\lambda)$ is the total absorption and $b_b(\lambda)$ is the total backscatter such that

$$a(\lambda)=a_w(\lambda)+a_{ph}(\lambda)+a_g(\lambda)+a_d(\lambda) \tag{2}$$

and

$$b_b(\lambda)=b_{bw}(\lambda)+b_{bph}(\lambda)+b_{bg}(\lambda)+b_{bd}(\lambda), \tag{3}$$

where the subscripts b_w, b_{ph}, b_g, and b_d correspond to backscatter due to seawater, phytoplankton, gelbstoff and detritus, respectively. Bulk inherent optical properties (IOPs), by definition, include the sum of the contributions from each of the optical components (*i.e.* water, particles, and dissolved material). A full list of symbols used in the paper can be found in Table 1

Phytoplankton absorption has been modeled using a wide range of mathematical approaches (Bricaud et al., 2004; Siegel, 2005; Uitz et al., 2006; Moisan et al., 2011). Phytoplankton backscatter values monotonically increase with decreasing wavelength and are also thought to vary considerably with cell size, taxonomic composition, and cellular carbon (Bricaud et al., 1996; Stramski et al., 2000), although a recent study was unable to detect any relationship with cell size (Whitmire et al., 2010). Successful modeling of absorption has led to the development of mathematical approaches to estimate photoprotective and photosynthetic pigments (Babin et al., 2003). Bricaud et al. (2004) demonstrated the relative importance of both pigment packaging effects and pigment composition on algal absorption, and noted that the majority of the observed deviations in absorption were due to variations in algal size and its impact on the pigment package effect. Using inherent optical properties, Garver et al. (1994) conducted an extensive review of the relationship between pigmentation and taxonomic composition and underscored the spectral limitations of present day ocean color remote sensing reflectance. Other mathematical approaches for understanding cellular absorption have separated the absorption spectrum

Table 1
Symbols used throughout the text.

λ	Wavelength (nm)
chl	Chlorophyll (mg m^{-3})
PAR	Photosynthetically available radiation (μmol quanta m^{-2} s^{-1})
a_{ph} (λ)	Absorption by phytoplankton (m^{-1})
a^*_{ph} (λ)	Chl-specific absorption of phytoplankton (m^2 mg chl a^{-1})
a_i (λ)	Pigment-specific absorption for the *i*th pigment (m^2 mg *i*th pigment a^{-1})
a'_{ph} (λ)	Reconstructed phytoplankton chlorophyll-specific absorption (m^2 mg chl a^{-1})
$\hat{a}_{ph}$ (λ)	Normalized phytoplankton absorption (m^{-1})
p_j	Concentration of jth pigment (mg *j*th pigment m^{-3})
R_{rs} (λ)	Above-water remote sensing reflectance (sr^{-1})
L_u (λ)	Upward ocean radiance above sea surface (W m^{-2} sr^{-1} nm^{-1})
E_d (λ)	Downward solar irradiance from direct and diffuse solar radiation (W m^{-2} nm^{-1})
a (λ)	Total absorption (m^{-1})
a_w (λ)	Seawater absorption (m^{-1})
a_{ph} (λ)	Phytoplankton absorption (m^{-1})
a_g (λ)	Gelbstof absorption (m^{-1})
a_d (λ)	Detritus absorption (m^{-1})
$\tilde{a}^*$ (λ)	Modeled pigment-specific absorption at λ (m^2 mg chl a^{-1})
b_b (λ)	Backscatter (m^{-1})
b_{bw} (λ)	Seawater backscatter (m^{-1})
b_{bph} (λ)	Phytoplankton backscatter (m^{-1})
b_{bm} (λ)	Mineral backscatter (m^{-1})
b_{bd} (λ)	Detritus backscatter (m^{-1})
b_T (λ)	Total backscatter (m^{-1})
c	HPLC pigment measurements (mg pigment m^{-3})
$\tilde{c}_j$	Inversion estimated concentration of pigment *j* (mg pigment m^{-3})
C_0 (λ)	Linear fit absorption model intercept coefficient (m^{-1})
C_E (λ)	Linear fit absorption model incident PAR coefficient (PAR^{-1} m^{-1})
C_T (λ)	Linear fit absorption model temperature coefficient (T^{-1} m^{-1})
HPLC	High-performance liquid chromatography (mg m^{-3})
R^2	Coefficient of determination
r^2	Pearson's coefficient of correlation (non-dimensional)
ACE	Aerosols-clouds-ecosystems
GEO-CAPE	Geostationary coastal and air pollution events
HyspIRI	Hyperspectral infrared imager