Identification of Phytoplankton Pigment Assemblages Using Derivative Spectroscopy of Hyperspectral Remote-Sensing Reflectances

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Abstract *– One of the major challenges of ocean color research is distinguishing phytoplankton groups from in situ, airborne and satellite measurements to better understand diversity of phytoplankton and some involved biochemical processes. In this framework, high spectral resolution measurements of remote-sensing reflectance, hyperspectral $R_{rs}(\lambda)$, can potentially yield more information about the presence of diverse phytoplankton groups than can be gleaned from traditional analyses of single band-ratios at discrete wavelengths (i.e. multispectral approaches). We introduce and discuss the feasibility of performing derivative spectroscopy and cluster analysis of hyperspectral $R_{rs}(\lambda)$ to improve the automatic identification of phytoplankton populations in open ocean waters.*

Keywords *– Ocean bio-optics, derivative spectroscopy, cluster analysis.*

I. INTRODUCCIÓN

Marine scientists have had a long term-interest in characterizing the diversity of phytoplankton communities in the ocean and understanding how diversity changes on spatial and temporal scales relevant to environmental and climate changes. The goal of this research is to estimate the diversity of phytoplankton communities from measurements of ocean color and to do so, a hyperspectral approach is proposed. We introduce and discuss the feasibility of performing derivative spectroscopy of hyperspectral remote-sensing reflectances ($R_{rs}(\lambda)$) [1, 2] to improve the identification of phytoplankton assemblages in open ocean waters. The full potential of hyperspectral optical information, as opposed to current multispectral measurements, in combination with development of algorithms for automatic assessment of phytoplankton composition is explored.

II. RESULTS AND DISCUSSION

The dataset analyzed corresponds to measured inherent and modeled apparent optical properties collected along a north-to-south transect in the eastern Atlantic Ocean during the German expedition ANT-XXIII/1 on R/V Polarstern (Fig. 1).

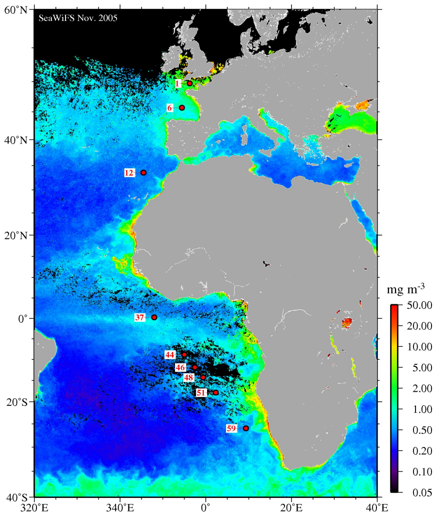

Figure 1. Location of the stations. Optical measurements and water sampling were conducted from October to November 2005. Stations selected for this study are shown with their station ID.

Stations were first classified into differing phytoplankton assemblages based upon the ratios of dominant accessory pigments to total Chlorophyll *a*, obtained through HPLC chromatography (Table 1). Next, numerical simulations with the Hydrolight radiative transfer model [3] were performed to estimate the aparent optical property of remote-sensing reflectance ($R_{rs}(\lambda)$) for each station (Fig. 2). Differences in each station $R_{rs}(\lambda)$ were further examined using tools such as derivative spectroscopy and hierarchical cluster analysis (HCA).

Table 1. Classification of stations into different groups based on phytoplankton community composition, as indicated by the ratios of two dominant accessory pigments to total Chlorophyll *a*.

Dominant accessory pigments to Chlorophyll *a*	**Station Label**
Fucoxanthin, 19'-Hex-Fucoxanthin	A ▬
Divinyl Chl a, Zeaxanthin (DV Chl a > Zea)	B ▬
Divinyl Chl a, Zeaxanthin (DV Chl a ≈ Zea)	C1,C2,C3,C4 ▬
19'-Hex-Fucoxanthin, Zeaxanthin (19'-Hex-Fuco > Zea)	D ▬
19'-Hex-Fucoxanthin, Zeaxanthin (19'-Hex-Fuco ≈ Zea)	E ▬
19'-Hex-Fucoxanthin, Fucoxanthin (19'-Hex-Fuco > Fuco)	F ▬

HCA is a common methodology consisting in creating a hierarchical cluster tree to partition a data set into subsets (clusters) using a single linkage algorithm. The linkage algorithm is based on a previously calculated pairwise distance between observations (i.e. each second derivative of a normalized Rrs(λ) spectrum). The selected distance measure determines how the similarity of two spectra is calculated. In this case, one minus the cosine of the included angle between two vectors was used as a distance measure (cosine distance). As a linkage algorithm, the shortest distance between vectors, also called the nearest neighbor (single linkage), was selected. The traditional representation of this hierarchical tree is a dendrogram, with individual elements at one end and a single cluster containing every element at the other. Note that the smaller the cosine distance between two observations, the more similar are the features of the two compared derivatives of normalized Rrs(λ) spectra. Therefore, spectra corresponding to observations with a similar phytoplankton composition are expected to appear closer in the dendrogram than those having a very different phytoplankton composition (Fig. 3).

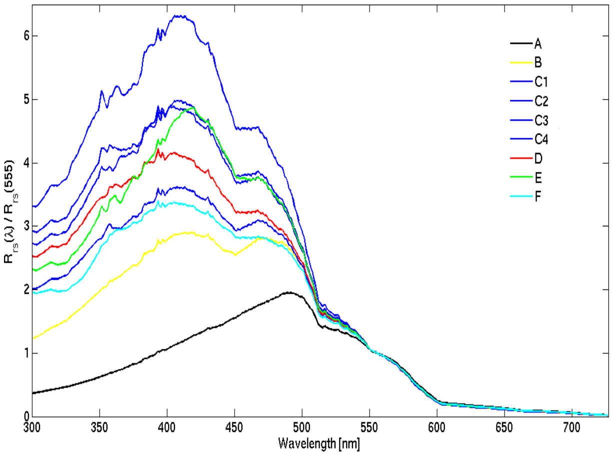

Figure 2. Normalized hyperspectral remote-sensing reflectance (Rrs(λ)) computed for each group of stations (cf. Table 1).

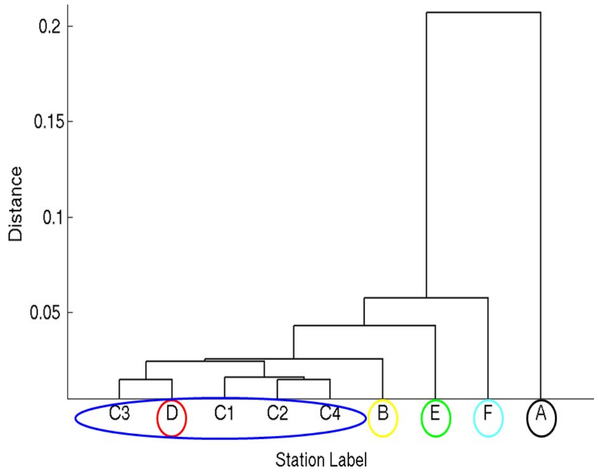

Figure 3. Classification of stations based on hierarchical cluster analysis for second derivative of normalized hyperspectral Rrs(λ) spectra shown in Fig. 2.

Different phytoplankton assemblages, previously identified by HPLC pigment analysis, were automatically classified from cluster analysis of the second derivative spectra of simulated hyperspectral $R_{rs}(\lambda)$. Our analysis indicates that utilizing derivative spectra of hyperspectral remote-sensing reflectance provides better separation between classified stations and the maximum distance between the clusters of classified stations. .

In order to evaluate the specific role that parameters involved in the derivative-based clustering approach play in the process (i.e. pre-smoothing filter window size – *WS* and derivative band separation – *BS*=*Δλ*), a sensitivity analysis has been also carried out (Fig. 4). We used a validation index - the so-called Cophenetic Index - so as to evaluate the performance of the clustering results for each set of processing parameters. It is worth noting that values of *WS* and *BS* parameters around 27 samples (i.e. 27 nm) provide the highest Cophenetic index, thus the best performance.

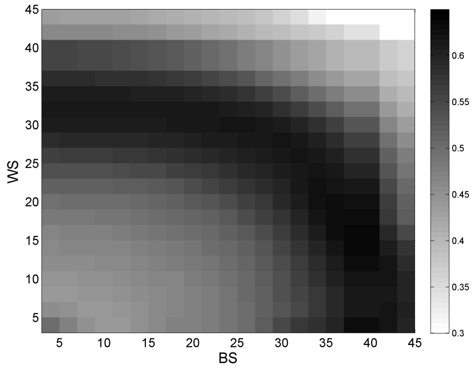

Figure 4. Sensitivity analysis of clustering results as a function of the parameters considered in the pre-smoothing and derivative analysis. X-axes indicate the derivative band separation (*BS*=*Δλ*) and Y-axes the smoothing filter window size (*WS*)..

III. CONCLUSIONS

The preliminary results suggest that the application of derivative spectroscopy to hyperspectral $R_{rs}(\lambda)$ provides an effective means to potentially characterize phytoplankton biodiversity in open ocean environments. Derivative spectroscopy has been satisfactorily applied to numerical simulations of hyperspectral remote-sensing reflectance (Rrs(λ)) corresponding to different environments. Its feasibility for identifying phytoplankton pigment assemblages in comparison with the use of raw Rrs(λ) spectra or traditional ratios of discrete spectral bands has been confirmed using a validation approach based on hierarchical cluster analysis (HCA).

For this simulated hyperspectral dataset, obtained based on detailed field measurements of inherent optical properties (i.e. absorption and scattering coefficients), a proper adaptation of parameters involved in the derivative analysis (i.e. pre-smoothing filter window size - *WS* and derivative band separation – *BS*=*Δλ*) was done according to the characteristics of the signals and particularly to its spectral resolution.

The experiments yield promising results when all the information contained in the second derivative of hyperspectral Rrs(λ) spectra is considered. This method can therefore provide a means for optical oceanographers to better characterize complex oceanic waters, detect harmful algal blooms or map phytoplankton functional types from hyperspectral oceanographic information. The recent advances in hyperspectral technology (e.g. miniaturization and power supply reduction) have given rise to a great number of sensor configurations that are suitable for incorporating in a large number of in situ and remote sensing platforms of oceanographic observing systems (e.g. satellites, gliders), which will allow these challenges to be overcome once hyperspectral data become more available.

Future work will be focused on assessing how the proposed methodology should be used depending on the spectral resolution of each dataset and exploring its potentiality within the framework of NASA Ocean Color Science projects for 2010 [4]. More research will also be focused on experiments based on larger field and modeled hyperspectral datasets, since the potential of integrating hyperspectral Rrs(λ) measurements and derivative spectroscopy has been emphasized in this work. However, the design of a more realistic approach when simulated-based experiments are employed would be useful for better validating the efficacy of the proposed method. An effort of detailed consideration of several factors involved in the analysis process is suggested. For instance, the accuracy of the derivative-based method for identifying different phytoplankton compositions would be improved if distortion experiments, caused by the sensor with which radiometric measurements would hypothetically be acquired (noise, spectral stray-light, thermal effects, etc.) were included in the simulation-based approach.

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