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Shape factors, two-flow models, and the problem of irradiance inversion in estimating optical parameters

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Abstract

The problem of the inversion of irradiance measurements for the inherent optical properties of a hydrosol such as the world ocean has been examined with the NOARL optical model. This model is a Monte Carlo simulation of the radiative transfer equation that, given the optical properties of a hydrosol, generates the zonal radiances and the commonly measured irradiances of that hydrosol. This information allows us to test the optical inversion capability of any irradiance model. We have demonstrated that the two-flow model, used often in atmospheric optics, cannot be inverted to yield the inherent backscatter coefficient of natural hydrosols due to the extreme asymmetry of the hydrosol volume scattering function. The asymmetry of the volume scattering function interacting with the radiance distribution introduces parameters called shape factors into the models for irradiance inversion. The presence of shape factors in an irradiance model renders it unsolvable; thus, simplifying assumptions are required for an inverse solution. ~~We inquire into~~ the possibilities for irradiance inversion given the existence of shape factors.

There is great interest in the problem of inversion of irradiance measurements in a hydrosol (pure water plus solutes plus suspensoids). Is it possible, given a suite of irradiance measurements of the submarine light field, to invert these measurements to determine the optical properties of a hydrosol such as the world ocean? The optical properties of interest are the absorption coefficient and the backscatter coefficient of the hydrosol. In many cases, the primary contribution to absorption and scattering comes from the suspended particles, which are primarily living cells. It is often possible to differentiate the living from the nonliving components by the variation in these optical properties at different wavelengths. The absorption and backscatter coefficients are linear functions of the hydrosol components they represent. Thus, they offer great potential for theoretical prediction of potential productivity of different oceanic regions, ecological energy budgets, and meteorological energy budgets.

The problem of optical inversion begins with consideration of the radiative transfer equation, accepted as the standard mathematical description of atmospheric and submarine light fields (Chandrasekhar 1960; Preisendorfer 1976). However, this equation has no simple analytical solution that is applicable to hydrosols and requires a large number of light radiance measurements to solve it for the inversion problem (Zaneveld 1974). These measurements are difficult and expensive to obtain, although recent developments in microprocessor-controlled instrumentation may allow the measurements required for the radiative transfer equation in the future (Voss 1988). If, however, the optical coefficients of a hydrosol are known, the radiant fluxes predicted from the radiative transfer equation can be simulated with Monte Carlo models such as the NOARL optical model. Thus any algorithm that inverts radiant flux to estimate optical parameters can be independently tested with this Monte Carlo model.

An approach to the problem of inverting radiant fluxes to obtain optical coefficients

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has been made by integrating the radiative transfer equation. This yields simpler equations in terms of the irradiances that can be conveniently measured in the field. The integration of the radiative transfer equation over all viewing angles yields the Gershun (1939) equation. Integrating the radiative transfer equation over the downwelling hemisphere and over the upwelling hemisphere of three-dimensional space yields Schuster-type equations, originally proposed by Arthur Schuster for stellar atmospheres in 1905. The Schuster equations were the original stimulus to the development of the radiative transfer equation and are still used to study the problem of optical inversion in aerosols and hydrosols. The most recently proposed integrations of these equations for hydrosols are from Aas (1987) and Preisendorfer and Mobley (1984). Zaneveld (1982) has proposed integrations of the radiative transfer equation that yield an equation utilizing the irradiances of the light field and the upwelling radiance.

In this paper we investigate the possibilities for inversion of simple irradiance measurements in the field to obtain the optical properties of Case 1 waters, which comprise 98% of the world ocean (Morel 1988).

Optical properties and the radiative transfer equation

All optical properties and radiant flux quantities discussed here are assumed wavelength-specific so that wavelength is not delineated in the properties and their derivations. Definitions of the radiance fluxes measured in the marine hydrosol are given in the list of symbols.

The optical properties we wish to obtain from the various inversion models depend only on the molecular composition and structure of the constituents of a hydrosol and are unaffected by changes in the distribution of radiant flux. Such optical properties were termed inherent optical properties by Preisendorfer (1976) because they are inherent to the medium being studied. These optical coefficients are strictly linearly related to the concentration of the various components of the hydrosol and their effects on light field transmission are thus precisely additive. The inherent optical properties on which we will focus are the absorption coefficient a and the backscatter coefficient b_b while the derivations will require consideration of the volume scattering function $\beta(\psi)$.

We will also consider the optical properties of the radiation field of the hydrosol. Among the most important of these properties are the mean cosines (Schellenberger 1965) of variously defined average photon paths. The mean cosines are used in the inversion models and are functions of the distribution of radiant flux in the marine hydrosol. These properties are descriptive of the structure of the light field penetrating the hydrosol and have thus been termed the light field properties by Kirk (1983).

Finally, there is a class of optical properties that represents combinations of inherent optical properties and light field structure. Preisendorfer (1976) termed this combination apparent optical properties. We will investigate the shape factors which, because they are a function of the hydrosol volume scattering function and the radiance distribution, are apparent optical properties. These parameters are derived below. Also in this class of optical properties are the radiance backscatter coefficients given in the list of symbols.

Radiative transfer equation—This equation is an integro-differential description of the absorption and scattering of the radiant energy in a specified radiance at a point z in the hydrosol

$$\frac{\mathrm{d}L(z;\theta,\phi)}{\mathrm{d}z}\cos\theta = -cL(z;\theta,\phi) + L^*(z;\theta,\phi) \quad (1)$$

where

$$L^*(z;\theta,\phi) = \int_{4\pi} \beta(z;\theta,\phi,\theta',\phi')L(z;\theta',\phi')\,\mathrm{d}\omega',$$

z is the depth in meters, θ the zenith angle, ϕ the azimuth angle, $c = a + b$, and $\mathrm{d}\omega = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$. The first term on the right-hand side of Eq. 1 is the loss of radiant energy from the radiance $L(z;\theta,\phi)$ due to absorption and scattering. The second term—the

Significant symbols

$L(z; \theta, \phi)$ Radiance—radiant flux per unit area per unit solid angle received at depth z from the bearing of zenith angle θ and azimuth angle ϕ by a tube or lens system pointing toward these coordinates, W m^{-2} sr^{-1}

$E_d(z)$, $E_u(z)$ Downwelling and upwelling irradiance—downward or upward flow or stream of radiant energy at depth z which represents the summed vertical downward- or upward-moving components of the radiances

$$= \int_{2\pi_d} L(z; \theta, \phi) \cos\theta \, d\omega, \ \mathrm{W\ m^{-2}}$$

$$= \int_{2\pi_u} L(z; \theta, \phi) \cos\theta \, d\omega, \ \mathrm{W\ m^{-2}}$$

$\mathbf{E}(z)$ Downwelling vector irradiance—the net flow of radiant energy at depth z; the upwelling irradiance subracted from the downwelling irradiance

$$= \int_{4\pi} L(z; \theta, \phi) \cos\theta \, d\omega = E_d - E_u, \ \mathrm{W\ m^{-2}}$$

$E_{0d}(z)$, $E_{0u}(z)$ Downwelling and upwelling scalar irradiance—the summation of all radiances in the downwelling or upwelling hemispheres at depth z

$$= \int_{2\pi_d} L(z; \theta, \phi) \, d\omega, \ \mathrm{W\ m^{-2}}$$

$$= \int_{2\pi_u} L(z; \theta, \phi) \, d\omega, \ \mathrm{W\ m^{-2}}$$

$E_0(z)$ Scalar irradiance—the summation of all radiances of three-dimensional space at depth z

$$= \int_{4\pi} L(z; \theta, \phi) \, d\omega, \ \mathrm{W\ m^{-2}}$$

$\bar{\mu}_d(z)$, $\bar{\mu}_u(z)$ Mean cosine of the average path traveled by downward- or upward-moving photons at depth z

$$= \frac{\int_{2\pi_d} L(z; \theta, \phi) \cos\theta \, d\omega}{\int_{2\pi_d} L(z; \theta, \phi) \, d\omega} = \frac{E_d(z)}{E_{0d}(z)}$$

$$= \frac{\int_{2\pi_u} L(z; \theta, \phi) \cos\theta \, d\omega}{\int_{2\pi_u} L(z; \theta, \phi) \, d\omega} = \frac{E_u(z)}{E_{0u}(z)}$$

$\bar{\mu}(z)$ Mean cosine of the average path traveled by all photons at depth z

$$= \frac{\int_{4\pi} L(z; \theta, \phi) \cos\theta \, d\omega}{\int_{4\pi} L(z; \theta, \phi) \, d\omega} = \frac{\mathbf{E}(z)}{E_0(z)}$$

a Absorption coefficient—a measure of radiant energy absorbed from a beam of radiant energy and converted into another form by an infinitesimally thin layer of hydrosol, m^{-1}

b Total scattering coefficient—a measure of radiant energy diverted from a beam of radiant energy by an infinitesimally thin layer of hydrosol

$= b_b + b_f$, m^{-1}

b_b Backscatter coefficient—a measure of radiant energy diverted by an infinitesimally thin layer of hydrosol from a reference beam of radiant energy and moving in a direction 90°–180° to the reference beam direction, m^{-1}

b_f Forward scattering coefficient—a measure of radiant energy diverted from a reference beam by an infinitesimal thickness of hydrosol and moving in a direction 0°–90° to the reference beam direction, m^{-1}

$\beta(\psi)$ Volume scattering function—a measure of radiant intensity diverted from a beam of radiant energy by an elemental volume of hydrosol into the direction indicated by the angle ψ relative to the orientation of the incident beam, m^{-1} sr^{-1}

$\bar{b}_d$, $\bar{b}_u$ Downwelling and upwelling radiance backscatter coefficients—measures of the amount of radiant energy backscattered from the downwelling or upwelling irradiance by an infinitesimal thickness of the medium, m^{-1}

r_d, r_u Downwelling and upwelling shape factors—the normalized contributions to the downwelling or upwelling radiance backscatter coefficient from the forward scattering lobe of the hydrosol volume scattering function path function—is the gain of radiant energy into the radiance $L(z; \theta, \phi)$ due to scattering of radiant energy out of all the other radiances in three-dimensional space. The zenith angle θ' and the azimuth angle ϕ' refer to the orientations in space of the contributing radiances. The notation for the volume scattering function differs from the list of symbols in that the angle ψ of intensity scattered into the radiance $L(z; \theta, \phi)$ from radiance $L(z; \theta', \phi')$ is the angle between the spatial coordinates θ, ϕ and θ', ϕ'.

Integrated forms of the radiative transfer equation for irradiances—Because of the difficulties in inverting the full radiative transfer equation, various integrations of this equation have been proposed that use the irradiances defined in the list of symbols. Integrating Eq. 1 over all viewing angles of three-dimensional space, we obtain

$$\frac{d\mathbf{E}(z)}{dz} = -a(z)E_0(z), \tag{2}$$

which is Gershun's (1939) equation—an expression of the net flow of radiant energy in a hydrosol and a fundamental physical statement of conservation of energy in the divergence of a radiative field. The inversion of this equation with the three-parameter model (Stavn 1981, 1987) gives only the absorption coefficient. Additional integrations are necessary to get expressions in terms of the scattering coefficients.

Integrating Eq. 1 first over the downwelling hemisphere and then separately over the upwelling hemisphere yields two differential equations in terms of the downwelling and the upwelling streams of radiant flux

$$\frac{dE_d(z)}{dz} = -\frac{a(z)}{\bar{\mu}_d(z)}E_d(z) - \frac{\bar{b}(z)}{\bar{\mu}_d(z)}E_d(z) + \frac{\bar{b}(z)}{\bar{\mu}_u(z)}E_u(z) \tag{3}$$

and

$$-\frac{dE_u(z)}{dz} = -\frac{a(z)}{\bar{\mu}_u(z)}E_u(z) - \frac{\bar{b}(z)}{\bar{\mu}_u(z)}E_u(z) + \frac{\bar{b}(z)}{\bar{\mu}_d(z)}E_d(z) \tag{4}$$

where $\bar{b}(z)$ is the *mean backscatter coefficient* at depth z. Equations 3 and 4 are the integrations proposed by Preisendorfer and Mobley (1984), which can be inverted and solved as a system of two equations in two unknowns. They represent the first real advance in the application of the concept of the two-flow equations of Schuster (1905) to hydrosols. Previous attempts combined the light field properties, inherent optical properties, and apparent optical properties in the right-hand side of Eq. 3 and 4 to yield poorly defined optical coefficients that could not be applied in any general sense to any part of the ocean.

The Preisendorfer and Mobley equations are stated in terms of a true hydrosol absorption coefficient and a mean backscatter coefficient applied to both irradiance streams. They defined the mean backscatter coefficient as a close approximation of the hydrosol backscatter coefficient. The backscatter coefficient of the hydrosol has been shown by Gordon et al. (1975) to be the most important aspect of the hydrosol scattering coefficient in terms of altering the radiance distribution and therefore the nature of the radiant flux in the marine hydrosol.

The mean backscatter coefficient approximates the hydrosol backscatter coefficient when the volume scattering function of the hydrosol is uniform or symmetrical. The essential justification for the mean backscatter coefficient approximation is the nearly uniform shape of the backscattering lobe of the hydrosol volume scattering function. This allows the backscattering of radiant flux to be treated in the same way as uniform scattering, i.e. we are dealing with half of a uniform scattering function. However, a problem arises because of the large forward scattering lobe of particles suspended in natural waters (Petzold 1972; Jerlov 1976) and the shape of the radiance distribution. It is well known (Smith 1974; Jerlov 1976) that the radiance distribution of the downwelling hemisphere is elongate and the maximum radiances occur within 40° of the vertical axis. In contrast, the maximum of the radiance distribution in the upwelling hemisphere occurs near the horizontal plane. The backscattering of the downwelling and upwelling irradiances arises not only from the backscattering lobe of the inherent volume scattering function of the hydrosol but also from the forward scattering lobe. The mean backscatter coefficient, strictly speaking, is therefore not directly referable to the backscattering lobe of the inherent volume scattering function of the hydrosol (Fig. 1). Preisendorfer and Mobley were well aware of this and suggested that how far a single mean backscatter coefficient for the two irradiance streams deviates from being an inherent optical property, an approximation of the hydrosol backscatter coefficient, and a quantitative estimate of this coefficient was worthy of theoretical and experimental investigation.

Aas (1987) also integrated the radiative transfer equation over the downwelling and upwelling hemispheres to yield the following pair of equations

$$\frac{dE_d(z)}{dz} = -\frac{a(z)}{\bar{\mu}_d(z)} E_d(z) - \frac{r_d(z)b_b(z)}{\bar{\mu}_d(z)} E_d(z) + \frac{r_u(z)b_b(z)}{\bar{\mu}_u(z)} E_u(z) \quad (5)$$

and

$$-\frac{dE_u(z)}{dz} = -\frac{a(z)}{\bar{\mu}_u(z)} E_u(z) - \frac{r_u(z)b_b(z)}{\bar{\mu}_u(z)} E_u(z) + \frac{r_d(z)b_b(z)}{\bar{\mu}_d(z)} E_d(z) \quad (6)$$

where b_b is the *hydrosol backscatter coefficient* and r_d and r_u are the shape factors. The combined coefficients $(r_d b_b)$ and $(r_u b_b)$ can be called the *radiance backscatter coefficients* which indicate the amount of irradiance backscattered from each irradiance stream divided by an infinitesimal thickness of the hydrosol. These coefficients serve the same function in Aas' integration as the mean backscatter coefficient in the Preisendorfer and Mobley integration and thus emphasize the fact that certain assumptions have to be made to obtain a mean backscatter coefficient. Aas' integration cannot be inverted because it is a statement of two equations in four unknowns.

Defining the radiance backscatter coefficients in terms of Preisendorfer and Mobley's notation, we review the particular integrations of the radiative transfer equation that produce them

$$\bar{b}_d = r_d b_b \quad (7)$$

$$\bar{b}_u = r_u b_b \quad (8)$$

and

$$\bar{b}_d(z) = \left\{ \int_{2\pi_d} \left[\int_{2\pi_u} \beta(\theta, \phi, \theta', \phi')\, d\omega \right] \cdot L(z; \theta', \phi')\, d\omega' \right\} \Big/ E_{0d}(z) \quad (9)$$

$$\bar{b}_u(z) = \left\{ \int_{2\pi_u} \left[\int_{2\pi_d} \beta(\theta, \phi, \theta', \phi')\, d\omega \right] \cdot L(z; \theta', \phi')\, d\omega' \right\} \Big/ E_{0u}(z) \quad (10)$$

where $2\pi_d$ and $2\pi_u$ indicate integrations of the three-dimensional space over the downwelling and upwelling hemispheres. From the above integrations we see that the backscatter coefficients of the irradiance streams involve truncated portions of the entire hydrosol volume scattering function. Therefore the forward lobe of the volume scattering function enters into the radiance backscatter coefficients. The shape factor is then seen as a measure of the contribution of the forward scattering lobe of the hydrosol, for a given radiance distribution, to the radiance backscatter coefficient. The shape factor normalizes the contribution of the forward scattering lobe of the hydrosol to the backscattering lobe. This results in a mathematical expression that ultimately relates changes in the irradiances to the backscatter coefficient of the hydrosol.

The inversion proposed by Preisendorfer and Mobley for obtaining the backscatter coefficient of the hydrosol is possible only if the mean backscatter coefficient defined from the two irradiance fluxes of the two-flow model has the following properties relative to the integration proposed by Aas:

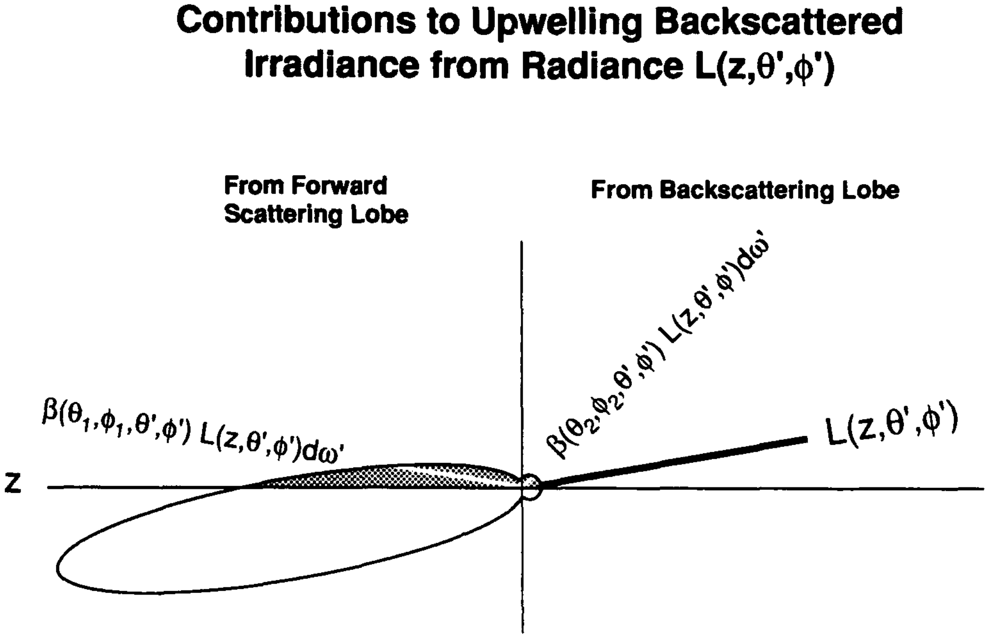

Fig. 1. Downward-moving radiance at depth z, $L(z;\theta',\phi')$, undergoing scattering by the hydrosol. Volume scattering function of intensities diverted from the radiance in plane of paper indicated by envelope of the thin line. Scattered intensities contributing to backscattered radiances come from shaded portion of volume scattering function. Contribution of $L(z;\theta',\phi')$ to two upward-moving radiances, $L(z;\theta_1,\phi_1)$ and $L(z;\theta_2,\phi_2)$, indicated by white lines in the shaded portion of volume scattering function. Backscattered radiances contributing to upwelling irradiance at depth z dominated by forward lobe of volume scattering function.

$$\bar{b} = \bar{b}_b = \bar{b}_u,$$

which is true only when

$$r_d = r_u.$$

However, for the mean backscatter coefficient to be equal to the inherent backscatter coefficient of the hydrosol, the following must be true

$$r_d = r_u = 1.0.$$

That is, the mean backscatter coefficient is a valid estimate of the hydrosol backscatter coefficient only when the foward scattering lobe of the hydrosol does not make a significant contribution to the backscattered flux of the irradiance field. Aas thus provided the analysis that allows the question of the inversion of two-flow-type models to be posed very simply and quantitatively: how much do the shape factors (r_d and r_u) deviate from 1.0 in ocean waters? His initial calculations of r_d and r_u indicated that in the most turbid coastal waters (Case 2 waters) the Preisendorfer and Mobley solution was probably not valid. Aas speculated that in the clearest ocean waters the deviation from 1.0 might not be too great and the two-flow model could be inverted. Based on the work of Aas, we extend the analysis of r_d and r_u to Case 1 waters with the NOARL optical model. This simulation of the radiative transfer equation allows a quantitative calculation of the magnitude of the shape factor and of the relative contributions of the various components of the marine hydrosol, a prediction of effects based on known optical properties of the open ocean as reported extensively by Morel and coworkers, and inclusion of the effect of hydrosol absorption which always reduces or ameliorates the effects of scattering. With this approach we can investigate the question of optical inversion in natural hydrosols and determine the limitations of the simple irradiance solutions so far proposed for the radiative transfer equation.

Case 1 waters: Optical parameters for the NOARL Monte Carlo simulation

Morel's optical classification of ocean waters represents a synthesis of various aspects of the remarkably useful and fruitful hypothesis on the biological origin of the optical properties of Case 1 ocean waters. The primary sources of this hypothesis are Smith and Baker (1978), Morel and Prieur (1977), and Morel (1980). The aspect of the Morel optical classification of ocean waters that we use here is the association of the total scattering coefficient of the hydrosol at 550 nm with the concentration of the chlorophyll-like pigments of the hydrosol, after the suggestion of Smith and Baker about the importance of chlorophyll-like pigments in Case 1 waters. The wavelength chosen for the simulations was 440 nm, which is close to the peak absorption for Chl *a*. This wavelength has been used extensively for ocean optical modeling.

Scattering parameters of the simulations—All of our simulations begin with the restricted version of the NOARL blue water model (Stavn and Weidemann 1988*a*) without emission sources. This model is equivalent to the Morel blue water model type 3 (Morel and Prieur 1977). The basis of the model is, of course, the optical properties of molecular water; the total scattering coefficient and volume scattering function of the water molecule (determined from fluctuation theory) are taken from Morel (1974). The other component of the model is finely divided quartzlike material which presumably has an aeolian source (Brown and Gordon 1973). The total scattering coefficient and volume scattering coefficient for this material are from Kullenberg (1968) and Gordon et al. (1975).

For the living component of the simulation we chose the alga *Platymonas* sp.; its optical properties are taken from Bricaud and Morel (1986). The total scattering coefficient and volume scattering function were then determined from these properties. The total scattering coefficient was normalized to the concentration of chlorophyll-like pigments. The cell size distribution from Bricaud and Morel had a median value of 4 μm in diameter. Multispecific assemblages can be modeled for the generation of Case 1 waters as the optical properties of other species become available.

The total scattering coefficient for organic detritus was estimated from the optical model of Prieur and Sathyendranath (1981). Their model scattering coefficients are normalized to 550 nm and converted to other wavelengths from the approximately λ^{-1} relationship of Morel (Morel 1973; Morel and Prieur 1977). Prieur and Sathyendranath estimated the quantitative contribution of organic detritus to the hydrosol total scattering coefficient by assuming the following. The minimal observed hydrosol scattering coefficients at 550 nm for all Case 1 waters are due to living algal cells plus water and quartz. The maximum hydrosol scattering coefficients observed for these waters result from the contribution of suspended organic detritus and bacteria added to the algal cell component. Such estimates are based on the empirical limits established by Morel (Morel 1980; Gordon and Morel 1983) and illustrated in Fig. 2. The difference between these two values constitutes the total scattering coefficient for suspended organic detritus.

We have modified this procedure as follows. For a given pigment concentration the total scattering coefficient at 550 nm due to *Platymonas* was calculated from Bricaud and Morel (1986) and then subtracted from the maximum hydrosol total scattering coefficient at 550 nm with water and quartz scatter removed. The result is an estimate of the total scattering coefficient of particulate organic detritus. This coefficient was then converted to its value at 440 nm. The hydrosol total scattering coefficient calculated for *Platymonas* plus the blue water component exceeded Morel's upper empirical limit at higher chlorophyll concentrations. Accordingly, an empirical curve fit between the organic detritus total scattering coefficient and the chlorophyll-like pigments at lower concentrations allowed extrapolation

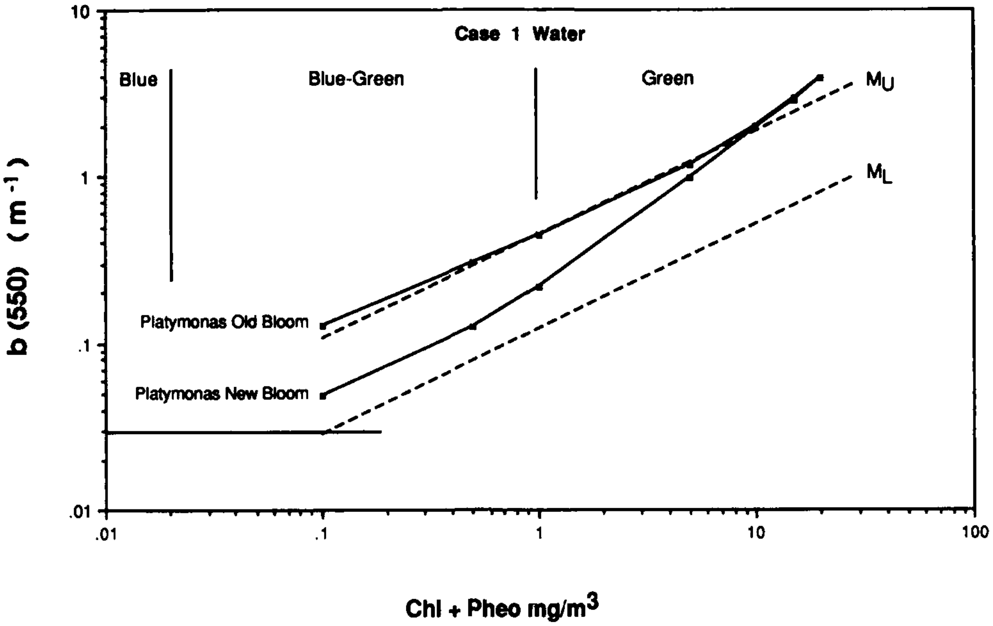

Fig. 2. Total scattering coefficients for hydrosols of NOARL simulations. Scattering coefficients for 550 nm shown to facilitate comparison with the Morel optical classification of ocean waters. Dashed line M_L represents Morel's lower limit for total scattering coefficient predicted from chlorophyll-like pigment concentration; $b(550) = 0.12(\text{pigment})^{0.63}$. Dashed line M_U represents Morel's upper limit for total scattering coefficient predicted from chlorophyll-like pigment concentration; $b(550) = 0.45(\text{pigment})^{0.62}$. Horizontal line is the hydrosol total scattering coefficient for the NOARL blue water model.

of the organic detritus component to the highest chlorophyll concentrations in the simulation. The result of the curve fit and extrapolation gave hydrosol total scattering coefficient values that were slightly higher than Morel's empirical limit but did not exceed the data limits reported by Gordon and Morel (1983). The volume scattering function of organic detritus was estimated from Petzold's (1972) measurements of the volume scattering function of San Diego Harbor water with the volume scattering function of molecular water (Morel 1974) subtracted.

Absorption coefficients of the simulations—The absorption coefficient for molecular water was taken from the tables of Smith and Baker (1981). Quartz was assumed to be nonabsorbing. The absorption coefficient for *Platymonas* was calculated from Bricaud and Morel (1986) where the specific absorption coefficient is normalized to the concentration of Chlorophyll-like pigments. The absorption coefficient for organic detritus was estimated from a regression relation in Prieur and Sathyendranath (1981) which is normalized to the total scattering coefficient of the organic detritus at 550 nm. Yellow substance absorption was estimated by the assumption that its absorption coefficient was 20.7% of the total hydrosol absorption coefficient as determined from the regression analysis of Prieur and Sathyendranath (1981).

NOARL Mo.ite Carlo simulations

The NOARL optical model is a Monte Carlo simulation of the radiative transfer equation (Eq. 1) written in structured Fortran 77 (Etter 1987). The fundamental algorithm is based on the work of Gordon and Brown (1973) with additions from Plass and Kattawar (1972) and Kirk (1981*a*). In brief, a photon enters the water and a random number generator chooses whether the photon is absorbed or scattered, based on the absorption coefficient and total scattering coefficient for the hydrosol. The random number generator subroutine uses a modified random number shuffler (Press et al. 1986) to minimize serial correlations. If an absorption event is chosen, the photon is terminated and a new photon enters the water. If a scattering event is chosen, the random number generator is reactivated and it selects the scattering event from a possible interaction with a water molecule, quartzlike particle, algal cell, or organic detritus particle depending on the value of the total scattering coefficient entered for each class of particle.

After the interacting particle is selected, the random number generator is reactivated and the new trajectory of the photon determined from the normalized volume scattering function (scattering phase function of Gordon and Brown 1973) for the interacting particle. A further reactivation of the random number generator determines the optical path based on the sum of the absorption and total scattering coefficient. The photons activate counters at specified depth intervals intersected by the photon trajectory, and the various photon sums are used to calculate zonal radiances, downwelling and upwelling irradiances, and downwelling and upwelling scalar irradiances. The accuracy of the photon fluxes is checked by calculating the absorption coefficient from the recorded fluxes using the three-parameter model solution of the Gershun equation. The model output was accepted for the depths from the surface down to the depth where the calculated absorption coefficient deviated by no more than 2% from the input absorption coefficient. Model output below this depth was judged to have too high a random variance. Duplicate simulation runs were made for each concentration of chlorophyll-like pigment chosen and each run used 2.5×10^6 photons.

The NOARL optical model was implemented as follows. A flat water surface was used with no skylight so that the only photons entering were of solar origin. On clear days the solar beam contributes ~85% of the entering irradiance (Kirk 1981*b*). The solar beam was set at an 11° zenith angle in air; the wavelength chosen for the simulations was 440 nm. The results from the irradiances generated for 440 nm should not vary widely from those of other wavelengths in the 400–490-nm waveband. We restrict consideration of our simulation without internal radiation sources to this waveband because the 500–600-nm waveband exhibits Raman emission effects in the clearest ocean waters (Marshall and Smith 1988; Stavn and Weidemann 1988*a,b*), while fluorescence emission strongly affects radiant flux in the 600-nm+ region (Gordon 1979; Morel and Prieur 1977). Internal source terms can always be added to simple irradiance equations after the situation without internal emission has been properly elucidated.

The purpose of this simulation of the radiative transfer equation is to estimate the shape factors defined by Aas (1987) which cannot be deduced directly from simple irradiance measurements. From the zonal (integrated over 2π) radiances at prescribed depth intervals and the hydrosol volume scattering function we can evaluate the integral

$$2\pi \int_{2\pi d} \left[\int_{2\pi u} \beta(\theta, \phi, \theta', \phi')\, d\omega \right] \cdot L(z; \theta', 2\pi')\sin\theta'\, d\theta',$$

which differs from the numerator of Eq. 9 in having the radiance $L(z; \theta, \phi)$ approximated with the zonal radiance $L(z; \theta, 2\pi)$. This approximation of the radiance is a common method of solving radiative transfer equations in a less computation-intensive fashion, and it is done both for empirical work and in the theory of radiative transfer (Zaneveld 1974; Kirk 1983; Kourganoff 1963). The zonal radiance distribution is a good approximation of the radiance distribution established at solar angles near the zenith direction.

The zonal radiance distribution is a less accurate estimate of the radiance distribution established at greater deviation of the solar bearing from the zenith. However, Kirk (1984), using a Monte Carlo model with zonal radiances, has successfully simulated optical relationships of various hydrosols dependent on the volume scattering function and radiance distribution at large solar zenith angles. We are assuming that the results obtained in this study at a large solar zenith angle are adequate approximations of results that would be obtained with a full radiance distribution with azimuth angles. This assumption deserves further study. This integral, which uses zonal radiances, is the backscattered scalar irradiance from the downwelling scalar irradiance. A similar term for the upwelling scalar irradiance results from replacing d with u and u with d. We then obtain the radiance backscatter coefficient for downwelling radiant flux from the integral and the downwelling scalar irradiance

$$\bar{b}_d(z) = \left\{ 2\pi \int_{2\pi_d} \left[\int_{2\pi_u} \beta(\theta, \phi, \theta', \phi')\, d\omega \right] \cdot L(z; \theta', 2\pi')\sin\theta'\, d\theta' \right\} \div E_{0d}(z). \quad (11)$$

Similarly for the upwelling radiant flux

$$\bar{b}_u(z) = \left\{ 2\pi \int_{2\pi_u} \left[\int_{2\pi_d} \beta(\theta, \phi, \theta', \phi')\, d\omega \right] \cdot L(z; \theta', 2\pi')\sin\theta'\, d\theta' \right\} \div E_{0u}(z). \quad (12)$$

The shape factors follow

$$r_d = \frac{\bar{b}_d}{b_b}$$

and

$$r_u = \frac{\bar{b}_u}{b_b},$$

since the b_b coefficient is evaluated from the given parameters of the Monte Carlo simulation.

To answer the questions posed by Preisendorfer and Mobley (1984) and quantified by Aas (1987), we have simulated the radiative transfer for the blue, blue-green, and green Case 1 waters and determined the r coefficients, using Eq. 11 and 12 on the Monte Carlo output.

Results

Two situations were modeled to generate the suite of optical water types in the Morel optical classification and obtain simulated irradiance fields that may represent the extreme values obtainable.

Platymonas new bloom: The surface layers of a parcel of blue water are ventilated with nutrient-rich water and this initiates a bloom of *Platymonas* cells. Growth is assumed rapid enough that no significant amounts of yellow substance or organic detritus are generated. Traganza (1969) described bloom situations in the Sargasso Sea that rapidly convert blue waters to a green water parcel and thereafter generate detrital organic matter. The pattern of formation of green Case 1 waters often seems to be one of a thick algal layer at the surface overlaying essentially blue water (Austin 1980). This situation is also possible near certain coasts where blue water can receive a rapid influx of nutrients from upwellng, etc. This *Platymonas* growth is postulated to be rapid enough to increase the chlorophyll concentration from neglible amounts to 20 mg m^{-3}.

Platymonas old bloom: At the concentration of chlorophyll-like pigments of 20 mg m^{-3}, it is assumed that the nutrients are exhausted and the bloom declines. During the period of decline the decay of old cells yields dissolved yellow substance, a decrease in chlorophyll-like pigments, and an increase in organic detritus representing decomposed cells, cellular fragments, and bacteria. This would generate the general conditions for Case 1 waters postulated by Morel. The scattering coefficient at 550 nm represents a higher concentration of organic detritus relative to live cells at lower concentrations of chlorophyll-like pigments and a relatively lower concentration of organic detritus at higher pigment concentrations.

The presumption here is that values of optical parameters for intermediate cases would fall between the range established for the *Platymonas* old bloom and new bloom. The new bloom is, admittedly, the least realistic situation.

The shape factors in each simulation were calculated both for individual components of the hydrosol and the total hydrosol. The shape factor for the total hydrosol would be determined from radiance data obtained from sensors directly measuring the radiances in the various optical water types. The values of the shape factors reported here are averages from the surface to the maximum depth of the simulations with acceptable statistical variation. The shape factors in this depth range varied by only a few percent. Shape factor values for simulations at large solar zenith angles are not reported as they were only a few percent greater than the values calculated from simulations at an 11° solar zenith angle.

Molecular water: This component serves as a check on the adequacy of the model implementation and the assumptions used to calculate the shape factor. Under all conditions the r_d for molecular water varied from 1.015 to 1.022, indicating the least accurate estimates of r_d would be in error by 2.2% and the most accurate estimates by 1.5%. The r_u coefficients for molecular water varied from 1.002 to 1.003 so that the worst error of estimate for r_u coefficients was 0.3%. The greatest error of estimate with a solar zenith angle of 70° was 2.3% for r_d and the r_u error was unchanged. We thus have a measure of the error involved in the common practice of using zonal radiances when calculating solutions for radiative transfer problems. The greater error in the r_d coefficient is, of course, explained by the fact that the radiances are more nearly uniformly distributed in the upwelling hemisphere than in the downwelling hemisphere. This inequality of the radiance distributions in the upper and lower hemispheres is of great importance in explaining the following results.

Quartz: The shape factors varied from 1.6 to 2.1 for r_d and 3.9 to 4.3 for r_u showing definite effects of the forward scattering lobe on the radiance backscatter coefficient and thus the backscattered flux of the irradiance field.

Organic detritus: The shape factors varied from 1.6 to 2.1 for r_d and 4.9 to 5.0 for r_u. We see increasing influence of the forward scattering in the r_u results as the backscattering lobe represents only ~1% of the total scattering coefficient for organic detritus (Morel and Prieur 1977).

Platymonas: The shape factors varied from 44 to 49 for r_d and 76 to 90 for r_u. The backscattering lobe is only about 0.06% of the total scattering coefficient for this alga which is not the lowest value recorded for algal cells (Bricaud et al. 1983; Bricaud and Morel 1986). Forward scattering is the dominant factor in the irradiance backscatter produced by this suspended particle.

Hydrosol: Total r_d and r_u coefficients for each optical water type investigated are in Fig. 3. The r_d coefficient varies from 1.3 for blue water to 10 for green water of 20 mg m^{-3} chlorophyll concentration. The r_u coefficient varies from 1.8 for blue water to 20 for green water of 20 mg m^{-3} chlorophyll concentration. Although the r coefficients for the individual components of the hydrosols varied by a maximum of about 23% for all the optical water types, the variation of these coefficients for all the hydrosols is an order of magnitude. At the lowest particle concentrations the shape factor is primarily an interaction between the volume scattering functions of the water molecule and suspended quartzlike particles. Adding suspended material such as algae or organic detritus, which is more strongly forward scattering, increases the magnitude of the shape factor for the hydrosol (Figs. 2 and 3, Table 1). The shape factors for the hydrosols show a tendency to increase to a limit imposed by the maximum shape factor for the dominant added component. The overall increase in the shape factor of the hydrosols represents the increase in particulate matter and the forward scattering of this material. This is correlated with an increase in the hydrosol backscatter coefficient—the parameter to which the shape factor is normalized.

Discussion

The question is under what conditions can simple irradiance models allow the inversion of irradiance data to yield the inherent optical properties of natural hydrosols? The simplest irradiance model—the three-parameter model—allows inversion of the net irradiant flux to yield the hydrosol

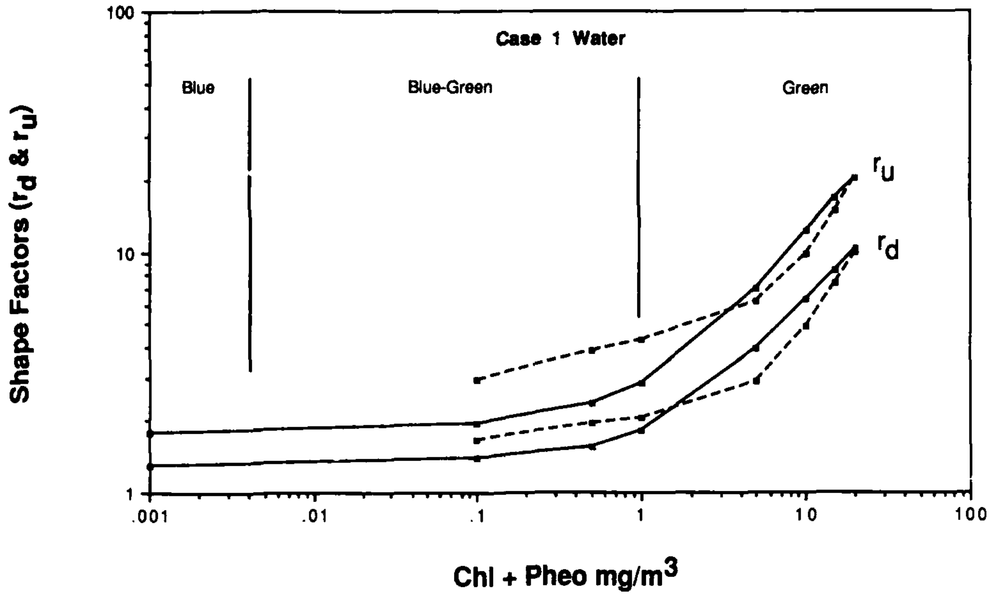

Fig. 3. Downwelling and upwelling shape factors plotted against pigment concentration of various ocean hydrosols. Solid lines represent shape factors for the *Platymonas* new bloom and dashed lines represent those for the *Platymonas* old bloom.

absorption coefficient in any hydrosol. Inversion for the backscatter coefficient, however, is problematical. After preliminary calculations indicated that the shape factors were too high in turbid Case 2 waters to allow inversion of the two-flow model, Aas (1987) noted that in clear ocean waters (blue and blue-green waters) the backscatter from molecular water is dominant, which implies that the shape factors might approach 1.0 and the two-flow model could be inverted. We have shown here that the smallest values for the shape factors, obtained from blue water (molecular water plus quartz), are 1.3 for r_d and 1.8 for r_u. The minimum error for an attempt to invert the two-flow equations in the clearest possible ocean water would be 55%. The inclusion of any other scattering material into the ocean will increase the error dramatically to an order of magnitude in Case 1 waters of 20 mg m^{-3} chlorophyll concentration. On the basis of this evidence we conclude that the mean backscatter coefficient ($\bar{b}$) is an apparent optical property that cannot be equated with the inherent hydrosol backscatter coefficient. Therefore inversion of the two-flow model produces a mean backscatter coefficient that is a backscatter coefficient for the irradiances and is not a backscatter coefficient for the hydrosol in which the irradiances are measured.

A more serious problem arises, however, when we consider that the ratio of the shape factors (r_u/r_d) for all simulations of blue-green and green waters ranges from 1.39 to 2.17 as shown in Table 2. Thus the radiance distribution in natural hydrosols, already noted as being rather different in the downwelling and upwelling hemispheres, renders $\bar{b}_d$ unequal to $\bar{b}_u$ with the hypothesis of a single mean backscattering coefficient unsupported. This extends the unknown parameters of Eq. 3 and 4 in natural hydrosols to three in each equation. There is, of course, no unique solution for such a system. We tried to correct for this by adding the three-parameter model solution to the two-flow model so that we would have a system of three equations in three unknowns (Eq. 13–15). A simple application of Cramer's rule for the solution of nonhomogeneous linear

Table 1. Optical coefficients (m^{-1}) used in simulations.

	Scattering coefficients						Absorption coefficients					
Chl concn ($mg\ m^{-3}$)	Water* $b_w(440)$	Quartzlike particulate† $b_q(440)$	*Platymonas*‡ $b_c(440)$	Hydrosol new bloom $b(440)$	Organic detritus∥ $b_d(440)$	Hydrosol old bloom $b(440)$	Water§ $a_w(440)$	*Platymonas*‡ $a_c(440)$	Hydrosol new bloom $a(440)$	Organic detritus∥ $a_d(440)$	Yellow subst.∥ $a_y(440)$	Hydrosol old bloom $a(440)$
0.0	0.0051	0.0342					0.0145					
0.1			0.0140	0.0533	0.0992	0.1525		0.0040	0.0185	0.0330	0.0135	0.0650
0.5			0.0700	0.1093	0.2203	0.3296		0.0202	0.0347	0.0737	0.0283	0.1367
1.0			0.1400	0.1793	0.2858	0.4651		0.0404	0.0549	0.0957	0.0393	0.1900
5.0			0.7000	0.7393	0.2534	0.9927		0.2020	0.2165	0.0849	0.0787	0.3800
10.0			1.4000	1.4393	0.1043	1.5436		0.4040	0.4185	0.0347	0.1183	0.5716
15.0			2.1000	2.1393	0.0365	2.1758		0.6060	0.6205	0.0120	0.1651	0.7976
20.0			2.8000	2.8393	0.0120	2.8513		0.8080	0.8225	0.0037	0.2157	1.0419

* Morel 1974.
† Kullenberg 1968.
‡ Bricaud and Morel 1986.
§ Smith and Baker 1981.
∥ Prieur and Sathyendranath 1981.

Table 2. Shape factor ratios.

Pigment concn ($mg\ m^{-3}$)	*Platymonas* new bloom (r_u/r_d)	*Platymonas* old bloom (r_u/r_d)
0.0	1.36	1.36
0.1	1.39	1.79
0.5	1.50	2.03
1.0	1.57	2.10
5.0	1.80	2.17
10.0	1.93	2.03
15.0	2.01	1.98
20.0	1.97	2.07

equations for the unknown coefficients a, $\bar{b}_d$, and $\bar{b}_u$ revealed that such a system is inconsistent (i.e. has no solution at all):

$$\frac{\mathrm{d}\mathbf{E}(z)}{\mathrm{d}z} = -\frac{a(z)}{\bar{\mu}(z)}\mathbf{E}(z), \tag{13}$$

$$\frac{\mathrm{d}E_d(z)}{\mathrm{d}z} = -\frac{a(z)}{\bar{\mu}_d(z)}E_d(z) - \frac{\bar{b}_d(z)}{\bar{\mu}_d(z)}E_d(z) + \frac{\bar{b}_u(z)}{\bar{\mu}_u(z)}E_u(z) \tag{14}$$

and

$$-\frac{\mathrm{d}E_u(z)}{\mathrm{d}z} = -\frac{a(z)}{\bar{\mu}_u(z)}E_u(z) - \frac{\bar{b}_u(z)}{\bar{\mu}_u(z)}E_u(z) + \frac{\bar{b}_d(z)}{\bar{\mu}_d(z)}E_d(z). \tag{15}$$

In this connection it is worthwhile to review some results of atmospheric work utilizing Schuster-type equations for an atmospheric two-flow model. Kondratyev (1969) reported that the atmospheric two-flow model with a uniform volume scattering function, which would give $r_d = r_u = 1.0$, provided an adequate solution. When he attempted a solution in the atmosphere for an asymmetric volume scattering function with no absorption, thus removing one unknown from the system, his conclusion was that the two-flow model yielded only rough estimates of the backscatter coefficient and not an accurate solution.

It is possible to make algebraic substitutions, however, in the above system to convert it to a form that does have a restricted solution dependent on the ratio of the shape factors—the same factors which originally rendered the equations inconsistent—

$$\bar{b}_u(z) = \bar{b}_d(z)\,\frac{r_u(z)}{r_d(z)};$$

and the following equation system does have a solution if r_u/r_d is known:

$$\frac{d\mathbf{E}(z)}{dz} = -\frac{a(z)}{\bar{\mu}(z)}\,\mathbf{E}(z), \tag{16}$$

$$\frac{dE_d(z)}{dz} = -\frac{a(z)}{\bar{\mu}_d(z)}\,E_d(z) - \bar{b}_d(z)\left(\frac{1}{\bar{\mu}_d(z)} - \frac{r_u(z)}{r_d(z)}\,\frac{R(z)}{\bar{\mu}_u(z)}\right)E_d(z) \tag{17}$$

and

$$-\frac{dE_u(z)}{dz} = -\frac{a(z)}{\bar{\mu}_u(z)}\,E_u(z) - \bar{b}_u(z)\left(\frac{1}{\bar{\mu}_u(z)} - \frac{r_d(z)}{r_u(z)}\,\frac{1}{\bar{\mu}_d(z)R(z)}\right)E_u(z) \tag{18}$$

where $R(z) = E_u(z)/E_d(z)$.

Equations 16–18 constitute what we term the net flow–two-flow model, which can be inverted to provide the inherent absorption coefficient for a hydrosol and the radiance backscatter coefficients for the light field which are one step removed from the hydrosol backscatter coefficient when r_u/r_d is known. The model represents three separate integrations of the radiative transfer equation (Eq. 1). The iterative techniques developed by Preisendorfer and Mobley (1984) appear to be the preferred mode for developing the inversion algorithm for this equation system.

Where do we stand, then, on the question of inverting the irradiances of natural light fields for the backscatter coefficient of a hydrosol? The problem stems from the asymmetry of the volume scattering function in natural hydrosols and the differences between the radiance distributions in the downwelling and upwelling hemispheres. These aspects of natural hydrosols require the use of shape factors when inversions are attempted, and we have shown that these parameters vary as a function of the concentration of suspensoids. Coupling the three-parameter model with the two-flow model (net flow–two-flow model) should allow the inversion for the radiance backscatter coefficient in most green Case 1 waters where the shape factor ratio (r_u/r_d) is close to 2.0 (Table 2). There is a regular increase in the magnitude of the radiance backscatter coefficient caused by the increase of the shape factors with the increase of the hydrosol backscatter coefficient (Figs. 2, 3). This fact will allow a functional relationship to be established between the radiance backscatter coefficient and the hydrosol backscatter coefficient from the results of NOARL Monte Carlo simulations. In this application, an improvement of up to an order of magnitude in the estimate of the hydrosol backscatter coefficient is to be expected over earlier estimates.

The situation is not as simple in the blue and blue-green Case 1 waters where the shape factor ratio varies downward somewhat from 2.0, depending on the relative concentrations of algal cells and organic detritus. Another approach to the inversion problem has been proposed by Zaneveld (1982); he rejects the two-flow approach in favor of integrations of the radiative transfer equation that give a statement of the optical factors affecting the transmittance and absorptance of the upwelling nadir radiance ratioed to the downwelling scalar irradiance. Shape factors are also involved with these integrations but they are defined differently from Aas' shape factors for the downwelling and upwelling irradiance streams. The solution of Zaneveld's model requires the same up- and downwelling irradiances required in the net flow–two-flow model plus measurements of the upwelling radiance received from the nadir viewing angle. The absorption coefficient can be obtained from the three-parameter model solution of the Gershun equation as is done in the net flow–two-flow approach. The assumptions required to solve the Zaneveld model are that the shape factor for the backscatter of downwelling scalar irradiance to the nadir radiance (f_b) and the radiance shape factor for the upwelling radiances (f_L) both be equal to 1.0. If these assumptions are met the model can be inverted for the backscatter coefficient of the hydrosol. Thus, inversion for the hydrosol backscatter coefficient can be accomplished from the integrations of the radiative transfer equation that yield the net flow–two-flow model or the integrations that yield the Zaneveld model.

The assumptions required to solve the net flow–two-flow model in the green Case 1 waters and the assumptions required to solve the Zaneveld model both imply errors in the range of ~30% with Zaneveld claiming this error range for all oceanic waters. However, this error range was estimated with a limited number of cases in which variations in suspensoid concentration were not accounted for and the volume scattering function for algal cells was not tested. It is important because the strongest effect on the shape factors determined in the NOARL simulations for the net flow–two-flow model was due to the volume scattering function for algal cells. An inversion with the net flow–two-flow model requires fewer light field measurements while an inversion with the Zaneveld model requires more light field measurements but may provide greater accuracy. NOARL simulations currently in progress which have a greater range of optical parameters, varying solar and sky conditions, and coverage of the 400–490-nm waveband will provide the data needed to investigate variance in all the shape factors proposed so far and determine the best inversion models for the various optical water types.

Conclusions

The two-flow model cannot be inverted to obtain the true backscatter coefficient b_b of natural hydrosols. The net flow–two-flow model at present can be inverted in all hydrosols to obtain the absorption coefficient a. When the ratio of the shape factors r_u/r_d is known, it has the potential to be inverted for the radiance backscatter coefficients $\bar{b}_d$ and $\bar{b}_u$. The NOARL simulation of the radiative transfer equation provides estimates of the shape factors r_d and r_u. The shape factors f_b and f_L can also be estimated. The estimates of r_d and r_u will establish the basis for a functional relationship between the hydrosol backscatter coefficient b_b and the radiance backscatter coefficients.

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