

Estimating chlorophyll-*a* concentration using first-derivative spectra in coastal water

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This study was intended to apply the technique of derivative analysis to estimate algal chlorophyll concentration in Pensacola Bay, Florida. The data collection was conducted over the 16 sampling sites on three separate occasions. A portable field spectroradiometer was used to collect the upwelling radiance of water and reference panel at each sampling station. The instrument records a continuous spectrum in 512 bands ranging from 350 nm to 1050 nm, with 1.37 nm spectral resolution. The first derivatives were computed and correlated with the chlorophyll-*a* concentration. The results indicated the first derivatives at 630–645 nm, 660–670 nm, 680–687 nm and 700–735 nm were correlated strongly with chlorophyll-*a*. The R values reached 0.858 for the wavelength at 686.7 nm. The results support the hypothesis that derivative spectra are less impacted by wave effects and, therefore, are an effective tool for estimating chlorophyll concentration.

Keywords: Spectral reflectance; Derivative spectra; Chlorophyll-a

1. Introduction

Estimating phytoplankton biomass and distribution through quantifying and mapping chlorophyll concentration has been one of the major applications of remote sensing of coastal waters (Johnson 1978, Khorram 1985, Harding *et al.* 1994). The biochemical processing of land-derived nutrients that takes place in estuaries and phytoplankton biomass has been found to be indicative of nutrient availability.

Hyperspectral sensors have been considered as the future sensors to measure chlorophyll concentration in water (Richardson 1996). Many narrow bands allow precise quantification of chlorophyll by measuring its pronounced spectral characteristics. As a fundamental research tool for the application of current and future hyperspectral and even multi-spectral sensing systems, a field spectro-radiometer was used to collect reflectance data. Some studies using field spectro-metry to measure algal chlorophyll concentration for inland and coastal waters have been conducted by other researchers. Aguirre-Gomez and others (2001) conducted research over Plymouth coastal waters using a ship-based hyperspectral radiometer to assess the potential of derivative analysis for retrieving information about photosynthetic pigments. They found that the derivatives of reflectance with different orders were useful in showing absorption and scattering characteristics of chlorophyll and other pigments. Gitelson (1992) studied the behaviour of the reflectance peak near 700 nm of algal water. It was found that the shift in peak position and an increase of the peak magnitude occurred as chlorophyll

concentration increased. Gitelson concluded that the 700 nm reflectance peak is important for the remote sensing of inland and coastal waters with regard to measuring chlorophyll. Gitelson et al. (1995) investigated chlorophyll distribution during a period of high chlorophyll concentration using a hyperspectral sensor in research conducted in Haifa Bay, Israel. Their findings not only supported the fact that the magnitude and location of the 700 nm peak were correlated closely with chlorophyll concentrations, but also proved that the reflectance height at 690 nm above the base line from 670 nm to 850 nm was a sensitive indicator for chlorophyll concentration. Han (1997) conducted research on characterizing the relationship between suspended sediment concentration (SSC) and reflectance in clear and algalladen waters. The author pointed out that the linearity in the SSC-reflectance relationship increased with wavelengths between 400 nm and 900 nm. Han and Rundquist (1997) compared the near-infrared (NIR) and red ratio and the first derivative of reflectance in modelling chlorophyll concentration in a turbid Midwestern reservoir. They observed that the first derivative was correlated better with the chlorophyll than the NIR/red ratio. The highest correlation between the first derivative and chlorophyll occurred at 690 nm. Fraser (1998) correlated reflectance and reflectance first derivatives with the chlorophyll-a and turbidity among 22 fresh to alkaline lakes in Nebraska. The author found that the first derivatives at 429 nm and 695 nm were correlated significantly with chlorophyll-a and turbidity.

Derivative spectra indicate the rate of change of reflectance with wavelength $(dR(\lambda)/d\lambda)$, which is the slope of the reflectance curve at wavelength λ . Derivative analysis allows one to correlate the shape of the reflectance pattern to chlorophyll concentrations. Derivative analysis has been applied by researchers in studying the spectral characteristics of chlorophyll and suspended sediments in water. Some major findings related to derivative analysis include: (1) the first-order derivative is able to remove pure water effects while the second derivative can remove suspended sediment effects (Goodin *et al.* 1993); (2) the first derivative at 690 nm is useful in estimating chlorophyll concentration in the presence of other water constituents (Han and Rundquist 1997); and (3) derivative spectra are an objective tool in isolating the absorption features of phytoplankton (Tsai and Philpot 1998).

The purpose of this study is to apply derivative analysis techniques to estimate algal chlorophyll concentration in the coastal water of Pensacola Bay, Florida, USA. The research is based on the hypothesis that, compared with the magnitude of spectral reflectance, derivative spectra are less impacted by wave effects. Therefore, derivative spectra can be an effective tool in estimating chlorophyll concentration.

2. Methodology

2.1 Study area

This research was conducted in Pensacola Bay, which is located in the north-west of Florida, USA. The estuary extends about 32 km inland from the Gulf of Mexico. The water area of the system is about 373 km^2 and the entire watershed is about $18 130 \text{ km}^2$. Escambia Bay, East Bay, Pensacola Bay, Escambia River, Blackwater River, and Yellow River are the major components of the system (figure 1). The Pensacola Bay system is regarded as a micro-tidal, partially stratified, drowned river valley estuarine system (Murrell *et al.* 2002). The significant usage of the Pensacola Bay system includes ecology, fisheries, military training, recreation and shipping.



Figure 1. Study area and sampling stations.

But the health and productivity of the system has been degraded in recent years due to point and non-point pollution, direct habitat damage and urban expansion (Thorpe *et al.* 1997). The systematic water quality monitoring programme for Pensacola Bay was started by the Gulf Ecology Division (GED) of the US Environmental Protection Agency (EPA) on a quarterly basis at 39 sampling stations throughout the system in 1997 (Lores *et al.* 2000). From 2000, the GED conducted monthly water sampling at 16 locations (P1–P16, figure 1). These sampling sites are distributed evenly over Escambia Bay and East Bay.

2.2 Water sampling

Water sampling and spectral data collection were conducted simultaneously on board the GED's water sampling boat for the 16 stations over the two-day period on three occasions in 2002: 14 and 15 May, 4 and 5 June and 27 and 28 August. The depths of the sampling sites range from 2.1 m (at P3 and P11) to 11.3 m (at P8). At each station, a hydrographic profile and light profile were obtained. Secchi disk depth was also recorded at each station. Surface and bottom water samples were collected and taken to the lab for chlorophyll-*a* and other pigment analyses. Figure 2 illustrates the measured chlorophyll-*a* in August seemed to be unexpectedly high and spatially variable $(14.3 \,\mu g 1^{-1}$ on average and ranging from $3.4-36.2 \,\mu g 1^{-1}$. The median chlorophyll-*a* concentration in Pensacola Bay is $4 \,\mu g 1^{-1}$ and normally



Figure 2. Chlorophyll-a concentrations at 16 sampling stations for three cruises.

ranges from $1-20 \ \mu g \ 1^{-1}$ (Murrell *et al.* 2002). The lowest chlorophyll concentration occurred in June, with the average concentration of chlorophyll-*a* being $3.85 \ \mu g \ 1^{-1}$. As expected, the sites that are closer to the river mouths had higher chlorophyll-*a* concentrations due to the greater nutrient loading from the rivers, e.g. sites P2, P3, P10, and P11.

2.3 Measurement of spectral reflectance

A field spectroradiometer (ASD FieldSpec ultraviolet/visible and near-infrared (UV/ VNIR)) was used to measure the upwelling radiance of the water at each sampling station during water sampling. The instrument records a continuous spectrum in 512 bands, ranging from 350 nm to 1050 nm with 1.37 nm spectral resolution. A fibre optic cable is built in for the radiance measurement. The light-receiving probe of the cable was held in a pistol grip and was placed at about 30 cm above the water surface. The diameter of the instantaneous field-of-view (IFOV) at the water surface (d) was calculated using the following equation:

$$d = h\beta, \tag{1}$$

where *h* is the height of the probe end of the fibre optic cable from the water surface, and β is the radiance of the forehead selected. In this study, *h* is 30 cm and β is 0.44 (10° forehead). Thus *d* is 13.2 cm.

A Spectralon reference panel was used to calibrate spectral data to downwelling solar radiation. At each sampling station, the reference panel was scanned first. The water reflectance (in percent) was calculated in real time with measurements of upwelling radiance from the water. There were ten measurements of upwelling radiance taken at each station, which resulted in ten replicate spectral reflectance curves. The average reflectance curves were smoothed using seven points averaging prior to the calculation of derivative spectra. The first derivatives were estimated by using the difference between successive reflectance values by the wavelength intervals separating them (Han and Rundquist 1994, Tsai and Philpot 1998). The interval between the wavelengths is at a constant 1.42 nm.

3. Results and discussion

The average reflectance curves for all 16 sampling sites were plotted against wavelength (figures 3(a)-(c)), which allows for visual inspection of spectral pattern and variation. Note that the spectral reflectance outside the 400–900 nm range was not included because of an excessive noise level. Among the three sampled occasions (May, June and August), the highest overall reflectance curves were found in May (figure 3(a)). The highest overall reflectance, ranging from 14.7% to 17% between



Figure 3. Spectral reflectance over 16 sampling stations: (a) May, (b) June and (c) August.

400 nm and 900 nm, was found at station P7 and the lowest overall spectra occurred at station P2, with reflectance ranging from 0.2% to 2.4%. This represents the biggest variable reflectance spectra among 16 sampling sites. It is believed that the greater variations of overall reflectance among the sampling stations were partly caused by wave effects, which generated specular reflection that leads to higher reflectance. The weather data indicated that the average wind speed during the data collection for 14 May and 15 May was 20.15 km h⁻¹. The wind speeds during the same time for 4 and 5 June and 27 and 28 August were 15.7 and 7.6 km h^{-1} , respectively. Also for May, for most of the 16 reflectance curves, the 680 nm absorption and 700 nm peak of chlorophyll were not obvious (Gitelson 1992), which revealed relatively low amounts of chlorophyll-a in the water. The overall reflectance for June was much lower than May (figure 3(b)). The most pronounced curve was the one occurring at station P9. It is believed that the white sand bottom is the reason for that. Again, the indicative spectral features of chlorophyll were not readily picked up. The spectral curves for August seemed to show much more 'peak and valley' characteristics than the other two months (figure 3(c)). It indicated higher chlorophyll-a concentrations in many sampling stations and was consistent with the measured results from water sampling.

To test if the reflectance value at a specific wavelength can be used to estimate chlorophyll concentration, correlation coefficients were calculated for all 512 ASD bands. As expected, the results were not promising. For all three cruises, the absolute values of correlation coefficients (R) between reflectance and chlorophyll-a concentration were less than 0.58 (figure 4).

Figures 5(*a*), (*b*) and (*c*) illustrate the first derivative spectra for May, June and August. The first derivatives for steeper slopes of reflectance curves tended to have higher absolute values. Note that the much greater variations among the 16 spectral curves that appeared in figures 3(a)–(*c*) did not appear this time for their derivative spectra. This phenomenon indicated that derivative spectra were less affected by the wave effects.

Figure 6 shows the results of correlation analysis performed on the first derivative and chlorophyll-*a* concentration. Compared with the correlation produced with the



Figure 4. Correlation coefficients (R) between reflectance and chlorophyll-a concentration.



Figure 5. First derivative spectra: (a) May, (b) June and (c) August.

reflectance (figure 4), the first derivative had much higher correlation with chlorophyll-*a* concentration. The higher correlation coefficients (|R| > 0.6) were found primarily in four spectral regions: 630–645 nm, 660–670 nm, 680–687 nm and 700–735 nm. These can be potential wavelength regions where the first derivative may be used to estimate chlorophyll-*a* concentration.

The 680–687 nm represented the ascending side of the so-called '700 nm peak' and was considered as the important spectral range where the first derivatives were indicative of the concentration of chlorophyll-*a*. Note that the spectral position of the '700 nm peak', generally varies with chlorophyll concentrations (Gitelson 1992). So the 680–687 nm may also vary in position accordingly. For example, a strong correlation between first derivative and chlorophyll was found at 690 nm for an inland water case (Han and Rundquist 1997). For this study, the effectiveness of the



Figure 6. Correlation coefficients (R) between first derivative and chlorophyll-*a* concentration.



Figure 7. Correlation between first derivative at 686 nm and chlorophyll-a concentration.

first derivative in 680–687 nm was examined. It was found that with all data combined, the first derivative at 686 nm produced the highest positive correlation with chlorophyll-*a* concentration (R=0.858) (figure 7).

4. Conclusions

The effectiveness of derivative analysis in estimating chlorophyll-*a* concentration from coastal water has been demonstrated in this paper. One of the serious problems in the remote sensing of oceans is the specular reflection caused by wave effects. This study proved that the derivative spectra were more independent of wave effects and therefore continued to show the absorption features of chlorophyll under windy conditions. This study further supported the usefulness of field spectrometry as a fundamental research tool in supporting the future hyperspectral sensors. In addition, the spectral regions 630–645 nm, 660–670 nm, 680–687 nm and 700–735 nm were found to be potential regions where the first derivatives can be used to estimate chlorophyll concentration.

Acknowledgements

This research has been supported by a grant from the US Environmental Protection Agency's Science to Achieve Results (STAR) Estuarine and Great Lakes (EaGLe) program through funding to the CEER-GOM, US EPA Agreement R 82945801. Although the research described in this article has been funded wholly or in part by the United States Environmental Protection Agency, it has not been subjected to the Agency's required peer and policy review and therefore does not necessarily reflect the views of the Agency and no official endorsement should be inferred. The Gulf Ecology Division of the EPA supported data collection.

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