Towards a unified approach for remote estimation of chlorophyll-a in both terrestrial vegetation and turbid productive waters

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Received 27 June 2003; revised 13 August 2003; accepted 15 August 2003; published 20 September 2003.

In this study we tested the applicability of a method, originally developed for terrestrial plant leaves, to retrieve chlorophyll-a concentrations from reflectance spectra of turbid productive waters. We tuned the conceptual model according to the optical characteristics of the aquatic medium, and accurately predicted chlorophyll-a concentrations in water bodies over a wide range of optical conditions. Our results provide evidence that this technique may be considered as a general solution, independent of the type of medium, for assessing chlorophyll concentration in optically deep media using remotely sensed data.


1. Introduction

[2] The photosynthetic pigment chlorophyll-a (chl-a) is an indicator of biomass and productivity of both terrestrial and aquatic ecosystems. Remote sensing of chl-a allows one to monitor ecosystem dynamics over large geographic areas at relatively low costs. Airborne and space borne sensors can detect the fraction of incoming solar irradiance reflected by any medium (e.g., water bodies or terrestrial plants), which is defined as reflectance, R, and is the wavelength of interest [e.g., Mobley, 1994]. The link between R and the concentrations of constituents in the medium is provided by the inherent optical properties [Preisendorfer, 1976], backscattering coefficient, bb, and absorption coefficient, ab, of all the constituents that interact with light in the medium [e.g., Kortum, 1969; Gordon et al., 1988].

[3] So far scientists have developed numerous medium specific, independent techniques to extract information on chl-a concentration from R. The normalized difference vegetation index (NDVI) [Rouse et al., 1974] is one of the most widely used algorithms to assess biomass in terrestrial vegetation. The blue to green reflectance ratio [e.g., Morel and Prieur, 1977] is widely used to estimate chl-a concentration in ocean waters. The near infrared to red reflectance ratio [e.g., Gitelson and Kondratyev, 1991], among many others, is used in productive waters (where chl-a is not correlated with the other optically active constituents). However, to the best of our knowledge, the differences and similarities of methods for extracting chl-a amounts from reflectance spectral data collected over different types of media (e.g., water bodies and plant leaves) have not been compared and generalized.

[4] Recently a conceptual model, relating remotedly sensed reflectance and pigment content in higher plant leaves was developed [Gitelson et al., 2003a]. The conceptual model was based on the fact that, for a wide range of reflectance values (0.01–0.50), the reciprocal reflectance of leaves was closely related to the Kubelka-Munk remission function, which is equal to a/bb, where ab is the absorption coefficient of the pigment of interest from reflectance spectra. The following relationship between leaf pigment content and reflectance was used:

\[ \text{Pigment content} \propto \frac{R_1 - R_2}{R_3}. \]

[5] Here \( \lambda_1 \) is a spectral region such that \( R_3 \) is maximally sensitive to the absorption of the pigment of interest; however, \( R_1 \) is also affected by the absorption of other constituents and backscattering. \( \lambda_2 \) is a spectral region such that \( R_2 \) is minimally sensitive to the pigment of interest, and for which the absorption by other constituents is almost equal to that at \( \lambda_1 \). The difference \( R_1 - R_2 \) was related to the content of the pigment of interest, but it was still affected by the variability in leaf structure and thickness [Gitelson et al., 2003a], i.e., the backscattering by the medium. \( \lambda_3 \) is a spectral region minimally affected by the absorption of pigments, and, therefore, was used to compensate for the variability in backscattering between samples. The model accurately estimated chlorophyll content in leaves (root mean square error, RMSE, less than 40 mg/m²) over a chlorophyll range spanning from 0.1 to 800 mg/m².

[6] The same conceptual model was also used for the quantification of different pigments in fruit peels [Merzlyak et al., 2003] as well as for non destructive estimation of leaf area index and biomass in agricultural crops [Gitelson et al., 2003b].

[7] In this paper we investigated the applicability of the conceptual model for remote estimation of chlorophyll-a in turbid productive waters. We hypothesized that the only requirement to apply the conceptual model to the aquatic medium is tuning of the spectral regions \( \lambda_1, \lambda_2, \lambda_3 \), according to the optical characteristics of the new medium.

2. Methods

[8] To tune and test the conceptual model for chlorophyll-a estimation in productive turbid waters, we carried...
out in situ and laboratory measurements in an as wide as possible range of constituent concentrations and compositions. The study areas included five of the Fremont sand pit lakes dominated by autochthonous organic suspended material; and two reservoirs (Glen Cunningham and Branched Oak) with a gradient of allochthonous organic and inorganic suspended materials from the inlet to the dam. All water bodies are located in Eastern Nebraska, USA. Measurements took place between July 2001 and October 2001, and between May 2002 and October 2002.

2.1. Field Measurements

[9] Spectral reflectance measurements were made from a boat using two inter-calibrated Ocean Optics USB2000 radiometers. Data were collected in the range 400–900 nm with a spectral resolution of about 1.5 nm. Radiometer #1, equipped with a 25° field-of-view optical fiber was pointed downward to measure the upwelling radiance from the lake ($L_{\text{water}}$). The tip of the optical fiber was kept just below the water surface. Radiometer #2, equipped with an optical fiber and a cosine collector, was pointed upward to simultaneously measure incident irradiance ($E_{\text{inc}}$). Spectral reflectance, $R_{\lambda}$, was computed as $R_{\lambda} = (L_{\lambda}/E_{\text{inc}})$. At each station, six reflectance spectra were measured, each averaging 15 consecutive scans.

[10] At each station, Secchi disk depth and turbidity were measured, and water was collected just below the surface and stored in the dark in a cooler with ice. Samples were filtered on Pall Gellman type A/E Glass Fiber Filters and frozen for successive laboratory analyses.

2.2. Laboratory Measurements

[11] Chlorophyll-a was extracted in hot ethanol, and its concentration quantified fluorometrically [Welshmeyer, 1994]. The concentrations of total suspended solids (TSS) and inorganic suspended solids (ISS) were determined gravimetrically [American Public Health Association, American Water Works Association, and Water Pollution Control Federation, 1989]. Spectral absorption measurements were carried out immediately after every 2002 field campaign with a Cary 100 Varian spectrophotometer. The optical densities of total suspended matter and tripton (suspended inorganic non-living organic material), after oxidation of pigments by means of diluted chlorine water [Tassan and Ferrari, 1995], were measured on filters [Fargion and Mueller, 2000] and corrected for scattering by subtracting the optical density at 750 nm from the entire spectrum. Conversion into absorption coefficient was accomplished by using published coefficients [Mitchell, 1990]. Pigment absorption was computed as the difference between total particles and tripton absorption coefficients. The colored dissolved organic matter (CDOM) absorption coefficients were measured as in Bricaud et al. [1981].

2.3. Model Tuning

[12] The data set was divided into two independent subsets, one for model development and the other for model validation. The former contained 47 samples, the latter 46. Based on the spectral characteristics of constituents in turbid productive waters (representative spectra are shown in Figure 1), we expected to find the optimal spectral regions $\lambda_1$, $\lambda_2$, and $\lambda_3$ for chl-a estimation as follows. The absorption by CDOM, tripton, and other pigments overlaps the absorption peak of chlorophyll-a in the blue spectral region (Figure 1a); this severely constrains the use of the blue range for chl-a estimation in turbid productive waters. In this type of waters, the only spectral range, $\lambda_1$, maximally sensitive to chlorophyll-a concentration is the red-NIR [e.g., Gitelson and Kondratyev, 1991; Gitelson, 1992]. However, reflectance in this spectral range is also affected by the residual absorption by CDOM and tripton. To remove these interferences and the variability between samples in backscattering, $\lambda_2$ should be as close as possible to $\lambda_1$. At the same time, it should be in a spectral region minimally affected by chlorophyll-a absorption (i.e., 690 $< \lambda_2$ $< 730$ nm). The variations in concentration, size, shape, and refractive index of all suspended particles affect the scattering coefficient [e.g., Mobley, 1994] and, thus, the difference ($R_{\lambda_1} - R_{\lambda_2}$). This leads to overestimating chlorophyll-a concentrations in water bodies with higher backscattering and underestimating it when backscattering is lower. Hence, this effect should be eliminated using reflectance in a spectral region $\lambda_3$ where the absorption by pigments, tripton and CDOM is negligible (i.e., $\lambda_3$ $> 740$ nm, [Babin and Stramski, 2002; Gons et al., 2002]).

[13] Using the model-development subset, we spectrally tuned the conceptual model by means of a stepwise technique. We linearly regressed $R_{\lambda_1}$ and ($R_{\lambda_1} - R_{720}$) versus chl-a to obtain a first estimate of $\lambda_1$. Then, regressing ($R_{670} - R_{\lambda_2}$) and ($R_{670} - R_{720}$)*$R_{\lambda_3}$ vs. chl-a, we found $\lambda_2$ and $\lambda_3$, respectively. Finally, we analysed the linear relationships between ($R_{\lambda_1} - R_{720}$)*$R_{750}$ and chl-a and identified the optimal $\lambda_1$. 

![Figure 1. Absorption coefficients of water constituents (a) and reciprocal reflectance (b) of a turbid productive lake (chl-a = 78 $\mu$g L$^{-1}$, Secchi depth = 49 cm, turbidity = 27 NTU).](image-url)
We then established a relationship between the model with 10-nm wide spectral bands and chl-a concentrations measured analytically. This relationship was finally used to predict chl-a concentrations using the model validation dataset.

3. Results and Discussion

[15] The water bodies sampled ranged from mesotrophic to hypereutrophic, and exhibited chl-a concentrations and turbidity values varying by a factor as high as 25. Absorption coefficients at 440 nm of CDOM and tripton varied 3 and 5 folds, respectively (Table 1). The dominant groups of algae encountered were Cyanophyta, Chlorophyta, and Chrysophyta. As an example, Figure 1 shows the absorption coefficients of water constituents and the corresponding reciprocal reflectance spectrum of a typical turbid productive lake.

[16] In the visible and NIR spectral range, the linear relationship between $R_{750}^1$ and chl-a concentration was not significant due to the variability between samples in backscattering and the interference of constituents different than phytoplankton. Subtraction of $R_{750}^1$ from $R_{544}^1$ decreased the effects of backscattering and of the residual absorption by tripton and CDOM. The best linear fit between ($R_{730}^1 - R_{544}^1$) and chlorophyll-a concentration was found for $\lambda_1$ around 670 nm and $\lambda_2$ near 720 nm ($r^2 = 0.72$).

[17] The optimal spectral region for $\lambda_3$ was found around 750 nm. The product of the difference ($R_{670} - R_{720}$) and $R_{750}$ allowed us to compensate for variation in backscattering between samples [Gons et al., 2002] and considerably increased the correlation with chl-a ($r^2 = 0.94$, $p < 0.0001$).

[18] The model in the form chl-a = $-28.3X^2 + 161.0X + 56.7$, where $X = (R_{660} - 670 - R_{720} - 730)R_{740} - 750$, accounted for 94% of the variance ($p < 0.0001$) of chl-a concentrations measured analytically. The RMSE of chl-a estimation was less than 11 $\mu$g L$^{-1}$.

[19] Using the above equation, chl-a concentrations were predicted for the model validation dataset and were compared to measured ones. The slope of the best-fit function chl-a predicted vs. chl-a measured was 0.990 (not significantly different from 1, $p = 0.86$), the intercept was not significantly different from zero ($p = 0.58$), and the RMSE of chl-a prediction was lower than 13 $\mu$g L$^{-1}$ (Figure 2).

4. Conclusions

[20] We spectrally tuned a conceptual model, developed for terrestrial plant leaves, and predicted accurately chlorophyll-a concentrations in productive water bodies. The wide range of optical conditions sampled support the robustness of the findings. Our results provide evidence that (a) the conceptual model can be applied for accurate remote estimation of chlorophyll-a in turbid productive waters; (b) the conceptual model may be considered as a unified approach for remote chlorophyll-a estimation in various media; and (c) fine tuning of the conceptual model can be carried out knowing the spectral characteristics of the specific medium of interest. To the best of our knowledge, this is the first time that a medium independent algorithm for remote assessment of chlorophyll-a concentration is presented. The conceptual model was previously used for the estimation of chlorophyll-a, carotenoids and anthocyanins in leaves [Gitelson et al., 2001; Gitelson et al., 2002; Gitelson et al., 2003a] and fruit peels [Merzlyak et al., 2003], as well as leaf area index assessment in crop canopies [Gitelson et al., 2003b]. The additional findings presented in this study lead us to believe that this conceptual model may be considered as a general solution for remote quantification of absorbing constituents in optically deep media.

[21] Acknowledgments. We would like to thank B. Leavitt and R. Perk for facilitating this research; A. Via for comments on the manuscript. We also acknowledge J. Holz, T. Barrow and the staff of the limnological laboratory of the Water Center of University of Nebraska-Lincoln for their support in the field and for laboratory analysis. This research was funded by U.S. Environmental Protection Agency under the contract R-82634501. A contribution of the University of Nebraska Agricultural Research Division, Lincoln, NE. Journal Series No. 14187. The research was supported in part by funds provided through the Hatch Act.

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