Modeling of Estuarine Chlorophyll a from an Airborne Scanner

SIAMAK KHORRAM, GLENN P. CATTTS, JAMES E. CLOERN, AND ALLEN W. KNIGHT
Abstract—Near simultaneous collection of 34 surface water samples and airborne multispectral scanner data provided input for regression models developed to predict surface concentrations of estuarine chlorophyll a. Two wavelength ratios were employed in model development. The ratios were chosen to capitalize on the spectral characteristics of chlorophyll a, while minimizing atmospheric influences. Models were then applied to data previously acquired over the study area three years earlier. Results are in the form of color-coded displays of predicted chlorophyll a concentrations and comparisons of the agreement among measured surface samples and predictions based on coincident remotely sensed data. The influence of large variations in fresh-water inflow to the estuary are clearly apparent in the results. The synoptic view provided by remote sensing is another method of examining important estuarine dynamics difficult to observe from in situ sampling alone.

I. INTRODUCTION

Knowledge of the location and concentration of chlorophyll a within an estuary provides greater ecological understanding. Phytoplankton, producers of chlorophyll a and other pigmented organics, are distributed throughout the San Francisco Bay estuary by wind and water circulation acting on areas of high productivity. In turn, areas of high biological productivity are relocated within the estuary based on dynamic environmental factors (i.e., fresh water inflow, volume, water depth, nutrient sources ([1])). The dynamic nature of these interrelationships makes cause and effect hypotheses difficult to formulate, and even more difficult to field verify.

Plankton field surveys conducted in the San Francisco Bay since the mid 1900’s have long been the standard yardstick against which anomalies in phytoplankton distribution patterns have been identified [2]. Field surveys are usually conducted by procuring and icing surface whole water samples for subsequent acetone extraction and laboratory spectrophotometric analysis for chlorophyll a concentration [3]. If many point samples are required, interpolation among sampling stations may adequately represent phytoplankton distribution. Extensive surface sampling is a costly monitoring technique. An alternative to point sampling is the use of shipboard fluorometers that provide a fluorometric "trace" of chlorophyll a concentration along the ship’s track.

Ship-borne fluorometers and field-measured surface samples both require interpolation among sampling stations to arrive at estimates of chlorophyll a concentration in unsampled areas. Phytoplankton distribution is often characterized by patchiness, which compounds the shortcoming of interpolation, especially among widely spaced surface observations. On the other hand, remotely sensed data is recorded for every picture element at a fixed resolution, creating wall-to-wall spectral coverage of the entire study area. If the reflected energy, as detected by the scanning device, is sufficiently related to surface chlorophyll a concentration, interpolation is unnecessary. The amount of costly surface sampling could be reduced to levels necessary for calibration of remotely sensed data and a more accurate synoptic "snapshot" view of phytoplankton distribution may be attained.

It was this line of reasoning that instigated initial studies involving the remote sensing of oceanic and coastal waters. Previous investigations concerning the spectral composition of ocean color have identified four sources governing water leaving radiance characteristics. The four sources are: 1) live phytoplankton, 2) associated biogenic and dissolved organic detritus, 3) terrigenous particles and resuspended sediment, and 4) particulate and dissolved terrigenous or anthropogenic organic matter gelbstoff or yellow substance [4], [5]. Furthermore, researchers have separated oceanic waters, whose spectral characteristics are due primarily to phytoplankton (and their detrital component's reflectance and absorbance (case 1)), from those waters wherein sediment and dissolved organic matter also exert an influence on the spectral properties of water leaving radiance (case 2). Case 1 waters tend to be oceanic in nature, while case 2 waters include coastal estuaries such as San Francisco Bay. Due to the simultaneous influence of sediment and phytoplankton on the spectral characteristics of case 2 waters, there is speculation among researchers that algorithms designed to extract chlorophyll a concentrations from spectral data may need to be tailored to a given geographic region and/or season [4], [5]. The normal range of chlorophyll a concentrations in case 2 waters (i.e., 0–100...
µg/l) is often an order of magnitude over the normal range for case 1 waters (i.e., 0–10 µg/l). These higher chlorophyll a concentrations of case 2 waters often produce measurable reflectance and absorbance in infrared wavelength regions weakly influenced by the lower chlorophyll a concentrations found in case 1 waters [6], [7]. Bressette and Lear [8] reported an aerial infrared photographic detection threshold of 30–50 µg/l of chlorophyll a in phytoplankton blooms. Therefore, work among researchers has utilized more than one wavelength region from different parts of the spectrum to obtain chlorophyll a concentration from remotely sensed spectral data acquired over case 2 waters [7], [15]. In addition to the aforementioned variables influential in dictating the spectral response from estuarine waters, the condition and type, as well as concentrations, of phytoplankton, present another set of factors. Age, vitality, and taxonomic group all affect reflectance and absorbance by phytoplankton [9], [16]. It seems plausible that because algorithms designed to extract chlorophyll a concentrations from spectral data acquired over case 2 waters may need to be tailored to meet specific estuarine situations, universal estuarine models may not be possible to establish.

A. Objective

A variety of remotely sensed data has been collected over the San Francisco Bay. Landsat multispectral scanner, thematic mapper, Daedalus 1260 multispectral scanner, and ocean color scanner data have all been acquired and analyzed [10]–[13]. Narrower wavelength channels facilitate the retrieval of chlorophyll a concentrations from remotely sensed data by allowing the selection of data from particular wavelength regions that are predominantly influenced by chlorophyll a reflectance and absorbance [17]. Catts et al. [12] utilized spectral data from four Daedalus wavelength channels centered at 475, 670, 745, and 1010 to establish a linear relationship between these data and surface measured chlorophyll a concentration values. These linear models were developed from data acquired over the same geographic region and at the same time of year as this current investigation. The objective of this study was to develop a model for predicting chlorophyll a surface concentrations for the 1983 data utilizing two wavelength ratios, one sensitive to lower concentrations and another sensitive to higher concentrations, that would also perform adequately with the data previously acquired by Catts et al. [12].

B. Selection of Channels

Due to the dynamic nature of the study area, chlorophyll a concentrations exhibit a broad range of values both spatially and temporally. Therefore, a model developed to predict chlorophyll a concentration based on spectral reflectance must be able to function in the presence of either high or low concentration levels. The four wavelength regions used in the ratios appear in Table I. The blue-green spectral region was chosen because it is greatly absorbed by chlorophyll a and is sensitive to variations in low chlorophyll a concentrations [4], [5], [14], [16]. Blue-green reflectance is influenced by atmospheric, bottom, and water surface backscatter. To remove these influences is desirable, even though high-altitude aircraft spectral data of the kind involved in this study are less atmospherically influenced than higher altitude platforms (i.e., satellites). Without surface sample site measurements of upwelling and downwelling irradiance, removal of these influences in a quantitative fashion is not possible. Gordon and Clark (14) used reflectance from the 670-nm wavelength region as a calibration value.

This calibration performs in oceanic case 1 waters where levels of biogenous and terrigenous suspended and dissolved matter are low enough not to contribute to reflectance in the 670-nm wavelength region. In case 2 waters, the red portion of the spectrum becomes an important indicator of chlorophyll a concentration [6]. For this reason the blue-green reflectance value is ratioed over the reflectance recorded by the scanner in the infrared II wavelength region. Water absorption of near-infrared energy in this spectral region infrared dominates over suspended and dissolved matter influences. However, atmospheric influence is not quantitatively the same in the blue-green and infrared II wavelengths. Therefore, this constitutes a relative, pixel by pixel, atmospheric correction method utilizing available information.

The second wavelength ratio employed was chosen to monitor the increasing absorption due to chlorophyll a in the red wavelengths and the increasing reflectance (including contribution from in vivo fluorescence) in the infrared I region with increasingly higher concentrations of chlorophyll a [6], [9], [15], [16]. This ratio becomes important when surface chlorophyll a values are high enough to cause significant reflectance in infrared wavelength regions of water absorption. The ratio technique was chosen to cancel out atmospheric and water surface backscatter similarly affecting these adjacent wavelength regions.

C. Research Methodology

Research methodology included: 1) acquisition of near-surface chlorophyll a measurements from boats and airborne Daedalus 1260 multispectral scanner (MS) visible and near-infrared reflectance measurements; 2) laboratory analysis of whole water samples to determine near-surface chlorophyll a concentrations for 34 sample sites; 3) extraction of reflectance measurements in the 485-, 660-, 720-, and 980-nm portions of the electromagnetic spectrum expressed at 8-bit digital count values from airborne Daedalus MS data for the 34 sample sites; 4) development of regression equations relating Daedalus 1260 MS reflectance data to near-surface chlorophyll a measurements utilizing wavelength ratios of 485 nm divided by 980 nm and 660 nm divided by 720 nm as independent variables; and, 5) production of color-coded maps representing near-surface chlorophyll a concentration predictions for the entire study area.
D. Collection of Near-Surface Water Samples and Laboratory Analysis

On September 13, 1983 during ebb-to-ebb slack tidal conditions, 34 whole water samples were collected just below the water surface. The 34 sample sites were located in the deeper channel regions of the study area. These sites were chosen to give good areal coverage of the study area and at the same time allow limited manpower to make as many measurements as close to the overflight time as possible without becoming mired in the shallows (see Fig. 1).

Surface sampling was conducted from 10:30 A.M. to 12:43 P.M. Pacific Daylight Time (PDT). This translates to water samples being acquired within 1.5 h of the scanner overflight.

In the laboratory, the 34 whole water samples were extracted in 90-percent acetone. These acetone extracts were analyzed spectrophotometrically to determine the chlorophyll \( a \) concentration for each sample [18].

E. Acquisition and Processing of Daedalus 1260 MSS Data

From 11:16 A.M. to 11:24 A.M. (PDT) on September 13, 1983, a NASA U-2 aircraft flew over the study area at about 70 000 ft MSL. Ground resolution was 91 ft, meaning that individual image pixels represented, on an average, roughly 28-m square at the bay surface. The electromagnetic wavelengths received by the Daedalus 1260 MS for this 1983 research are shown in Table I.

Overflight data on 1600 bit/in magnetic tapes were procured from the NASA Ames Research Center and redensitized to 800 bit/in to be compatible with the University of California, Berkeley, Remote Sensing Research Program’s image-processing system. Fifty-five digitized control points from both the image files and NOAA nautical charts (1:40 000 scale) were used to develop a second-order polynomial regression equation. This equation was used in conjunction with 34 surface sample site coordinates digitized from the NOAA nautical charts to determine the image file coordinates of all 34 surface measured sample sites. Even with the highly correlating fits and low residuals obtained by the regression method, accurately locating a 28 m\(^2\) block in an estuary is not ensured. To help ensure accurate reflected energy values representing the sample sites, a 5 × 5 pixel matrix, centered on each of the 34 predicted sample site locations, was averaged, and this value was used to represent the reflected energy in each of the four selected wavelengths 485, 660, 720, and 980 nm. Each 5 × 5 pixel matrix was examined for homogeneity of reflected energy measurements. Standard deviations for these sample site matrices ranged from 0–5 percent of the matrix mean. Fortunately, there were no apparent bad scanline data in any image file.

F. Development of Coefficients Used in Modeling

Using the two wavelength ratios as independent variables and the 34 measured near-surface chlorophyll \( a \) concentrations (in micrograms per liter) as dependent variables, least squares regression was employed to determine coefficients that would be used to produce final images of chlorophyll \( a \) concentration predictions for the entire study area. The near-surface chlorophyll \( a \) concentration distributions in dynamic estuarine regions may change quickly. In the study area, tidal speeds range from 1–3 m/s and riverine inflow speeds are even greater [19]. Therefore, establishment of stable predictor coefficients can be a problem when surface measurements are made at times far away from the scanner overpass. Alterations in river inflow, wind direction and speed, tidal action, and net productivity are some of the influences on the chlorophyll \( a \) concentration of a given water parcel during a particular time. It follows that the establishment of coefficients for a given set of surface measured data is best accomplished using sites measured as close to the time of the scanner overflight as possible. The drawback of such a strategy is that it severely reduces the size of the sub-sample selected from the original data set used to determine coefficients. It may also reduce the range of near-surface chlorophyll \( a \) measurements input to regression as dependent variables. For these reasons, both models whose coefficients

<table>
<thead>
<tr>
<th>TABLE I</th>
<th>DAEDALUS 1260 MS CHANNELS FOR TWO ACQUISITION DATES</th>
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<tbody>
<tr>
<td></td>
<td>1980 DATA COLLECTION</td>
</tr>
<tr>
<td></td>
<td>BLUE-GREEN CHANNEL</td>
</tr>
<tr>
<td></td>
<td>450–500nm (c=475nm, ( bw=90nm ))</td>
</tr>
<tr>
<td></td>
<td>450–520nm (c=485nm, ( bw=70nm ))</td>
</tr>
</tbody>
</table>

\( c \) = center of wavelength channel  
\( bw \) = width of wavelength channel  
\( nm \) = nanometers
were developed from regression using the full data set \((n = 34)\) and those whose coefficients were determined by regression using only data measured within 15 min of the scanner overpass \((n = 11)\) were examined. Plots of residual versus actual data from full data-set regressions revealed strong positive linear trends. As expected, these residual trends became random scattering when time partitioned data input to regression techniques. The linear trend of plots of residual versus actual values behaved similarly in all three data sets (two from 1980 and one from 1983).

Coefficients for the data set composed of 34 sample sites and those established for the data set partitioned by time were different but produced similar general patterns of predicted chlorophyll \(a\) concentrations in image files of the entire study area. Models based on all 34 sample sites predicted near-surface chlorophyll \(a\) concentration distributions that exhibited less range and lower maximum values than models based on data from sites measured within 15 min of the scanner overflight. The statistical summary of the full and time partitioned data sets are shown in Table II. The form of the full model was: Chlorophyll \(a\) (in micrograms per liter) \(= \ a + b \) \((485 \text{ nm}/980 \text{ nm}) + C \) \((660 \text{ nm}/720 \text{ nm})\).

From the last column in Table II it is apparent that the test of significance of coefficients (PROB > T) is not at the 95-percent level for the wavelength ratio red/infrared I indicates that the coefficient assigned to this ratio is not significantly different from zero and, therefore, this independent variable could be dropped from the model. The nonsignificance of the red/infrared I wavelength ratio in this case is to be expected. The highest surface-measured concentration of chlorophyll \(a\) in the study area was 13.54 \(\mu g/l\) on the day of the overflight. This is an extremely low value for a maximum considering that in 1980 surface samples in excess of 60 \(\mu g/l\) were measured. The red/infrared I wavelength ratio was developed on 1980 data, including high values of chlorophyll \(a\) concentration. This ratio is an indicator of higher near-surface chlorophyll \(a\) concentrations where absorption of the 720-nm wave-length by bay water occurs until chlorophyll \(a\) concentrations in the water become high enough to cause measurable reflectance. In any case, this ratio was left in the time-partitioned model used to produce the final color-coded map to deal with unmeasured portions of the study area where chlorophyll \(a\) concentrations might exceed the highest observed measurement of 13.54 \(\mu g/l\).

G. Application of Models to the Entire Study Area

In order to examine the spatial distributions of near-surface chlorophyll \(a\) concentrations predicted by the models in Table II, each linear equation was applied to image files of the entire study area on a pixel by pixel basis. Land areas were first masked from the image files before application of models by using reflectance characteristics of near-infrared wavelengths to delineate the water/land boundary. Reflected energy values of the wavelength bands centered on 485, 660, 720, and 980 nm were ratioed first \((485 \text{ nm}/980 \text{ nm}; 660 \text{ nm}/720 \text{ nm})\) and then the ratio image files were combined using the linear equations of Table II. Predicted values of chlorophyll \(a\) concentration were separated into nine classes. Each class represented a range of chlorophyll \(a\) concentrations and was assigned a color. The final color-coded result and key appears in Fig. 2(b) and is based on (2) of Table II.

H. Discussion of Results

The spatial pattern of predicted chlorophyll \(a\) concentration shown in Fig. 2(a) and (b) includes two data sets from 1980 and one from 1983. Conditions in the northern portion of San Francisco Bay estuary were markedly different in 1980 than in 1983. In 1983 fresh water inflow from the Sacramento/San Joaquin rivers delta was 27 000 compared with 2900 ft\(^3\)/s average for the 1980 conditions (U.S. Bureau of Reclamation, Sacramento, CA). The high volume of fresh water inflow appears to have relocated the highest chlorophyll \(a\) concentrations westward into eastern San Pablo Bay. This situation is similar to winter hydrographic conditions in this portion of the estuary where a high volume of fresh water inflow may flush phy-
TABLE II
Statistical Summary of Model Coefficient Development on September 13, 1983 Data Set

<table>
<thead>
<tr>
<th>MODEL #</th>
<th>Adjusted R Square</th>
<th>F Prob&gt;F</th>
<th>Residual Mean Squared Error</th>
<th>Model Coefficient Values</th>
<th>Standard Error of Coefficients</th>
<th>Prob&gt;F for coefficient Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Full Model using all Data (n = 34)</td>
<td>.35</td>
<td>10.1</td>
<td>2.02</td>
<td>a = 4.63</td>
<td>b = 0.11</td>
<td>c = 4.33</td>
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<tr>
<td></td>
<td></td>
<td>.0004</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>2. Full Model using Time-Partitioned Data</td>
<td></td>
<td>84.7</td>
<td>0.78</td>
<td>a = 3.58</td>
<td>b = 0.55</td>
<td>c = 0.41</td>
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<td>(n = 11) (Data required within 15 minutes of</td>
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<td>overflight)</td>
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<tr>
<td>3. Model with 485nm/980nm ratio only</td>
<td></td>
<td>19.5</td>
<td>2.00</td>
<td>a = 2.41</td>
<td>b = 0.12</td>
<td>c = 0.38</td>
</tr>
<tr>
<td>using all data</td>
<td></td>
<td>.0001</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>(n = 34)</td>
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<td></td>
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<td></td>
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</tr>
<tr>
<td>4. Model with 485nm/980nm ratio only</td>
<td></td>
<td>190.4</td>
<td>0.74</td>
<td>a = 2.89</td>
<td>b = 0.55</td>
<td>c = 0.38</td>
</tr>
<tr>
<td>using time partitioned data</td>
<td></td>
<td>.0001</td>
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<td>(n = 11)</td>
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</table>

toplankton productivity zones westward into suitable salinity ranges [19]. In the 1980 data, Grizzly and Honker Bays were areas of high chlorophyll a as well as turbidity values. In 1983, the highest field measured turbidity values were still recorded in Grizzly and Honker Bays. The chlorophyll a maximum for 1983 is no longer coupled with high turbidity and appears in eastern San Pablo Bay, although chlorophyll a concentrations are predicted to be slightly greater than their immediate surrounding for both Grizzly and Honker Bays. The uncoupling of high turbidity and high chlorophyll a concentration suggests that the model based predominantly on blue-green reflectance in the 1983 data is not adversely influenced by variations in turbidity. This does not preclude turbid waters from influencing the red/infrared ratio instrumental in models predicting chlorophyll a concentrations for the 1980 data. However, suspended sediment reflectance should be similar and cancel out in the ratio of red/infrared.

The performance and form of linear chlorophyll a prediction equations from all three data sets is displayed in Table II. Neither of the full ebb tide sampled data (mornings of 1980 and 1983) have adjusted R square values of any magnitude; while the full data set from flood tide conditions (afternoon of 1980) has an adjusted R² value of 0.72. All three time partitioned datasets show high adjusted R² values. Sampling during this flood tide condition resulted in a greater surface water parcel residence time. For this reason, sampling away from scanner overflight time displayed less temporal change then during ebb tidal conditions.

Average chlorophyll a concentration for corresponding locations of surface measured samples was higher in 1980 than in 1983, and the wavelength ratios behave quite differently in each instance. Table IV is composed of simple correlation coefficients comparing several surface measured (turbidity and chlorophyll a) and spectral data ratio variables among one another for each of the three dates. In 1980, turbidity for chlorophyll a exhibited a strong positive correlation in both morning and afternoon data sets (R = 0.93 and R = 0.80, respectively), whereas in 1983, their correlation was lower (R = –0.48). These correlation values are for time partitioned data only. In 1980, wavelength ratio red/infrared had a strong negative correlation with chlorophyll a concentration for both times of day (R = –0.85 and R = –0.84), while the wavelength ratio blue-green/infrared II was less influential (R = 0.07). On the other hand, in 1983, chlorophyll a concentration was highly correlated with wavelength ratio blue-green/infrared II in a positive fashion (R = 0.98) and only slightly correlated with the wavelength ratio red/infrared I (R = 0.11). Obviously, one wavelength ratio is better suited to remotely sensed monitoring of chlorophyll a of a particular concentration range than the other. Higher chlorophyll a concentrations will be better represented in the red/near infrared I wavelength region [6], [7], whereas lower concentrations of chlorophyll a are representative of more oceanic conditions and will be better represented by information in the blue-green portion of the electromagnetic spectrum [5].

II. CONCLUSIONS

Several conclusions can be drawn from the analysis of these data.

1) Wavelength ratios employing blue-green and infrared II spectral information and those employing red near infrared I wavelengths are influenced by the surface concentration of chlorophyll a. These ratios may be used as independent variables in regression analysis in order to
Fig. 2. Predicted spatial patterns of surface chlorophyll a concentration based on surface data acquired within 15 min of Daedalus 1260 MSS overflight. (a) Morning and afternoon data of August 28, 1980. (b) Morning data of September 13, 1983.
establish a linear equation capable of predicting relative spatial distribution of surface chlorophyll a concentrations as determined and calibrated by surface sampling methods under drastically different fresh water inflow regimes.

2) These wavelength ratios are best utilized by providing surface measured data within minutes of spectral data acquisition, especially when surface water movement is rapid.

3) The blue-green/near infrared II ratio explains the most variation in the surface measured observations when measured chlorophyll a concentrations are relatively low. The red/infrared I wavelength ratio functions most effectively when higher chlorophyll a concentrations exist.

4) Certain portions of the tidal cycle are associated with the longest calm surface condition and are, therefore, the most desirable times to simultaneously acquire surface and airborne observations.

5) Due to the complexity of estuarine systems and the number of variables affecting the distribution and concen-
tration of algal chlorophyll $a$, additional data sets need to be acquired and analyzed in order to provide conclusive evidence of model predictive performance.

6) Remote monitoring of estuarine chlorophyll $a$ can produce visual mappings that could be invaluable in the further understanding of the interrelationships among estuarine water quality parameters.

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REFERENCES


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James E. Cloern, photographs and biography not available at the time of publication.

Allen W. Knight, photograph and biography not available at the time of publication.