Remote sensing of ocean chlorophyll: consequence of nonuniform pigment profile

Shubha Sathyendranath and Trevor Platt

Remote sensing of ocean color, applied to the estimation of chlorophyll biomass, is discussed for the case where the vertical distribution of phytoplankton pigments is nonuniform. Using a spectral model of reflectance, the consequences of vertical structure are evaluated by sensitivity analysis on a generalized pigment profile. It is shown that the assumption of a vertically homogeneous chlorophyll distribution can lead to significant errors (relative error exceeding 100%) in the estimation from satellite data of photic depth and total pigment content in the photic zone. The errors are shown to be functions of the parameters of the pigment profile. It is further shown that, if the shape of the pigment profile is known from independent data, the entire pigment profile may be recovered from the satellite data by making slight changes in the existing algorithms for chlorophyll retrieval.

I. Introduction

Two features of remote sensing make it an indispensable tool for oceanographic monitoring at large horizontal scale: (1) synoptic coverage and (2) the possibility of data dissemination in near real time. In the last decade, increasing use has been made in oceanographic research of maps of chlorophyll distribution derived from measurements made by satellite-borne color scanners. But, to date, it is the patterns and features of the maps that have been emphasized, rather than the absolute values of pigment concentration themselves. One reason for this is that only the first optical attenuation length is accessible to the satellite, which returns a weighted average over this depth interval. If the pigment distribution is not uniform, the satellite-weighted surface concentration *per se* ceases to have ecological significance. To optimize oceanographic exploitation of ocean color data, these limitations have to be removed.

In this paper, we discuss the estimation of photic zone depth and of total pigment content of the photic zone using only remotely sensed data when the pigment profile is nonuniform. By sensitivity analysis on a generalized pigment profile, we calculate the magnitude of the potential errors incurred through ignoring vertical structure in the pigment distribution. We show that if prior information is available on the shape of the pigment profile for a particular scene, it is possible to recover water-column biomass and photic depth with only slight modifications to the conventional algorithms for retrieval of satellite-weighted surface chlorophyll concentration.

II. Background and Theory

A. Empirical Algorithm for Chlorophyll Retrieval.

An ocean-color sensor receives upwelling radiance L (flux per unit area per unit solid angle) from the sea surface after modification by the intervening atmospheric path. Empirical relationships have been established that link changes in radiance (corrected for atmospheric effects) with changes in concentration of phytoplankton pigments (including phaeopigments) in the water. The most commonly used algorithm is the form

$$C = A[L(\lambda_1)/L(\lambda_2)]^B, \tag{1}$$

where L is the radiance, λ_1 and λ_2 are wavelengths, C is the concentration of phytoplankton pigments (mg m^{-3}), and A and B are empirically determined constants. In the case of the Coastal Zone Color Scanner (CZCS), the wavelengths used are 443 and 550 nm for low pigment concentrations and 520 and 550 nm for high pigment concentrations. The algorithm has been found to be most successful in open ocean waters.[1,2]

Shubha Sathyendranath is with Dalhousie University, Oceanography Department, Halifax, Nova Scotia B3H 4J1, Canada, and Trevor Platt is with Bedford Institute of Oceanography, Biological Oceanography Division, Box 1006, Dartmouth, Nova Scotia B2Y 4A2, Canada.

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B. Theory of Ocean Color

Simultaneously with the development of empirical relationships, advances have also been made in the theory of ocean color. Let $E_d(\lambda)$ be the downwelling irradiance (flux per unit area) received by a flat plate collector facing upward at the sea surface, and $E_u(\lambda)$ the upwelling irradiance (sensor facing downward), also at the sea surface. Intrinsic ocean color is determined by the spectral values of reflectance $R(\lambda)$, defined as the ratio of $E_u(\lambda)$ to $E_d(\lambda)$. Radiance ratios are treated analogously to reflectance ratios at the same wavelengths.[2] It has been shown[2–7] that the reflectance $R(\lambda)$ can be expressed in terms of the absorption and backscattering coefficients. The simple relationship[5,6,8]

$$R(\lambda) = 0.33 b_b(\lambda)/a(\lambda), \tag{2}$$

where b_b is the backscattering coefficient and a is the absorption coefficient, has been found to be adequate for most oceanic cases.[7,9]

Reflectance spectra from various marine regions can be reconstructed by accounting for absorption and backscattering by phytoplankton, yellow substances and nonchlorophyllous particles.[10–12] We use such an approach with some minor modifications. In open ocean waters, phytoplankton and covarying material are the major substances responsible for changes in ocean color. It is this simple case that is considered here. The coefficients $a(\lambda)$ and $b_b(\lambda)$ are, therefore, expressed as

$$a(\lambda) = a_w(\lambda) + Ca_c^*(\lambda) + Ya_y^*(\lambda), \tag{3a}$$

$$b_b(\lambda) = \tilde{b}_{bw} b_w(\lambda) + \tilde{b}_{bc} b_c(\lambda), \tag{3b}$$

where $a_w(\lambda)$ is the absorption coefficient of pure seawater (m^{-1}); $a_c^*(\lambda)$ is the specific absorption coefficient of phytoplankton [$m^{-1}(mg\ m^{-3})^{-1}$]; Y is the concentration of yellow substances, expressed in terms of their absorption at 440 nm (m^{-1}); $a_y^*(\lambda)$ is the specific absorption coefficient of yellow substances (dimensionless); $\tilde{b}_{bw}$ is the backscattering ratio of pure seawater, i.e., the ratio of backscattering to total scattering; $b_w(\lambda)$ is the total scattering coefficient of pure seawater (m^{-1}); $\tilde{b}_{bc}$ is the backscattering ratio for phytoplankton; and $b_c(\lambda)$ is the total scattering coefficient of phytoplankton (m^{-1}).

The absorption coefficient is parametrized according to Prieur and Sathyendranath.[13] With this parametrization, the spectral form of the specific absorption coefficient of phytoplankton is held invariant, but its magnitude is allowed to vary (the value of the specific absorption coefficient at 440 nm is specified, and the other values are scaled accordingly). At 440 nm, we have taken the specific absorption by yellow substances to be 20% of the absorption by phytoplankton.[13] The backscattering coefficient is modeled as described in Sathyendranath and Platt.[14]

C. Comparison of Model and Empirical Results

In Fig. 1 are plotted various relationships linking the reflectance ratio with the chlorophyll concentration in the water. Using the 440/550 (blue-green) ratio, we have computed this dependence by four different methods [Figs. 1(a)]: first, with the coefficients A and B of Eq. (1) based on the results of Gordon and Morel,[1] as used by NASA in their algorithms for chlorophyll retrieval; second, with slightly different coefficients based on Morel[15]; third, according to an analytical model of Gordon and Morel[1]; and fourth, with the blue-green ratio computed according to our spectral reflectance model, the parameters of which are known to vary depending on the phytoplankton population and the water type. As pointed out by Gordon and Morel,[1] the theoretical results are sensitive to changes (within plausible ranges) in the values of these parameters (the backscattering ratio for phytoplankton and its spectral dependence, the magnitude of the specific absorption coefficient for phytoplankton, and the absorption of yellow substances). The curve obtained using our model was computed with a specific absorption coefficient of phytoplankton at 440 nm = 0.077 [$m^{-1}(mg\ m^{-3})^{-1}$] for chlorophyll concentrations of <1 mg m^{-3} and $a_c^*(440) = 0.025$ [$m^{-1}(mg\ m^{-3})^{-1}$] for chlorophyll concentrations of >1 mg m^{-3}. The computations are based on the assumption that the pigment concentration is uniform with depth.

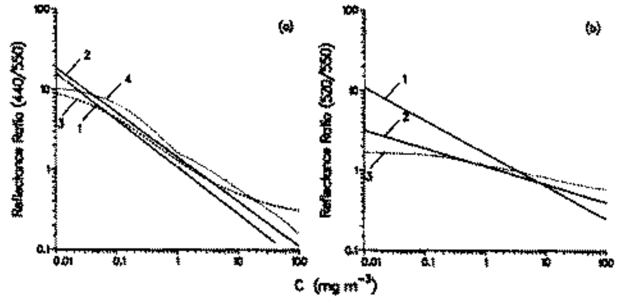

Fig. 1. (a) Relationship between the reflectance ratio for wavelength pair 440/550 and pigment concentration in water: 1, Eq. (1) with parameters $A = 1.13$ and $B = -1.71$ after Gordon and Morel,[1] the NASA algorithm for retrieval at low chlorophyll concentrations; 2, Eq. (2) with parameters $A = 1.92$ and $B = -1.8$ from Morel[15]; 3, analytical relation proposed by Gordon and Morel[1]; 4, results of reflectance model used in this study. (b) Relationship between reflectance ratio for wavelength pair 520/550 and pigment concentration in the water: 1, Eq. (1) with parameters $A = 3.326$ and $B = -2.439$, the NASA algorithm for retrieval at high chlorophyll concentrations; 2, Eq. (2) with parameters $A = 1.69$ and $B = -4.45$ after Clark[16]; 3, result of the reflectance model used in this study.

It is seen from Fig. 1(a) that all four of these approaches yield similar results for the 440/550 ratio. This is not the case, however, if the wavelengths are changed and the 520/550 ratio is used instead [Fig. 1(b)]. We have computed the dependence of this reflectance ratio on chlorophyll concentration by three methods: first, using the standard NASA coefficients for chlorophyll retrieval; second, with coefficients given by Clark[16]; and, third, according to our own model. It can be seen from Fig. 1(b) that the results for the 520/550 ratio are more divergent than those for the 440/550 ratio. The small slope of the curve and the low radiometric resolution of the CZCS contribute to the divergence for the 520/550 ratio. We conclude that further study is required before this ratio can be exploited to maximum advantage. All the analyses in the rest of the paper are, therefore, based only on the 440/550 ratio.

D. Penetration Depth

The depth of the water column sampled by the CZCS is variable. About 90% of the radiance leaving the water surface originates from the first optical attenuation length.[17] If $K(\lambda)(\mathrm{m}^{-1})$ is the diffuse attenuation coefficient for downwelling light at wavelength λ, the penetration depth for that wavelength, $z_{90}(\lambda)(\mathrm{m})$, is defined as

$$z_{90}(\lambda) = 1/K(\lambda). \tag{4}$$

If the optical properties are nonuniform with depth, $K(\lambda)$ is the mean attenuation coefficient above the penetration depth.

E. Satellite-Weighted Surface Concentration.

The contribution of a given layer to the water-leaving radiance is a decreasing function of its depth, a factor whose significance becomes greater when the optical properties are not vertically homogeneous. Let us consider the case of a nonuniform chlorophyll profile $C(z)$ ($\mathrm{mg\,m^{-3}}$). Then, according to Gordon and Clark,[18] the effective signal at wavelength λ would be the same as that from a homogeneous water column with concentration C_s, where C_s is the satellite-weighted pigment concentration defined as

$$C_s(\lambda) = \int_0^{z_{90}(\lambda)} C(z)f(z)dz \bigg/ \int_0^{z_{90}(\lambda)} f(z)dz, \tag{5a}$$

where

$$f(z) = \exp\left[-\int_0^z 2K(\lambda,z')dz'\right]. \tag{5b}$$

The case of the nonuniform pigment profile is further complicated by the fact that at least two wavelengths are used in algorithms for chlorophyll retrieval. Since the optical properties of the water are wavelength dependent, the satellite-weighted pigment concentration and the penetration depth are both wavelength dependent. Sathyendranath *et al.*[19] showed that changes in the shape of the pigment profile produce some spread in the relationship between the blue-green ratio and the satellite-weighted pigment concentration determined at 520 nm.

F. Generalized Pigment Profile

To study the consequences of nonuniform chlorophyll distribution, we use a generalized pigment profile $C(z)$ constructed from a Gaussian curve superimposed on a constant background[20]

$$C(z) = C_0 + \frac{h}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(z-z_m)^2}{2\sigma^2}\right]. \tag{6}$$

Here z_m is the depth of the chlorophyll maximum, σ is its standard deviation or spread, C_0 is the background

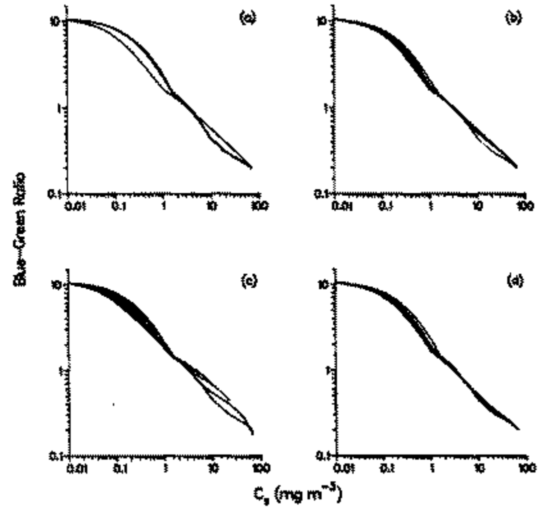

Fig. 2. Reflectance ratio (440/550) plotted against the satellite-weighted surface concentration for 520 nm, C_s ($\mathrm{mg\,m^{-3}}$) for various nonuniform pigment profiles. In each of the subplots, one of the parameters of the pigment profile is varied while the other three are held constant at their assigned typical values. In each subplot, the relationship is plotted for eleven values of the parameter at equal intervals within the range over which the parameter is varied: (a) h is varied from 0.1 to 250 ($\mathrm{mg\,m^{-2}}$); (b) σ is varied from 2 to 22 m; (c) z_m is varied from 0 to 85 m; (d) C_0 is varied from 0.05 to 1.5 ($\mathrm{mg\,m^{-3}}$).

concentration, and $h/(\sigma\sqrt{2\pi})$ determines the height of the peak above the background.

G. Light Penetration and Photic Depth

Attenuation of light in water for photosynthetically active radiation (PAR, irradiance in range from 400 to 700 nm) is computed using the model of Sathyendranath and Platt.[14] The photic depth (depth where the PAR is reduced to 1% of its surface value), defining the lower boundary of the zone suitable for photosynthesis, is computed using the same model. The irradiance field at the surface is computed assuming clear skies for local apparent noon on 23 Sept. at the Equator.

III. Effect of Profile Parameters on Blue-Green Ratio

In Fig. 2, we have plotted the blue-green ratio as a function of $C_s(520)$ for various values of the profile parameters. In computing the blue-green ratio, the effective concentration was calculated for 440 and 550 nm according to Eq. (5) and substituted into Eq. (3) to calculate coefficients suitable for estimation of reflectance ratio at these wavelengths from Eq. (2). The sensitivity analysis was carried out around a typical profile with the following parameter values: $C_0 = 0.1$ ($\mathrm{mg\,m^{-3}}$), $h = 18.8$ ($\mathrm{mg\,m^{-2}}$), $\sigma = 5$ m, and $z_m = 42.5$ m. In each of the subplots, one of the parameters was varied over a range of plausible values while the others were held constant at their assigned values.

Figure 3 shows more directly the dependence of the blue-green ratio on the parameters of the pigment profile, varied one at a time. For comparison, the blue-green ratio for a homogeneous water body with the same mean pigment concentration in the photic zone as the nonuniform case is also shown. The influence of each of the profile parameters on the blue-green ratio is discussed next.

A. Effect of h

Initially, when h is increased, the mean pigment concentration in the photic zone increases. But, correspondingly, the photic depth z_p decreases until it becomes smaller than z_m. Any further increase in h has no effect on the mean photic-zone concentration of pigments. As h is increased, there is an initial increase in the blue-green ratio (corresponding to the increase in biomass) for both the uniform and nonuniform cases. But for $h > 50$ (mg m^{-2}), the blue-green ratio is hardly affected by increasing h. Note, however, that since the chlorophyll maximum is at 42.5 m, much of the increase in biomass in the nonuniform case is undetectable by the satellite. Therefore, a given change in biomass has a smaller effect on the nonuniform profile than on the equivalent uniform profile.

B. Effect of σ

Change in σ does not change the total biomass, provided the whole peak is contained in the photic zone. The increase in σ broadens the peak with a consequent increase in near-surface biomass. As a result, more biomass is accessible to the satellite so that the blue-green ratio decreases. The redistribution of biomass with changing σ also changes the photic depth slightly and, therefore, changes the mean pigment concentration in the photic zone. Consequently, the corresponding uniform case shows a weak dependence on σ.

C. Effect of z_m

As z_m increases, the peak becomes less visible to the satellite, and the blue-green ratio increases. When the peak is at the surface, only the lower half of the Gaussian curve lies in the photic zone. When z_m is increased, the entire peak falls within the photic zone so that the biomass in the peak doubles, resulting in a decrease in the blue-green ratio for an initial increase in z_m. Mean photic-zone biomass is little affected by z_m as long as the entire peak lies within the photic zone. When the peak lies close to either the surface or the bottom of the photic zone, the mean photic-zone biomass decreases. This results in an increase in the blue-green ratio for the uniform case for very high and very low values of z_m.

D. Effect of C_0

The increase in the background pigment concentration C_0 increases the biomass at all depths with a consequent decrease in the blue-green ratio. But the uniform redistribution of the total biomass within the photic zone brings more biomass to the surface. The blue-green ratio for the nonuniform case is, therefore, higher than that of the corresponding uniform case, unless the background biomass is so high that it dominates the total biomass in the photic zone.

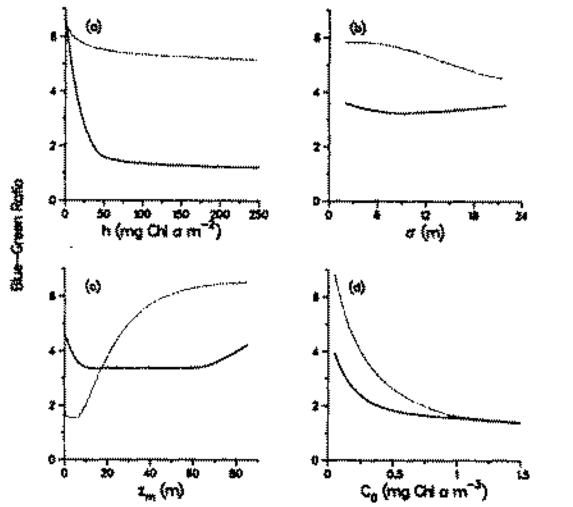

Fig. 3. Reflectance ratio (440/550) plotted against the parameter values of the pigment profiles. When one of the parameters is varied, the others retain their constant typical values. Dotted line—nonuniform pigment profile; continuous line—uniform pigment profile with concentration the same as the mean photic-zone concentration in the nonuniform case.

IV. Error in Estimating Photic Depth and Photic-Zone Biomass

The previous section has shown that the water-leaving radiance is markedly different depending on whether the water column is homogeneous with respect to the vertical distribution of pigment biomass. In applying the algorithms for chlorophyll retrieval, our interpretation of the signal would be erroneous if we assumed uniform distribution when the water column was in fact vertically structured. We now examine the magnitude of such errors as might be incurred in the estimation of photic-zone depth and photic-zone biomass if uniform biomass profile is incorrectly assumed.

We proceed as follows:

(1) For a given pigment distribution, the reflectance is computed at 440 and 550 nm using the weighted pigment concentration for those wavelengths. An estimate of the pigment concentration is then obtained from the blue-green ratio using the NASA algorithm [Fig. 1(a)]. Call this concentration C_s.

(2) C_s is assumed to be uniformly distributed through the water column.

(3) The depth of the photic zone z_p is then computed for noon irradiance according to the model of Sathyendranath and Platt.[14]

(4) The total pigment concentration in the photic zone is computed as $C_s z_p$.

(5) The estimates of photic depth and photic-zone biomass are compared with those computed directly from the given nonuniform pigment profile.

The satellite-estimated photic depth, the true photic depth, and the relative error in estimation are plotted in Fig. 4 as a function of the four profile parameters. As before, the sensitivity analysis is carried out

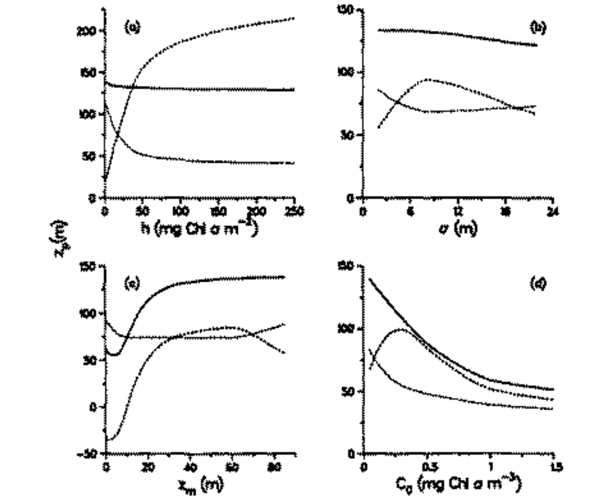

Fig. 4. Photic depth z_p (m) plotted against the four profile parameters. Continuous line—photic depth estimated from the satellite-weighted surface concentration, assuming uniform pigment profile; dotted line—real photic depth computed with the given nonuniform pigment profile; dashed line—relative error (%) in estimated photic depth computed as (estimated depth–real depth)/real photic depth. As in the previous figure, when one parameter is changed, the others are held constant.

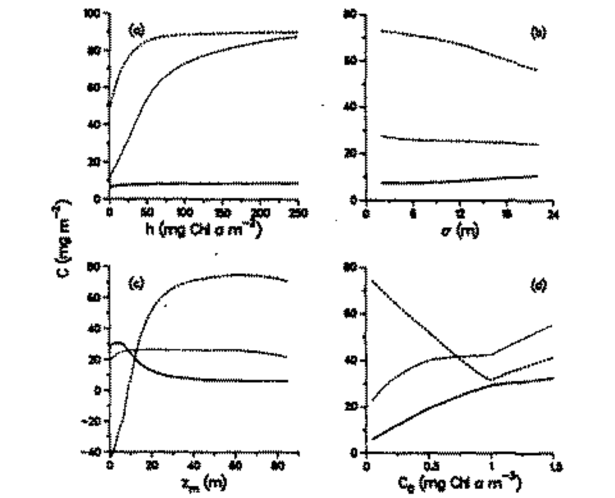

Fig. 5. Total pigment in the photic zone (mg m^{-2}) plotted against the four parameters of the pigment profile. Continuous line—estimated pigment content, calculated as product of C_s and the estimated photic depth; dotted line—the actual pigment content [integral of $C_s(z)$ from surface to bottom of photic zone]; dashed line—relative error in estimated photic-zone pigment content computed as (estimated value–real value)/real value.

around the typical profile, varying one parameter at a time. The relative error is positive (the assumption of uniform pigment distribution leads to overestimate) and maximal (relative error of the order of 200%) for high values of h. Minimum errors are found for low values of h and for extreme values (large or small) of σ. The relative error is negative when the peak is at the surface, $z_m = 0$, and reaches a positive maximum (~80%) when the peak is situated just above the photic depth. The relative error is a decreasing function of background pigment concentration.

Figure 5 shows the errors associated with estimation of photic zone pigment content. When the chlorophyll maximum is well below the surface, most of it is inaccessible to the satellite. The photic-zone depth, computed on the basis of the low surface concentration, is then overestimated (see Fig. 4). As a consequence, the total photic-zone pigment content is also overestimated. Conversely, the pigment content is underestimated when the chlorophyll maximum is at or near the surface. The relative error in the photic-zone pigment content is seen to be strongly dependent on the values of the parameters of the pigment profile: the maximum relative error exceeds 90%.

V. Case Where Shape of Pigment Profile is Known

The deep chlorophyll maximum is a well-known and ubiquitous feature of the oceans. The results presented above might, therefore, be seen as a severe limitation on the applicability and utility of remotely sensed data on ocean color.

There is, however, a possible way out. Recent work[21] has shown that, within seasons and regions, the shape of the pigment profile is a fairly stable property.

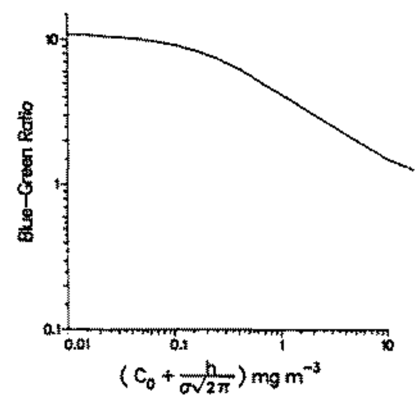

Fig. 6. Blue-green reflectance ratio plotted against $\{C_0 + h/[\sigma\sqrt{(2\pi)}]\}$ (mg m^{-3}) for a given profile shape defined by $z_m = 20$ m, $\sigma = 5$ m and $h/[C_0\sigma\sqrt{(2\pi)}] = 10$.

If, therefore, information is available on the typical shape of the profile for a given locality and season, it can be combined with the satellite data, with slight modification of existing algorithms, to yield information that is ecologically useful. We suggest the following approach.

The shape of the profile is defined by three parameters: z_m, σ, and the ratio of peak height to background, $h/[C_0\sigma\sqrt{(2\pi)}]$. Using our spectral reflectance model for a nonuniform pigment profile, the blue-green ratio is computed for various values of $\{C_0 + h/[\sigma\sqrt{(2\pi)}]\}$, the sum of peak height and background concentration. The results (see Fig. 6, for example) constitute a look-up table with which it becomes possible to use the satellite-derived blue-green ratio to estimate $\{C_0 + h/[\sigma\sqrt{(2\pi)}]\}$. Combining this with the three parameters of the profile shape, one can estimate the pigment profile in absolute terms. The spectral transmission model can then be applied to the absolute profile to compute the photic-zone depth and the total pigment content within the photic zone.

VI. Conclusion

Satellite-weighted surface concentration of phytoplankton pigments has only limited value when the pigment profile is nonuniform. Our sensitivity analysis has shown that photic depth, and the total pigment content within the photic zone, as computed by conventional methods from the satellite-weighted concentration, can be much in error. If independent information is available on the shape of the pigment profile, the chlorophyll retrieval algorithm is easily modified so that the entire profile can be recovered.

Thus by combining oceanographic measurements of relatively stable parameters (defining the shape of the pigment profile) with satellite measurements of the more responsive ocean color field (specifying the absolute value of the biomass field), it is possible to obtain a more complete picture of the ocean than would be possible by either method alone. The principal requirement for sea truth data follows directly from this view. We need a relatively small number of carefully chosen stations at which detailed profiles are measured rather than a large number of surface observations. This is the approach we have taken for computation of primary production at regional and global scales.[21]

In our analysis, we have used a normal curve to parametrize the chlorophyll profile, because it has already been found capable of representing profile data from a variety of oceanographic regimes.[20] But the general method presented here is by no means limited to the use of the normal curve. If, in modeling data from a given locality, an alternative parametrization is found to be more suitable, the method is easily adjusted to account for it.

Shubha Sathyendranath is on leave from the National Institute of Oceanography, India.

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