Invited paper

Inverse methods in hydrologic optics

OCEANOLOGIA, 44 (1), 2002.
pp. 9–58.

KEYWORDS
Radiative transfer
Inverse methods
Apparent optical properties
Inherent optical properties
Inelastic processes

Howard R. Gordon
Department of Physics,
University of Miami,
Coral Gables, FL 33124, USA;
e-mail: hgordon@miami.edu

Manuscript received 5 February 2002, accepted 11 February 2002.

Abstract

Methods for solving the hydrologic-optics inverse problem, i.e., estimating the inherent optical properties of a water body based solely on measurements of the apparent optical properties, are reviewed in detail. A new method is developed for the inverse problem in water bodies in which fluorescence is important. It is shown that in principle, given profiles of the spectra of up- and downwelling irradiance, estimation of the coefficient of inelastic scattering from any wave band to any other wave band can be effected.

Acknowledgements

The author is grateful to the U.S. Office of Naval Research (ONR) for the generous support of his investigations in inverse methods under Grants N00014-89-J-1985, N00014-97-I-0069, and N00014–99-I-0007. In the fall of 1967, I had the opportunity to begin my researches in hydrologic optics in collaboration with Dr. J. Dera. The friendship that developed during our year together has lasted thirty-five years. I dedicate this paper to that friendship.

1. Introduction: marine optics and radiative transfer

In this paper I examine the various methods that have been proposed and developed for estimating the inherent optical properties (IOPs) of water bodies from measurements of the apparent optical properties (AOPs). (See Appendix 1 for a list of acronyms, such as IOP, used in this work.) This is the so-called inverse problem of hydrologic optics: given measurements of the natural light field in a water body determine the fundamental optical characteristics of the medium. It is to be distinguished from the direct (or forward) problem of radiative transfer: calculating the AOPs given the IOPs. I will limit the discussion to measurements of the *natural* light field, i.e., illumination of the water by only the sun and sky. I will not address inverse problems in which artificial light sources are introduced into the medium for the purpose of estimating the IOPs (e.g., Maffione et al. 1993); however, I will discuss one inversion technique in which a primary goal is to detect the presence of artificial internal sources (Tao et al. 1994), but which also yields IOPs. I will further limit the analysis to methods that are based on rigorous solutions to the radiative transfer equation, e.g., I will not examine 'two-flow' methods (Preisendorfer & Mobley 1984), which have been shown to require additional assumptions, e.g., constant backscattering 'shape factors' (Aas 1987), to remove parameters that are difficult to estimate (Stavn & Weidemann 1989, Mobley 1994). An analog of the inverse problem problem in atmospheric optics is the estimation of aerosol properties (scattering phase function, single scattering albedo, etc.) from measurements of sky radiance (Gordon & Zhang 1995, Zhang & Gordon 1997, Cattrall 2001). Finally, I regret that because of my own ignorance of works published in languages other than my own, I must confine my discussion mostly to those published in English.

We begin in this section by reviewing basic marine optics and radiative transfer. Next, several methods for effecting solutions to the inverse problem, conveniently divided in time at 1994, are described in detail. Then, I provide a new inverse approach for fluorescent media in which the AOPs at a given wavelength also depend on the IOPs at all shorter wavelengths. Finally, I discuss and compare the various methods for inversion in realistic natural water settings.

1.1. Fundamental radiometric quantities

Here, I provide a very brief definition of two fundamental radiometric quantities. We assume the existence of a detector of electromagnetic radiation in the visible that can measure the radiant power $P(\lambda)$ in a narrow spectral region ($\Delta\lambda$) around a central wavelength λ. (See Appendix 2 for a list of symbols that are used frequently in this work.) There are two

fundamental quantities that we will be concerned with. In the case of an extended source, e.g., the sky, the quantity is called the *radiance*. If the detector has an area ΔA and measures a radiant power $\Delta P(\vec{r}, \hat{\xi}, \lambda)$ when its normal is pointed in the direction $-\hat{\xi}$ with its field of view limited to a set of directions specified by the solid angle $\Delta\Omega$, then radiance $L(\vec{r}, \hat{\xi}, \lambda)$, where $\vec{r}$ is the spatial position and the unit vector $\hat{\xi}$ is in the direction of the propagation, is defined through

$$L(\vec{r}, \hat{\xi}, \lambda) \stackrel{\text{def}}{=} \frac{\Delta P(\vec{r}, \hat{\xi}, \lambda)}{\Delta A \, \Delta\Omega \, \Delta\lambda}.$$

The quantity $\Delta P(\vec{r}, \hat{\xi}, \lambda)$ divided by $\Delta A \, \Delta\lambda$ is called the spectral *irradiance* (or just the irradiance) falling on the detector from $\hat{\xi}$ in $\Delta\Omega$.

In contrast to radiance, if the source of radiation is confined to a small (compared to the viewing distance) region of space, e.g., a star or planet in the night sky, the radiometric quantity of importance is called the radiant *intensity*. If the detector is oriented normal to the direction of propagation (along the line from the source to the detector) and records a power $\Delta P(\vec{r}, \hat{\xi}, \lambda)$, then the intensity $I(\vec{r}, \hat{\xi}, \lambda)$ defined to be

$$I(\vec{r}, \hat{\xi}, \lambda) \stackrel{\text{def}}{=} \frac{\Delta P(\vec{r}, \hat{\xi}, \lambda)}{\Delta\Omega_d \, \Delta\lambda},$$

where $\Delta\Omega_d$ is the solid angle subtended by the detector at the source (area of the detector divided by the square of the distance between the source and detector). It is understood that in the definitions above, the independent quantities ($\Delta\lambda$, $\Delta\Omega$, $\Delta\Omega_d$, and ΔA) are sufficiently small that reducing their size further would result in a negligible change in the radiometric quantities. In what follows, I will assume the existence of instrumentation capable of measuring both $L(\vec{r}, \hat{\xi}, \lambda)$ and $I(\vec{r}, \hat{\xi}, \lambda)$.

1.2. The inherent optical properties

Consider a parallel beam of irradiance $E(\lambda)$, where λ is the wavelength. If $\Delta E(\lambda)$ is the irradiance having left the beam (by absorption and scattering) after traversing a length $\Delta\ell$ of the medium, then the beam attenuation coefficient $c(\lambda)$ is defined through

$$c(\lambda) \stackrel{\text{def}}{=} \frac{\Delta E(\lambda)}{E(\lambda)\Delta\ell}.$$

If the parallel beam is incident on a small volume of medium Δv and an intensity $\Delta I(\Theta, \lambda)$ is measured at an angle Θ from the direction of the beam, the volume scattering function for *elastic* scattering is defined by

$$\beta(\Theta, \lambda) \stackrel{\text{def}}{=} \frac{\Delta I(\Theta, \lambda)}{E(\lambda)\Delta v}.$$

Similarly, if a parallel beam of irradiance $E(\lambda_e)$, within a narrow band of wavelengths between λ_e and $\lambda_e + \Delta\lambda_e$, where $\lambda_e < \lambda$, is incident on a small volume of medium Δv and an intensity $\Delta I(\Theta, \lambda)$ is measured at an angle Θ from the direction of the beam, the volume scattering function for *inelastic* scattering is defined by

$$\beta_{in}(\Theta, \lambda_e \to \lambda) \stackrel{\text{def}}{=} \frac{\Delta I(\Theta, \lambda)}{E(\lambda_e)\Delta v \Delta\lambda_e}.$$

Note that the elastic and inelastic volume scattering functions do not have the same units. The elastic and inelastic scattering coefficients are defined, respectively, by

$$b(\lambda) \stackrel{\text{def}}{=} \int\int_\Omega \beta(\Theta, \lambda)\, d\Omega,$$

$$b_{in}(\lambda_e \to \lambda) \stackrel{\text{def}}{=} \int\int_\Omega \beta_{in}(\Theta, \lambda_e \to \lambda)\, d\Omega,$$

where the element of solid angle $d\Omega = 2\pi \sin\Theta\, d\Theta$. The absorption coefficient $a(\lambda)$ is defined in terms of the lost irradiance from a parallel beam at wavelength λ that is not associated with elastic or inelastic scattering, i.e.,

$$a(\lambda) \stackrel{\text{def}}{=} c(\lambda) - b(\lambda) - \int_{\lambda'>\lambda} b_{in}(\lambda \to \lambda')\, d\lambda'.$$

The inelastic term represents the scattering of radiant power at λ to *all* wavelengths $> \lambda$, i.e., the loss from λ to all other wavelengths. This term can sometimes be related to the absorption by some constituent of the medium, e.g., in the case of fluorescence a photon must be absorbed before it is fluoresced (Gordon 1979), and if one used an instrument that truly measured absorbed photons, the associated $\int_{\lambda'>\lambda} b_{in}(\lambda \to \lambda')\, d\lambda'$ would be included implicitly in $a(\lambda)$. However, as we will treat all inelastic processes as scattering (with a change of wavelength), it is consistent to include the integral term explicitly in the definition of $a(\lambda)$. Thus, by 'a' we refer to the absorption of radiant energy that is converted into another form in the medium and *not* re-radiated at a longer wavelength. The quantities $c(\lambda)$, $\beta(\Theta, \lambda)$, and $\beta_{in}(\Theta, \lambda_e \to \lambda)$ are usually referred to as *inherent optical properties* (IOPs). In media such as natural waters, the IOPs are all dependent on position within the medium.

1.3. The apparent optical properties

We assume here that the radiance in natural waters $L(\vec{r}, \hat{\xi}, \lambda)$ depends only on the depth. Also, we specify the unit vector $\hat{\xi}$ by the angles θ and ϕ ($\xi_x = \sin\theta\cos\phi$, $\xi_y = \sin\theta\sin\phi$, $\xi_z = \cos\theta$) in a spherical coordinate system centered on the sea surface with the z axis directed into the ocean, i.e., $L(\vec{r}, \hat{\xi}, \lambda) \stackrel{\text{def}}{=} L(z, \theta, \phi, \lambda)$. It is observed that the downwelling $E_d(z, \lambda)$,

upwelling $E_u(z,\lambda)$, and scalar $E_0(z,\lambda)$ irradiances defined by

$$E_d(z,\lambda) \stackrel{\text{def}}{=} \int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi/2} \mid \cos\theta \mid L(z,\theta,\phi,\lambda) \sin\theta \, d\theta \, d\phi,$$

$$E_u(z,\lambda) \stackrel{\text{def}}{=} \int_{\phi=0}^{\phi=2\pi} \int_{\theta=\pi/2}^{\theta=\pi} \mid \cos\theta \mid L(z,\theta,\phi,\lambda) \sin\theta \, d\theta \, d\phi,$$

$$E_0(z,\lambda) \stackrel{\text{def}}{=} \int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} L(z,\theta,\phi,\lambda) \sin\theta \, d\theta \, d\phi,$$

respectively, decay approximately exponentially with depth in the water. It is therefore tempting to characterize as 'properties' of the medium the (almost depth-independent) exponential decay coefficients,

$$K_x(z,\lambda) \stackrel{\text{def}}{=} -\frac{d\ell n[E_x(z,\lambda)]}{dz},$$

where $x = d$, u, or 0. Similarly the irradiance ratio or irradiance reflectance

$$R(z,\lambda) \stackrel{\text{def}}{=} \frac{E_u(z,\lambda)}{E_d(z,\lambda)}$$

is often almost independent of z and might also be considered to be a 'property' of the water body. However, these 'properties' are dependent on the illumination at the water's surface, e.g., the solar zenith angle and the cloud cover. Because of this they are referred to a *apparent optical properties* (AOPs) (Preisendorfer 1961).

Treating $L(z,\theta,\phi,\lambda)$ as a probability density for photon directions, another important AOP is the mean cosine ($\overline{\mu}$) of the radiance distribution:

$$\overline{\mu}(z,\lambda) \stackrel{\text{def}}{=} \frac{\int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} \cos\theta L(z,\theta,\phi,\lambda) \sin\theta \, d\theta \, d\phi}{\int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} L(z,\theta,\phi,\lambda) \sin\theta \, d\theta \, d\phi} = \frac{E_d(z,\lambda) - E_u(z,\lambda)}{E_0(z,\lambda)}.$$

In a manner similar to K_x and R, $\overline{\mu}$ is a weak function of depth, but is dependent on the surface illumination.

1.4. The radiative transfer equation

The radiative transfer equation (RTE) governs the propagation of radiance in the ocean-atmosphere system:

$$\begin{aligned} \cos\theta \frac{dL(z,\theta,\phi,\lambda)}{dz} &= -c(z,\lambda)L(z,\theta,\phi,\lambda) \\ &+ \int_{\Omega'} \beta(z,\theta' \to \theta, \phi' \to \phi, \lambda) L(z,\theta',\phi',\lambda) \, d\Omega' \\ &+ \int \int_{\Omega'} \beta_{in}(z,\theta' \to \theta, \phi' \to \phi; \lambda_e \to \lambda) \times \\ &\times L(z,\theta',\phi',\lambda_e) \, d\Omega' \, d\lambda_e, \end{aligned} \tag{1}$$

where $\beta(z,\theta'\to\theta,\phi'\to\phi,\lambda)$ is the volume scattering function describing the *elastic* scattering of radiance of wavelength λ from direction (θ',ϕ') to direction (θ,ϕ), etc. The subscript Ω' on the integrals implies integration over the full range of solid angle (4π). To derive the light field at λ, eq. (1) must be solved subject to the boundary conditions that the radiance incident at the top of the atmosphere (TOA) is that due to the sun, or equivalently, with prescribed radiance from the sun and sky incident on the sea surface. Here, we use the RTE to compute only the irradiances or the nadir-viewing radiance, so it is sufficient to solve only the azimuthly averaged RTE for the azimuthly averaged radiance $L^{(0)}$:

$$\begin{aligned}\cos\theta\frac{dL^{(0)}(z,\theta,\lambda)}{dz} &= -c(z,\lambda)L^{(0)}(z,\theta,\lambda)\\ &+\int_0^\pi \beta^{(0)}(z,\theta'\to\theta,\lambda)L^{(0)}(z,\theta',\lambda)\sin\theta'\,d\theta'\\ &+\int_0^\pi \beta^{(0)}_{in}(z,\theta'\to\theta,\lambda_e\to\lambda)L^{(0)}(z,\theta',\lambda_e)\sin\theta'\,d\theta'\,d\lambda_e,\end{aligned}\tag{2}$$

where

$$L^{(0)}(z,\theta,\lambda)\stackrel{\text{def}}{=}\frac{1}{2\pi}\int_0^{2\pi}L(z,\theta,\phi,\lambda)\,d\phi,$$

$$\beta^{(0)}(z,\theta'\to\theta,\lambda)\stackrel{\text{def}}{=}\frac{1}{2\pi}\int_0^{2\pi}\beta(z,\theta'\to\theta,\phi'\to\phi,\lambda)\,d\phi,$$

$$\beta^{(0)}_{in}(z,\theta'\to\theta,\lambda_e\to\lambda)\stackrel{\text{def}}{=}\frac{1}{2\pi}\int_0^{2\pi}\beta_{in}(z,\theta'\to\theta,\phi'\to\phi;\lambda_e\to\lambda)\,d\phi.$$

The last term in eq. (2) is called the inelastic 'source function' indicated by J_{in}. Expressions for the J_{in} have been given by Ge et al. (1993) for fluorescence, J_f, and for Raman scattering, J_r:

$$J_f(z,\theta,\lambda)=\frac{1}{4\pi}\int b_f(z;\lambda_e\to\lambda)E_0(z,\lambda_e)\,d\lambda_e,\tag{3}$$

and

$$\begin{aligned}J_r(z,\theta,\lambda) &= \frac{1}{4\pi}\int b_r(z;\lambda_e\to\lambda)E_0(z,\lambda_e)\times\\ &\times\left[1+\frac{1}{2}\left(\frac{1-\rho(\lambda_e)}{1+2\rho(\lambda_e)}\right)\frac{E_2(z,\lambda_e)}{E_0(z,\lambda_e)}P_2(\cos\theta)\right]d\lambda_e,\end{aligned}\tag{4}$$

where $\rho(\lambda_e)$ is the Raman depolarization factor. In these expressions,

$$E_\ell(z,\lambda)=2\pi\int_0^\pi P_\ell(\cos\theta')L^{(0)}(z,\theta',\lambda)\sin\theta'\,d\theta',\tag{5}$$

and P_ℓ is the Legendre polynomial of order ℓ. E_0 is the scalar irradiance and E_1 is often called the vector (or net) irradiance. E_1 is easily seen to be

$E_d - E_u$, i.e., the difference between the downwelling and upwelling irradiance at depth z. Note that that the mean cosine can be written

$$\overline{\mu}(z,\lambda) = \frac{E_1(z,\lambda)}{E_0(z,\lambda)}.$$

Based on the discussion thus far, the inverse problem can be succinctly stated: given the external sources and measurements of $L(z,\theta,\phi,\lambda)$ or its moments, e.g., $E_1(z,\lambda)$, $E_0(z,\lambda)$, $E_d(z,\lambda)$, $E_u(z,\lambda)$, etc., estimate $a(z,\lambda)$, $b(z,\lambda)$, $b_{in}(z,\lambda_e \to \lambda)$, $\beta(z,\theta' \to \theta,\phi' \to \phi,\lambda)$, and $\beta_{in}(z,\theta' \to \theta,\phi' \to \phi;\lambda_e \to \lambda)$.

1.5. The raison d'être of inverse methods

Several methods exist for solving the RTE given the IOPs, and instrumentation exists for measuring the IOPs (although not routinely for β and β_{in}), therefore one might reasonably ask why bother with the inverse problem? There are in fact three very valid reasons for considering it.

First, the AOPs are far easier to measure than the complete IOP suite. The AOP instrumentation is simpler (cheaper) and readily available. Because of this there are far more measurements of the AOPs than the IOPs. Historical AOP data can be subjected to inversion yielding IOPs for time periods prior to the existence of modern instrumentation (providing additional value to such data). The important endeavor of interpretation of the AOPs for other applications, e.g., relating them to constituent concentrations for remote sensing ocean color (Gordon & Morel 1983), is best accomplished with the IOPs, as they are linearly additive over the concentrations.

Second, inverse methods provide IOPs that are characteristic of different (larger) sampling volumes than can be addressed with conventional instruments. For example, it is argued in Gordon & Boynton (1997) that inverse methods provide the IOPs at the proper sampling scale for remote sensing (an inverse problem in its own right). When IOPs are used with the RTE to develop interpretative algorithms for remote sensing, these IOPs should be measured at a scale ($\sim$ a few m^3) significantly larger than presented by typical IOP-measuring instruments ($\sim$ a few cm^3).

Third, the inverse methods of finding IOPs provide an alternate route to closure — the estimation of IOP-measuring instrument accuracies through comparison with IOPs determined by other means (with due caution required by the sampling volume mismatch).

2. Initial inversion algorithms (1939–1994)

Following McCormick (1992) and Mobley (1994) inverse problems can be classified as *explicit*, where formulas are used to provide IOPs given AOPs,

and *implicit*, where IOPs are estimated, inserted in the RTE to assess their efficacy in providing the AOPs, and then updated in an iterative manner.

2.1. Explicit algorithms – rigorous methods

Explicit algorithms can be divided into those that use rigorous or exact relationships between AOPs and IOPs, and those that use approximate relationships (usually, but not always, based on simulations). In the absence of inelastic processes, rigorous relationships can be developed to estimate the absorption coefficient given $E_0(z)$ and $E_1(z)$, or all of the IOPs given $L^0(z)$. We review these now.

2.1.1. The absorption coefficient

The best known example of an explicit rigorous method is the use of the so-called Gershun equation (Gershun 1939). This can be derived directly from the RTE in the following manner. Multiplying eq. (1) by $d\Omega$ and integrating over all directions, noting that

$$\begin{aligned}\int_\Omega \int_{\Omega'} \beta(z,\theta' \to \theta, \phi' \to \phi, \lambda) L(z,\theta',\phi',\lambda)\, d\Omega'\, d\Omega \\ = \quad b(z,\lambda) \int_{\Omega'} L(z,\theta',\phi',\lambda)\, d\Omega' = b(z,\lambda) E_0(z,\lambda)\end{aligned}$$

and

$$\begin{aligned}\int_\Omega \int \int_{\Omega'} \beta_{in}(z,\theta' \to \theta, \phi' \to \phi; \lambda_e \to \lambda) L(z,\theta',\phi',\lambda_e)\, d\Omega'\, d\lambda_e\, d\Omega \\ = \quad \int b_{in}(z,\lambda_e \to \lambda) \int_{\Omega'} L(z,\theta',\phi',\lambda_e)\, d\Omega'\, d\lambda_e \\ = \quad \int b_{in}(z,\lambda_e \to \lambda) E_0(z,\lambda_e)\, d\lambda_e,\end{aligned}$$

it is easy to see that

$$\frac{dE_1(z,\lambda)}{dz} = -a(z,\lambda)E_0(z,\lambda) + \int b_{in}(z,\lambda_e \to \lambda) E_0(z,\lambda_e)\, d\lambda_e. \qquad (6)$$

This can be rearranged to

$$a(z,\lambda) = \overline{\mu}(z,\lambda) K_1(z,\lambda) - \frac{1}{E_0(z,\lambda)} \int b_{in}(z,\lambda_e \to \lambda) E_0(z,\lambda_e)\, d\lambda_e,$$

where we have used the notation

$$K_1(z,\lambda) \stackrel{\text{def}}{=} -\frac{d\ell n[E_1(z,\lambda)]}{dz}.$$

This relationship, which to my knowledge was first derived by Højerslev (1975), is exact; however, it is not simple to solve because it requires information from λ_e as well as λ. We will return to this equation later

(Section 4); however, if inelastic processes are ignored, we have an explicit equation for $a(z,\lambda)$ as a function of the AOPs:

$$a(z,\lambda) = \overline{\mu}(z,\lambda)K_1(z,\lambda).$$

This shows that at least one IOP can be estimated from AOPs in a rigorous manner.

Use of the Gershun equation for the direct estimation of a has been limited because of the difficulty of measuring the scalar irradiance E_0, although examples of its direct application in estimating a can be found in Højerslev (1973), Pegau et al. (1995), Tyler (1960), and Voss (1989). More usefully, a is estimated from E_1 through approximations to $\overline{\mu}$, e.g., Højerslev (1996) shows that $0.62 < \overline{\mu} < 0.93$ for a wide range of solar zenith angles, wavelengths, and water types.

2.1.2. The absorption coefficient and volume scattering function

The only other rigorous explicit method of inverting the RTE is that proposed by Zaneveld (1974). This is based on expanding the azimuthally averaged volume scattering functions (elastic and inelastic) and radiance in a series of Legendre polynomials, to wit:

$$L^{(0)}(z,\theta,\lambda) = \frac{1}{2\pi}\sum_{n=0}^{\infty}\frac{(2n+1)}{2}P_n(\cos\theta)E_n(z,\lambda),$$

$$\beta^{(0)}(z,\theta'\to\theta,\lambda) = \frac{b(z,\lambda)}{2\pi}\sum_{n=0}^{\infty}\frac{(2n+1)}{2}\varpi_n(z,\lambda)P_n(\cos\theta)P_n(\cos\theta'),$$

$$\beta_{in}^{(0)}(z,\theta'\to\theta,\lambda_e\to\lambda) = \frac{b(z,\lambda_e\to\lambda)}{2\pi}\times \\ \times\sum_{n=0}^{\infty}\frac{(2n+1)}{2}\varepsilon_n(z,\lambda_e\to\lambda)P_n(\cos\theta)P_n(\cos\theta'),$$

where $\varpi_0 = 1$ and $\varepsilon_0 = 1$. Inserting these into eq. (2) and using the orthogonality properties of the Legendre polynomials provides a set of equations that can in principle be solved for the unknowns. These are

$$(n+1)\frac{dE_{n+1}(z,\lambda)}{dz} + n\frac{dE_{n-1}(z,\lambda)}{dz} = (2n+1)[-c(z,\lambda)+b(z,\lambda)\varpi_n(z,\lambda)]\times \\ \times E_n(z,\lambda) + (2n+1)\int b_{in}(z,\lambda_e\to\lambda)\varepsilon_n(z,\lambda_e\to\lambda)E_n(z,\lambda_e)\,d\lambda_e,$$

where $E_{-1}(z,\lambda)$ and $E_{-1}(z,\lambda_e)$ are taken to be zero. It is easy to see that the E_n's in this equation are identical to those defined in the previous section. In an inverse procedure, the E_n's are known and the ϖ_n's and ε_n's are the unknowns. Clearly, $n = 0$ yields Gershun's law. For the two inelastic processes of importance in natural waters, fluorescence and Raman

scattering, the ε coefficients are $\varepsilon_n(z) = 0$ for all $n > 0$ for fluorescence and $\varepsilon_n(z) = 0$ for all $n > 0$, excluding $n = 2$, for Raman scattering. Thus, for most values of n, the last term above is zero.

Ignoring the inelastic contribution, we see that these equations can be used to find $a(z, \lambda)$, $b(z, \lambda)$, and $\varpi_n(z, \lambda)$, i.e., they show that solution of the inverse problem by explicit methods is formally possible. However, as pointed out by Mobley (1994), except for $n = 0$, they are virtually useless. To represent a typical volume scattering function, e.g., similar to those measured by Petzold (1972), with reasonable accuracy requires $n \sim 1000$ or more. Recall that $P_n(\cos\theta)$ has n zeros approximately equally spaced in θ between 0 and π. Thus, to evaluate the integrals required to form the E_n's requires measurements of radiance at very fine increments in θ, e.g., $< 0.1^\circ$. Furthermore, the oscillatory nature of $P_n(\cos\theta)$ causes significant cancellation in the integrations, so as the light field becomes more diffuse (as with increasing z) a small amount of random noise will disrupt the cancellation and result in significant errors in E_n for large n. Thus, even given measurements of radiance at fine increments in θ, this sensitivity to random noise makes the inversion unstable. Holl & McCormick (1995) have examined the performance of these equations (elastic scattering only) and conclude that they are not 'expected to be of practical use in ocean-optics applications.' However, these difficulties are not present in Gershun's law ($n = 0$).

Two important conclusions result from the above analysis of Zaneveld's solution: (1) explicit inversion for the volume scattering function is possible in principle; but (2) explicit inversion with these exact formulas derived from the RTE is likely to be unsuccessful. The difficulty was realized early in research on inversion methods, and most work on explicit methods was based on inversion with approximate formulas that were developed from analysis of direct (or forward) solutions of the RTE for the AOPs in terms of the IOPs. As inelastic processes usually make small contributions to the AOPs, initial work was centered on deriving AOPs for elastically scattering media only.

2.2. Explicit algorithms – approximate methods

Morel & Prieur (1975b) provide one of the earliest applications of using Gershun's law to estimate a in the *absence* of E_0, i.e., from E_1 alone (see also Prieur & Sathyendranath (1981)). In the absence of inelastic scattering, Gershun's law can be rewritten

$$a(z) = K_d(z)\left[1 - R(z) + \frac{1}{K_d(z)}\frac{dR(z)}{dz}\right]\frac{E_d(z)}{E_0(z)}.$$

It is easy to show that

$$\frac{E_0(z)}{E_d(z)} = \frac{1}{\overline{\mu}_d(z)} + \frac{R(z)}{\overline{\mu}_u(z)},$$

where

$$\overline{\mu}_d(z) = \frac{E_d(z)}{E_{0d}(z)}, \qquad \overline{\mu}_u(z) = \frac{E_u(z)}{E_{0u}(z)},$$

and

$$\begin{aligned} E_{0d} &= \int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi/2} L(z,\theta,\phi,\lambda) \sin\theta \, d\theta \, d\phi, \\ E_{0u} &= \int_{\phi=0}^{\phi=2\pi} \int_{\theta=\pi/2}^{\theta=\pi} L(z,\theta,\phi,\lambda) \sin\theta \, d\theta \, d\phi. \end{aligned}$$

Note that E_{0d} and E_{0u} are the same as E_{0+} and E_{0-} defined in Section 3 below. The quantities E_d, E_u, E_{0d}, and E_{0u} are often referred to as the 'irradiance quartet' (Mobley 1994). Thus, when only E_d and E_u are available from measurements, it is necessary to estimate $\overline{\mu}_u$ and $\overline{\mu}_d$ to find a. Noting that $1/\overline{\mu}_u$ is multiplied by R, which is $\ll 1$, it is clearly of much lesser importance than $\overline{\mu}_d$. Through examination of previous measurements (Tyler & Preisendorfer 1962) and their own radiative transfer simulations (Prieur & Morel 1971), they settled on $\overline{\mu}_u = 2.5$. In the case of $\overline{\mu}_d$, if sky light is ignored one would expect a good approximation (at least near the surface) to be $\mu_w \equiv \cos\theta_w$, where θ_w is the solar zenith angle *in* the water. This is the value $\overline{\mu}_d$ would have if there were *no* scattering in the water. However, as sky light can make an important contribution to the light field incident on the sea surface, they estimated $\overline{\mu}_d$ for diffuse illumination by computing it for a cardioidal radiance distribution incident on the sea surface with no scattering in the water. The diffuse source $\overline{\mu}_d$ was 0.859. They then combined the contribution for the sun and sky to estimate $\overline{\mu}_d$ as

$$\frac{1}{\overline{\mu}_d} \approx \frac{0.6}{\mu_w} + \frac{0.4}{0.859},$$

and noted that for sun angles between 8°and 62°, the variation in μ_w is from 0.99 to 0.75, so $1.005 \leq 1/\mu_w \leq 1.33$ and $1/\overline{\mu}_d$ varies only from 1.069 to 1.265. Because of the small variation in μ_w the relative weights given to the sun and the sky in $\overline{\mu}_d$ (0.6 and 0.4, respectively) are not critical. From 400 to 700 nm, the variation in the estimated $\overline{\mu}_d$ caused by variations in the relative contributions of sunlight and skylight is $\sim 7\%$.

One of the first exercises in developing approximate methods over and above Gershun's law was that of Gordon et al. (1975) based on earlier studies of the diffuse reflectance of the ocean (Gordon 1973, Gordon & Brown 1973). They solved the RTE for a homogeneous ocean (sun in a black sky) with realistic IOPs using Monte Carlo methods. They showed that the AOPs

depended on the scattering phase function ($P = \beta/b$) of the ocean mostly through the probabilities of backscattering ($\tilde{b}_b$) and forward scattering ($\tilde{b}_f$) defined by

$$\tilde{b}_b \stackrel{\text{def}}{=} \frac{2\pi}{b}\int_{\pi/2}^{\pi}\beta(\Theta)\sin\Theta\, d\Theta,$$

and $\tilde{b}_f \stackrel{\text{def}}{=} 1 - \tilde{b}_b$. The backscattering coefficient b_b is $b\tilde{b}_b$, etc. Explicitly, their relationships were

$$R(\tau) \cong \sum_{n=0}^{3} r_n(\tau)\left[\frac{\omega_0\tilde{b}_b}{1-\omega_0\tilde{b}_f}\right]^n \tag{7}$$

and

$$\overline{\mu}_0(\tau)\frac{K_d(\tau)}{c} \cong \sum_{n=0}^{3} k_n(\tau)[\omega_0\tilde{b}_f]^n, \tag{8}$$

where τ was the optical depth $\tau = cz$, ω_0 the single scattering albedo ($\omega_0 = b/c$), and $\overline{\mu}_0(\tau)$ the value of $\overline{\mu}(\tau)$ at the given depth computed in the absence of scattering (this involves only the distribution of radiance on the sea surface and the surface roughness, and should *not* be confused with μ_w, which is independent of depth). Values of the coefficients $r_n(\tau)$ and $k_n(\tau)$ were provided in tabular form for a medium illuminated with the sun at the zenith in a black sky and a completely overcast sky. The $\overline{\mu}_0(\tau)$ term in the K_d equation removed nearly all of the dependence of the relationship on the incident illumination, but illumination effects were included in the R equation only through the parameters r_n that were derived for specific illumination conditions. It is easy to see that the parameter in the R equation can be rewritten

$$\frac{\omega_0\tilde{b}_b}{1-\omega_0\tilde{b}_f} = \frac{b_b}{a+b_b},$$

which shows that the diffuse reflectance of the ocean is a function of only a and b_b. Later, Gordon (1989b) carried out a much larger set of simulations (for a homogeneous water body) and replaced eq. (8) with

$$\overline{\mu}_0(0)\frac{K_d(0)}{c} \cong \sum_{n=1}^{2} k_n[1-\omega_0\tilde{b}_f]^n, \tag{9}$$

and

$$\overline{\mu}_0(0)\frac{\langle K_d\rangle}{c} \cong \sum_{n=1}^{3}\langle k\rangle_n[1-\omega_0\tilde{b}_f]^n, \tag{10}$$

where $\langle K_d\rangle \stackrel{\text{def}}{=} -\ell n[E_d(z_{10})/E_d(0)]/z_{10} \approx 2.3/z_{10}$, with z_{10} the depth at which the downwelling irradiance falls to 10% of its value at the surface. These papers also provided the inverse of the relationships, i.e., explicit

formulas for IOP combinations in terms of the AOPs, which could be used in explicit inversions.

In eq. (9) $k_1 \approx 1 \gg k_2$, so

$$\overline{\mu}_0(0)K_d(0) \approx a + b_b,$$

and we see that both $R(0)$ and $K_d(0)$ appear to be functions only of a and b_b and the incident water surface illumination. Although illuminating, relationships involving $K_d(0)$ are of little practical use because of the near impossibility of measuring this quantity in natural waters with surface waves. However, we shall see later that this relationship is helpful in developing a useful expression for b_b. In the equation for $\langle K_d \rangle$ the approximate dependence on $a + b_b$ seen for $K_d(0)$ is not valid because of the larger contribution of the $n > 1$ terms. This is a serious shortcoming in using $\langle K_d \rangle$ if c is not measured simultaneously with the irradiances. As commercial instruments for measuring c were not widely used until the mid 1980's, most AOP data acquired prior to that time would not be accompanied by c measurements.

Gordon (1989a) removed the influence of the incident illumination on $R(0)$ by showing that $R(0) \propto 1/\overline{\mu}_0(0)$. This allowed a reformulation of the equation for $R(0)$ in terms of the value the reflectance would have with the sun at the zenith $R_{\mu_w=1}(0)$ (Gordon 1991). The latter was to be estimated by measuring $R(0)$ as a function of the solar zenith angle and using the $1/\overline{\mu}_0(0)$ dependence of $R(0)$. Although this required measurement of $R(0)$ as a function of the solar zenith angle, it was shown that it provided the possibility of also estimating the volume scattering function over a limited range of angles.

Morel & Prieur (1975b) applied the first-order approximation to the Gordon et al. (1975) equation for R, i.e., $R \approx b_b/3(a + b_b)$, to estimate the spectral backscattering coefficient of a number of different waters. They inverted this to give

$$b_b \approx a\frac{3R}{1 - 3R}. \tag{11}$$

They also used a relationship for R that they had developed earlier (Prieur & Morel 1971, Morel & Prieur 1975a),

$$R = 0.33\frac{b_b}{a}(1 + \Delta),$$

where Δ depends on the incident radiance distribution and the phase function. When molecular scattering is unimportant, they reduce this to

$$R \approx \frac{b_b}{3(a - b_b)},$$

which gives

$$b_b \approx a\frac{3R}{1+3R}. \tag{12}$$

For waters with $b_b/a \ll 1$, eqs. (11) and (12) converge to $b_b \approx 3aR$. They applied these formulas to the analysis of the same irradiance data for which they derived a in Section 2.1.1. They used the resulting two values of b_b as a measure of the order of magnitude of the uncertainty in the retrieved b_b. They stipulate that eq. (11) is more appropriate for clear water (molecular scattering important) and eq. (12) is more appropriate for turbid water (molecular scattering unimportant).

During roughly the same time Gordon and coworkers were developing the approximate explicit relationships above for application to the marine environment, Kirk was developing relationships along the same lines focusing on turbid lakes. Kirk's work is documented in a series of papers from 1981 to 1994 (Kirk 1981a, 1981b, 1984, 1991, 1994a, 1994b) and in his book (Kirk 1983). His approach was to use the diffuse reflectance $R(0)$ and the mean attenuation coefficient for downwelling irradiance at the midpoint of the euphotic zone (same as $\langle K_d \rangle$) or averaged over the entire euphotic zone. The latter is $\langle K_d \rangle_e \stackrel{\text{def}}{=} -\ell n[E_d(z_e)/E_d(0)]/z_e \approx 4.6/z_e$, where z_e is the euphotic depth. As he was interested in turbid lakes, Kirk fixed the phase function (β/b) to be that measured by Petzold (1972) in very turbid water. He then carried out simulations varying a and b, but keeping the same phase function. He wrote the expression for either $\langle K_d \rangle$ or $\langle K_d \rangle_e$ as

$$K_d = \frac{a}{\mu_w}\sqrt{1 + G(\mu_w)\frac{b}{a}}$$

for the sun in a black sky. Kirk's simulations show that $G(\mu_w)$ is approximately a linear function of μ_w, i.e., $G(\mu_w) \cong g_1\mu_w + g_2$, with the parameters g_1 and g_2 depending on whether one is considering $\langle K_d \rangle_e$ ($g_1 = 0.425$ and $g_2 = -0.190$) or $\langle K_d \rangle$ ($g_1 = 0.473$ and $g_2 = -0.218$).

It is clear that this relationship (with the given g_1 and g_2) cannot be applied to all waters because the attenuation of irradiance must depend on the phase function. Clearly, for given values of a and b, if scattering is almost all in the near-forward direction its effect on K_d will be smaller than if it is more isotropic. Kirk looked for a quantity that would parameterize the effect of the phase function on K_d, and settled on the mean cosine of scattering $\overline{\mu}_s$ (Kirk 1994a) defined by

$$\overline{\mu}_s \stackrel{\text{def}}{=} \frac{\int_0^\pi \beta(\Theta)\cos\Theta\sin\Theta\, d\Theta}{\int_0^\pi \beta(\Theta)\sin\Theta\, d\Theta}.$$

Then he found that the average downwelling irradiance attenuation coefficient could be written

$$\langle K_d \rangle = \frac{a}{\mu_w} \sqrt{1 + G(\mu_w, \overline{\mu}_s) \frac{b}{a}}, \tag{13}$$

where

$$G(\mu_w, \overline{\mu}_s) \cong \mu_w \left[\frac{2.127}{\overline{\mu}_s} - 1.895 \right] - \frac{0.618}{\overline{\mu}_s} + 0.490.$$

Thus, given the IOPs, $\langle K_d \rangle$ can be estimated with good accuracy from these expressions. Note that this is essentially equivalent to the Gordon (1991) expression (eq. (10)), where $\tilde{b}_b$ or $\tilde{b}_f$ is used to parameterize the phase function rather than $\overline{\mu}_s$.

Kirk also studied the diffuse reflectance $R(0)$ as a function of the IOPs. Rather than relating R to $b_b/(a + b_b)$, following Morel & Prieur (1975a) he related it to b_b/a:

$$R(0) = C(\mu_w) \frac{b_b}{a}, \tag{14}$$

where $C(\mu_w) \cong -0.629\mu_w + 0.975$. The linear variation of C with μ_w is close to the inverse variation given by Gordon (1989a), which for Petzold's turbid water phase function with $\omega_0 \leq 0.8$ ($b/a \leq 4$) can be written as

$$R_{\mu_w}(0) \cong \left[\frac{1.6}{\overline{\mu}_0} - 0.6 \right] R_{\mu_w = 1}(0).$$

It is important to note that Gordon, Morel and Prieur, and Kirk all followed the same approach: carry out a large number of forward radiative transfer simulations using realistic values of the IOPs for the waters of interest and develop semi-empirical relationships between the IOPs and AOPs. These relationships then become the explicit equations to be used in the inversions.

Given measurement of only the irradiances $E_d(z, \lambda)$ and $E_u(z, \lambda)$, neither Gordon's nor Kirk's relationships can be inverted because there are more unknowns than the two equations (Gordon: a, b_b, and $\tilde{b}_b$; and Kirk: a, b, and $\overline{\mu}_s$). However, if the phase function is assumed to be known, i.e., a specific phase function is chosen to effect the inversion, this eliminates $\tilde{b}_b$ and/or $\overline{\mu}_s$. Then the inversion is straightforward. The R equation can be used to provide b/a with the $\langle K_d \rangle$ equation then providing a or c. Unfortunately, the results for both b and c depend strongly on the assumed phase function.

Gordon was able to circumvent somewhat the need for assuming a phase function. Noting that $\overline{\mu}_0(0) K_d(0) \approx a + b_b$ and $R_{\mu_w = 1}(0) \approx b_b/(a + b_b)$, he suggested that $R_{\mu_w = 1}(0) \approx b_b/(\overline{\mu}_0(0) K_d(0))$ or more usefully,

$\approx b_b/(\overline{\mu}_0(0)\langle K_d\rangle)$. Thus Gordon (1991) expanded $R_{\mu_w=1}(0)$ as follows:

$$\frac{b_b}{\overline{\mu}_0(0)\langle K_d\rangle} \cong \sum_{n=1}^{3} r'_n [R_{\mu_w=1}(0)]^n.$$

This would give b_b directly if $R_{\mu_w=1}(0)$ could be found. Gordon suggested measuring $R_{\mu_w}(0)$ by making irradiance measurements for a range of μ_w, e.g., as the sun sets or rises, and using this to estimate $R_{\mu_w=1}(0)$ by extrapolation. In addition, if one picks a functional form for the volume scattering function, e.g., the Beardsley & Zaneveld (1969) formula

$$\beta(\Theta) = \frac{\beta(90^\circ)}{(1 - e_f \cos\Theta)^4 (1 + e_b \cos\Theta)^4},$$

where e_f and e_b are unknown parameters, he showed that the dependence of $R_{\mu_w}(0)$ on μ_w can be used to estimate the unknown parameters. Then the retrieved b_b can be used to estimate $\beta(90^\circ)$; however, the derived volume scattering function would be realistic only for $\Theta \gtrsim 50^\circ$.

If it is further assumed that c is known, i.e., if c is measured along with the irradiances, it can be used in the $\langle K_d\rangle$ equation to estimate $\omega_0\tilde{b}_f$. However, $\omega_0\tilde{b}_b$ is b_b/c, and this is known, as b_b was estimated above. Thus,

$$\omega_0 = \omega_0\tilde{b}_f + \omega_0\tilde{b}_b = \omega_0\tilde{b}_f + \frac{b_b}{c},$$

and $b = \omega_0 c$ and $a = (1 - \omega_0)c$. Thus measurement of the irradiances and c allow estimation of both a and b, *without* any assumption regarding the phase function. Note that the c measurement is critical here – without it only b_b and the $\Theta \gtrsim 50^\circ$ volume scattering function could be directly estimated.

In Kirk's formulation even knowing c does not allow an inversion without assuming the correct phase function because of the dependence of G on $\overline{\mu}_s$ in eq. (13). Given c, and assuming a phase function, one uses eq. (13) to estimate a, and then eq. (14) to estimate b_b. From b_b and $c - a$, $\tilde{b}_b$ can be estimated, and if $\tilde{b}_b$ turns out to be the same as that for the assumed phase function, then the IOPs will form a consistent set. If the estimated $\tilde{b}_b$ is not in agreement with that assumed, then a new phase function must be tried. The difficulty with this approach is that, although for a given phase function both $\tilde{b}_b$ and $\overline{\mu}_s$ can be determined, there is only weak correlation between the two: $\tilde{b}_b$ depends on the volume scattering function in the backward direction, while $\overline{\mu}_s$ depends mostly on the volume scattering function in the forward direction. Both $\overline{\mu}_s$ and $\tilde{b}_b$ are needed for Kirk's inversion algorithm, but only $\tilde{b}_b$ for Gordon's; however, Gordon's requires measurements of $R(0)$ as a function of μ_w.

It should be obvious from analysis of the Gordon and Kirk equations that it is impossible to estimate the scattering coefficient from the irradiances alone without guessing at the scattering phase function. This suggests that c

has little influence on $K_d(z)$ and $R(0)$. Gordon (1993) explicitly showed this by computing the irradiances using truncated forms of the volume scattering function. Specifically, the Petzold (1972) turbid water volume scattering function $\beta(\Theta)$ was truncated by replacing it by $\beta(\Theta_0)$ for $\Theta \leq \Theta_0$ (but without changing the absorption coefficient or the backscatttering coefficient) and the RTE solved for a homogeneous ocean to give the irradiances as a function of Θ_0. Note that as Θ_0 increases, the corresponding scattering coefficient (and therefore c as well) decreases because small angles contribute most to b. The results indicated that the irradiances were almost independent of Θ_0, suggesting that if irradiances are inverted, it is possible to estimate a and b_b, but *not* b or c.

Finally, Zaneveld (1989) developed a method to estimate b_b from a solution to the RTE that involved parameters similar to the Aas (1987) two-flow shape factors. This will not be discussed, as Weidemann et al. (1995) show that these unknown factors are variable enough to induce significant error in b_b (-20% to $+40\%$). So, accurate inversion required some knowledge of β in backward directions.

3. Modern inversion algorithms (1994–2001)

In the mid 1990's a major advancement in the improvement of empirical relationships was the development of the radiative transfer code 'Hydrolight' (Mobley et al. 1993, Mobley 1994). This computer code allowed rapid computation of AOPs given IOPs, replacing the time-consuming Monte Carlo methods used by Kirk and Gordon. It allowed orders of magnitude more cases (including some inelastic processes) to be used as input to empirical relationships for explicit algorithms. In addition, more powerful computation tools enabled relating the AOPs to the IOPs in the asymptotic light field with relative ease. These developments led to explicit inversion methods that are described in this section, and provide a convenient demarcation between the initial and more modern inversion algorithms.

3.1. Explicit algorithms based on asymptotic theory

McCormick (1996) shows that away from the surface, for an infinitely deep homogeneous medium, the azimuthally-averaged radiance can be expanded in a series of eigenfunctions of the source-free RTE and written

$$L(z,\mu) = \sum_{j=1}^{N} C(\nu_j)\phi(\nu_j,\mu)\exp[-cz/\nu_j], \tag{15}$$

where $\mu = \cos\theta$, $C(\nu_j)$ are constants, $\phi(\nu_j,\mu)$ are the eigenfunctions, and the ν_j are the associated eigenvalues. The ν_j are roots of a transcendental equation involving the phase function and ω_0. The number N of roots

depends in a simple manner in the phase function. All the ν_j's are > 1. If the ν_j's are arranged in decreasing order, i.e., $\nu_1 > \nu_2 > \nu_3 \cdots$, then as $z \to \infty$

$$L(z, \mu) \to \phi(\nu_1, \mu) \exp[-cz/\nu_1].$$

Note that in this state, the depth dependence and angular dependence of the radiance decouple and all moments of the radiance distribution E_0, E_1, etc., decay with depth exponentially with decay coefficient $c/\nu_1 \equiv K_\infty$. This demonstrates the existence of what is called the asymptotic regime (see also Højerslev & Zaneveld 1977, Preisendorfer 1959, and McCormick 1992), and given $P(\Theta)$ and ω_0, provides a way to compute its properties. In this regime the reflectance $R(z) = E_u(z)/E_d(z)$ becomes R_∞ and is independent of depth. It is important that this condition is independent of the radiance distribution incident on the sea surface (although the *rate* of approach to it is not), and hence all quantities with the subscript ∞ are IOPs. Given the usual IOPs, a and β, the RTE is relatively simple to solve for R_∞ and K_∞, and vice versa (Prieur & Morel 1971, Kattawar 1975, McCormick 1992). (Gordon & Xu (1996) developed the properties of the asymptotic light field in the presence of inelastic processes.)

Tao et al. (1994) use asymptotic theory directly to effect an approximate inversion of the RTE. Their method is also capable of handling internal sources. Rather than describing their method in detail (complete with internal sources), I will demonstrate the basis of their inversion by providing a source-free, inelastic-free, homogeneous-medium example. We assume that *both* E_1 and E_0 are measured, and consider the Zaneveld (1974) equations for $n = 0$ and $n = 1$:

$$\frac{dE_1}{dz} + aE_0 = 0$$

$$2\frac{dE_2}{dz} + \frac{dE_0}{dz} = 3(-c + b\varpi_1)E_1,$$

where we have left off all of the arguments on the E_n's. The first equation gives a directly. To use the second we must relate E_2 to E_1 and/or E_0. This is effected through asymptotic theory, from which

$$\begin{aligned} E_n &= C(\nu_1) \exp[-cz/\nu_1] \int_{-1}^{1} P_n(\mu)\phi(\nu_1, \mu)\, d\mu \\ &= C(\nu_1) \exp[-cz/\nu_1] g_n(\nu_1). \end{aligned}$$

They show that $g_n(\nu_1)$ satisfies the recursion relationship

$$(n+1)g_{n+1} - h_n\nu_1 g_n + ng_{n-1} = 0,$$

where $g_{-1} = 0$, $g_0 = 1$ and $h_n = (2n+1)(1 - \omega_0 \varpi_n)$. Therefore, we see that

$$E_2 = g_2(\nu_1)E_0 = \frac{1}{2}[3(1-\omega_0)(1-\omega_0\varpi_1)\nu_1^2 - 1]E_0,$$

so the second Zaneveld equation becomes

$$(1-\omega_0)\nu_1^2 \frac{dE_0}{dz} + cE_1 = 0.$$

ν_1 is a function of ω_0 and the phase function. Assuming a particular phase function for the medium (as all inverse algorithms must) provides $\nu_1(\omega_0)$. Then the equation can be solved numerically for ω_0, which after having already found a, yields b. The value of b will depend strongly on the phase function, but $b_b = b\tilde{b}_b$ should not. This algorithm should provide a and b_b and should perform best in the near-asymptotic regime. Tao et al. (1994) show that this method is equivalent to using asymptotic theory to estimate the Aas (1987) two-flow shape factors.

Although we are not treating inversion methods with artificial sources, natural internal sources, e.g., bioluminescence, do exist and they have been incorporated into the Tao et al. (1994) algorithm when the source is isotropic and the source function depends only on z. They add to the Zaneveld (1974) equations an equation for $E_{\ell+}(z,\lambda) - E_{\ell-}(z,\lambda)$, where

$$E_{\ell+}(z,\lambda) = 2\pi \int_0^{\pi/2} P_\ell(\cos\theta') L^{(0)}(z,\theta',\lambda) \sin\theta' \, d\theta',$$

and

$$E_{\ell-}(z,\lambda) = 2\pi \int_{\pi/2}^{\pi} P_\ell(\cos\theta') L^{(0)}(z,\theta',\lambda) \sin\theta' \, d\theta',$$

are downward and upward partial moments of the radiance distribution. (Note $E_{\ell+}(z,\lambda) + E_{\ell-}(z,\lambda) = E_\ell(z,\lambda)$.) They use asymptotic theory to estimate all of the moments of the radiance distribution $E_{\ell\pm}(z)$ for $\ell \geq 2$, and estimate the IOPs and source density given the irradiance quartet, $E_{0\pm}(z)$ and $E_{1\pm}(z)$. Simulations show that an explicit version of this formulation works well as the depth increases and the asymptotic regime is approached, but works poorly near the surface. Note that in the application with sources, both E_{0+} and E_{0-} must be measured individually rather than only their sum.

Leathers et al. (1999) used asymptotic theory to derive IOPs from the $E_u(z)$ and $E_d(z)$ combination or from the $L_u(z)$ and $E_d(z)$ combination, where $L_u(z) \stackrel{\text{def}}{=} L^{(0)}(z, \theta = \pi)$. This approach differs from the Tao et al. (1994) algorithm in that E_0 is not used. Explicit empirical relationships are not obtained, rather at every depth $R(z)$, $R_L(z) \stackrel{\text{def}}{=} L_u(z)/E_d(z)$, $K_d(z)$, or $K_L(z) \stackrel{\text{def}}{=} -d\ell n[L_u(z)]/dz$, are equated to the asymptotic values R_∞, K_∞, etc. The latter are computed in the absence of inelastic processes.

Gordon et al. (1993) have shown that under many circumstances $K_d(z)$ in a homogeneous medium approaches its asymptotic value rapidly. For diffuse illumination, e.g., from a completely overcast sky, K_d is within 5% of K_∞ at a depth $\sim 1/K_d$ or less for $\omega_0 \geq 0.4$. The situation for R and R_L is not as clear, although R does not change rapidly with depth anywhere in the medium except possibly near the surface (at least for a homogeneous, infinitely deep water body). Given the scattering phase function and ω_0, R_∞ and K_∞ are not difficult to compute. Leathers et al. (1999) use the singular eigenvalue approach (Leathers & McCormick 1997) to compute them as a function of the IOPs. Because asymptotic relationships are used, no knowledge of the surface illumination is required. Of course, the AOPs are functions of the surface illumination, so this will lead to error, and one would assume that the quality of the retrievals of IOPs would be degraded near the surface.

Leathers et al. (1999) compared their retrieval of $a(z)$ profiles with direct measurements in situations where the water was strongly stratified. Good agreement was found; however, there was a consistent offset between the two, with the retrievals lower than the direct determinations. Large variations in a with depth were well recovered in the inversions from the AOPs, even though the asymptotic light field exists only for a homogeneous medium. This is attributable to the fact that, in Gershun's law, $\overline{\mu}$ varies slowly with IOPs and depth, so variations in the retrieved a closely follow variations in K_d, which are directly observed. No measurements were available to examine the quality of the $b_b(z)$ retrieval.

An extension of the asymptotic method was also developed by McCormick (1996) inspired by the empirical approximation developed by Zaneveld (1989) to describe the approach of $\overline{\mu}$ to the asymptotic value (also see McCormick 1995). The goal was to get a better approximation to the values of R_∞ and K_∞ than those generated by simply equating them to $R(z)$ and $K_d(z)$. McCormick's idea was that a better approximation to the asymptotic quantities could be obtained by keeping the second largest term in the radiance expansion eq. (15) as well as the first, i.e.,

$$L(z,\mu) \rightarrow C(\nu_1)\phi(\nu_1,\mu)\exp[-cz/\nu_1] + C(\nu_2)\phi(\nu_2,\mu)\exp[-cz/\nu_2].$$

Using this, and estimates of the relative magnitudes of the $C(\nu_j)$'s and ν_j's, he suggested that

$$Q(z) = Q(\infty) + [Q(z_r) - Q(\infty)]\exp[-P(z - z_r)], \tag{16}$$

where $z > z_r$, Q is any one of the quantities $1/\overline{\mu}$, R, K_0, K_1, and K_d, and $P = c(1/\nu_2 - 1/\nu_1)$. The depth z_r is a reference depth below which the

two-eigenfunction expansion of the radiance is valid. Given measurement of $Q(z)$ at three depths z_0, z_2 and $z_1 = (z_0 + z_2)/2$, one can readily show that

$$Q(\infty) = \frac{Q(z_0)Q(z_2) - Q^2(z_1)}{Q(z_0) + Q(z_2) - 2Q(z_1)}. \tag{17}$$

This equation was first derived by Zaneveld (1989) for $Q = K_1$. Thus, measuring these quantities at three depths provides estimates of the asymptotic values *without* measurements in the asymptotic regime. Leathers & McCormick (1997) show that for a homogeneous medium, these relationships provide a much better estimate of R_∞ and K_∞ than are obtained by approximating them as $R(z)$ and $K_d(z)$, respectively.

Zaneveld (1989) was one of the first to use the notion of the asymptotic light field to estimate AOPs from IOPs. He referred to this as 'asymptotic closure.' He started from eq. (16) as an assumption (P unknown). Then from measurements of E_0 and E_1, and an empirical relationship linking K_∞/c to ω_0, he was able to estimate a, b, and c. Of course, the results depend critically on the K_∞/c to ω_0 relationship, which in turn can be valid only within a limited range of phase functions.

3.2. Explicit algorithms based on numerical simulations

Stramska et al. (2000) were the first to use Hydrolight for the purpose of developing empirical formulas for use in explicit algorithms. They carried out a large number of homogeneous-ocean simulations using models relating the IOPS to the water's chlorophyll a concentration (Gordon & Morel 1983, Morel 1988, Morel & Gentili 1991) and the Petzold (1972) scattering phase function. They also used additional parameter values to break the covariation between a and b built into the models. As it is now apparent that Raman scattering can significantly affect the upwelling light field in clear waters in the green and red portions of the spectrum (Sugihara et al. 1984, Stavn & Weidemann 1988, Marshall & Smith 1990, Stavn 1990, Kattawar & Xu 1992, Ge et al. 1993, Waters 1995, Hu & Voss 1997, Gordon 1999), and can cause significant error in the retrieved IOPs, particularly $b_b(z)$, Raman scattering was included using the Morel & Gentili (1991) optical properties. However, the analysis was limited to $\lambda < 560$ nm to avoid Raman contamination in the upper layers as much as possible. Because they wanted to use Gershun's law to estimate a, they focussed on estimating the mean cosine from the measured AOPs. They used the observation that the reflectance is roughly proportional to $1/\overline{\mu}(z)$ (Gordon 1989a), while in contrast the radiance reflectance, $R_L(z) = L_u(z)/E_d(z)$, is almost independent of $\overline{\mu}(z)$. They developed a relationship between R_L and b_b/a, and tried to find a simple relationship between $\overline{\mu}(z)$ and R_L/R that was good for all wavelengths, optical parameters, sun angles and depth.

This led to a relationship that showed significant error in the estimation of $\overline{\mu}(z)$, considering its total range of variation. They tried to improve on $\overline{\mu}(z)$ by writing

$$\overline{\mu}(z) \cong \text{slope} \times \frac{L_u}{E_u} + \text{intercept},$$

and relating the slope and intercept to ω_0 and $\tilde{b}_b$. As before, in the analysis, all solar zenith angles, depths, and wavelengths are lumped together, so their relationships can in some sense be considered to be independent of these quantities, but since in reality they are not, this leads to increased scatter in the relationships. To estimate $\overline{\mu}(z)$ the two unknown quantities ω_0 and $\tilde{b}_b$ must be estimated. They use two methods. In the first, they assume a phase function providing $\tilde{b}_b$ directly. Then using their coarse estimate of $\overline{\mu}(z)$, a is found from Gershun's law, and b_b from R_L. The resulting b_b is combined with $\tilde{b}_b$ to give an estimate of b, which with a gives ω_0. The estimates of ω_0 and $\tilde{b}_b$ are then used to improve the estimate of $\overline{\mu}(z)$, providing a better estimate of a, etc. If c is measured, then one can estimate b (and thus ω_0) from $c - a$ using the coarse estimate of a. This is averaged with the b found by assuming a phase function and the procedure is carried out as before. They try to make a case that the algorithm will work in a stratified medium; however, in the examples that are provided, the reflectances are weak functions of IOPs and the vertical variations are nearly all in the asymptotic field, so $\overline{\mu}$ does not vary much across the structure.

There are two basic differences between the Stramska et al. (2000) algorithm and those of Kirk and Gordon: (1) the use of L_u along with E_u and E_d; and (2) the combining of various sun angles, depth, and wavelengths in a single analysis for $\overline{\mu}(z)$. The measurement of all three quantities (L_u, E_u, and E_d) are not typically carried out, and the pooling of quantities that would normally be known in the analysis must lead to error in the final relationships. However, it is difficult to argue with success, comparison of retrievals in the blue (minimum Raman contribution) with direct measurements of a and b_b show excellent correlation between the two (see Section 5).

Loisel & Stramski (2000), building on a series of Monte Carlo simulations by Morel & Loisel (1998), extended Kirk's formulation by including significantly more simulations, and by including Raman scattering in Hydrolight simulations. In the Morel & Loisel (1998) simulations (no inelastic processes), the elastic scattering phase function was decomposed into that due to particles $P_p(\Theta)$ and that due to the water itself $P_w(\Theta)$, according to

$$P(\Theta) = \eta P_w(\Theta) + (1 - \eta) P_p(\Theta), \tag{18}$$

where η is the fraction of total scattering due to the water, b_w/b, and b_w is the scattering coefficient of water. They use the Petzold (1972) turbid water phase function for P_p, and the Morel (1974) determinations for P_w and b_w. They carried out simulations for a homogeneous medium with $a = 1\ \mathrm{m}^{-1}$ and b/a from 0 to 10. The variation allowed in η was $0 \le \eta \le 0.2$. These simulations were analyzed in a manner similar to Kirk (1994b); however, rather than using $\langle K_d \rangle$ or $\langle K_d \rangle_e$, they studied $\langle K_d \rangle_1$, the mean attenuation coefficient over the first irradiance optical depth z_1, where $E_d(z_1)/E_d(0) = 1/e$. In their formulation, they write

$$\frac{b}{a} = g(\eta, \mu_w)\frac{R(0)}{1 - R(0)}$$

and

$$\langle K_d \rangle_1 = \frac{a}{\mu_w}\sqrt{1 + \frac{b}{a}\Gamma(\eta, \mu_w)}.$$

The first equation was suggested by an equation developed by Kirk (1994b) showing that at the depth z_{10}, b/a is proportional to $R/(1 - R)$. Note the similarity between the $\langle K_d \rangle_1$ equation and Kirk's $\langle K_d \rangle$ equation. In essence, they replaced $\overline{\mu}_s$ in Kirk's $G(\overline{\mu}_s, \mu_w)$ with η in $\Gamma(\eta, \mu_w)$ to represent the variation of K_d with the scattering phase function. They determined relationships for $\Gamma(\eta, \mu_w)$ and for $h(\eta, \mu_w) \equiv g(\eta, \mu_w)\Gamma(\eta, \mu_w)$. The result was for $0.03 \le \eta \le 0.2$, $h(\eta, \mu_w)$ depended almost entirely on μ_w and could be replaced by an average value $\overline{h}$ that depends only on μ_w, i.e.,

$$\overline{h}(\mu_w) \cong 2.54 - 6.54\mu + 19.89\mu_w^2.$$

The parameter $g(\eta, \mu_w)$ was also studied alone and found to be

$$g(\eta, \mu_w) \cong \frac{1}{(0.0215 - 0.0149\mu_w) + (0.1652 - 0.0358\mu_w)\eta}.$$

Thus, the Loisel and Stramski equations can be combined to give a from measurements of $R(0)$ and $\langle K_d \rangle_1$,

$$a = \frac{\mu_w \langle K_d \rangle_1}{\sqrt{1 + \overline{h}(\mu_w)R(0)/(1 - R(0))}},$$

and $b = b_w/\eta$, from either the b/a or $\langle K_d \rangle_1$ equation (their analysis shows the b/a equation is better). However, it must be noted that the value of b is completely dependent on the assumed $P_p(\Theta)$. At this point, η is known, so $\tilde{b}_b$ is as well. Therefore b_b could be determined as $b_b = \tilde{b}_b b$. This b_b should be almost independent of $P_p(\Theta)$, as $K_d(z)$ and $R(0)$ depend mostly on a and b_b (Gordon 1993).

Loisel and Stramski preferred to derive b_b from an equation similar to that developed by Gordon (1991) for $b_b/\langle K_d \rangle$ as a function of $R_{\mu_w=1}(0)$.

However, rather than using the measurement of $R(0)$ at several values of μ_w as suggested by Gordon, they chose to make an empirical fit involving η and μ_w, i.e.,

$$\frac{b_b}{\langle K_d \rangle_1} = 10^{\alpha} \left[R(0)\right]^{\delta},$$

with

$$\alpha \cong [-0.83 + 5.34\eta - 12.26\eta^2] + \mu_w[1.013 - 4.124\eta + 8.088\eta^2]$$

and

$$\delta \cong 0.871 + 0.40\eta - 1.83\eta^2.$$

Because of η, this equation cannot be used without an estimate of b. The b estimate is determined from the earlier relationships for a and b.

Tests of this algorithm suggest that a and b_b can be obtained with excellent accuracy, while the error in b is significantly larger and totally dependent on the assumptions for P_p. In the opinion of this author, the weakest part of the Loisel and Stramski algorithm is the reliance on b in the derivation of b_b; however, it is shown that the correct b_b can be found even in the presence of large errors in b, e.g., $\sim 100\%$. The algorithm has a significant advantage over others in that all of the required quantities can be estimated from space borne ocean color sensors (Gordon & Morel 1983).

The equations above for the Loisel-Stramski algorithm were developed in the absence of inelastic processes, i.e., $\langle K_d \rangle$ and $R(0)$ do not include any effects of inelastic processes. Loisel and Stramski included Raman scattering in their algorithm by estimating its contribution using Hydrolight. As Raman scattering has little effect on $\langle K_d \rangle$, they chose to correct only $R(0)$ for the presence of Raman scattering. The procedure they used was to compute the reflectance ratio $\kappa \stackrel{\text{def}}{=} R_{\text{Elastic}}/R_{\text{Total}}$, where 'Elastic' and 'Total' refer to the absence and presence of Raman scattering, respectively. κ was determined as a function of b_b/a and wavelength using the Morel & Gentili (1991) model of the IOPs as a function of chlorophyll a as provided in the subroutines in Hydrolight. Note that in the Morel and Gentili model, specifying the chlorophyll a concentration specifies all of the IOPs except P_p. Loisel and Stramski again used the Petzold (1972) turbid water phase function for P_p. The correction scheme they used was iterative: first, take $\kappa(\lambda) = 1$ and find the IOPs to form b_b/a, use this b_b/a to find a new $\kappa(\lambda)$, which gives a new b_b/a, etc.

In Loisel et al. (2001) IOPs estimated this inversion method were compared with direct measurements. Good agreement was found for a and b_b measured in waters ranging from oligotrophic to turbid. In contrast, the retrievals of b were quite poor, indicating that the Petzold (1972) turbid water phase function was not appropriate for their data set. An important

aspect of the Loisel et al. (2001) paper is the development of a way of using their algorithm with remote sensing data. Their idea is that $\langle K_d \rangle_1$ can be estimated at 490 nm from current remote sensing algorithms using the reflectances at 443 and 555 nm (Mueller & Trees 1997), and that $\langle K_d \rangle_1$ at any wavelength can be estimated (empirically) given that at 490 nm (Austin & Petzold 1981, Kishino et al. 1996). Thus, $R(0, \lambda)$ provides the required $\langle K_d(\lambda) \rangle_1$. This method was tested in the data set and the retrievals of a and b_b were found to be only slightly degraded.

3.3. Implicit algorithms

Tao et al. (1994) presented a *quasi*-implicit version of their asymptotic-based algorithm. Thus, the exact RTE is not solved, but an approximation to it is. They construct an objective functional that depends on the IOPs, the measured AOPs, and the source function, and minimize it using standard minimization techniques (Press et al. 1992). In reality they simply used minimization techniques to solve a complicated set of non-linear equations that are nearly impossible to solve analytically. The implicit version of their algorithm was better than the explicit version (which uses the same physics, but a simplified source function to make the solution tractable) in retrieving the absorption coefficient and the internal source function, but did not improve the estimates of the scattering coefficient. Their resultant solution would not be expected to be a solution to the RTE, except at great depth, where asymptotic theory is valid.

At this time, the only truly implicit algorithms known to the author are those developed by Gordon and Boynton (Gordon & Boynton 1997, 1998; Boynton & Gordon 2000). The Gordon and Boynton algorithms are based on trying to achieve the following goal: given the illumination on the sea surface and measurements of depth profiles of either $E_u(z)$ and $E_d(z)$ or $L_u(z)$ and $E_d(z)$, find IOPs which, when inserted into the RTE, reproduce the measured AOP profiles exactly (actually, within experimental error). This is really the ultimate goal of inverse methods as the incident illumination and the RTE are the only links between the AOPs and IOPs.

In Gordon & Boynton (1997) an implicit algorithm is presented for the inverse problem in a homogeneous water body that is infinitely deep or of finite depth with a reflecting bottom. The basic procedure is very simple. Consider the case where $E_u(z)$ and $E_d(z)$ are measured. The algorithm starts with an initial guess for the absorption coefficient, $a^{(0)}(z) = \mu_w K_1(z)$. This is averaged over depth according to

$$a^{(0)} = \frac{\int_0^{z_m} a^{(0)}(z)\, f(z)\, dz}{\int_0^{z_m} f(z)\, dz}, \tag{19}$$

where z_m is the maximum depth of the measurements. Gordon & Boynton (1997) used a weighting in which $f(z) = \ell n[E_d(z)]$, yielding a near-linear weighting with depth, but found the results were not sensitive to the form of f. Then recalling $R(0) \approx 0.33 b_b/a$, they estimated the initial b_b from $b_b^{(0)}(z) = 3R(z)a^{(0)}$ averaged over depth in a manner identical to $a^{(0)}(z)$. As in all inverse algorithms, an assumption must be made for the scattering phase function, and this provides $\tilde{b}_b$, and $b^{(0)} = b_b^{(0)}/\tilde{b}_b$. These guesses for the IOPs are then inserted into the RTE, which is solved for $E_u^{(0)}(z)$, $E_d^{(0)}(z)$, *and* $E_0^{(0)}(z)$, yielding an estimate for the $\overline{\mu}$ profile, $\overline{\mu}^{(0)}(z)$. The estimated $\overline{\mu}$ provides a new estimate of $a(z)$, i.e., $a^{(1)}(z) = \overline{\mu}^{(0)}(z)K_1(z)$. The crucial part is the revised estimate of $b_b(z)$. Calling the computed value of $R(z)$ after the initial iteration $R^{(0)}(z)$, $\Delta R(z) = R(z) - R^{(0)}(z)$ is formed, and the change in $b_b(z)$ is taken to be $\Delta b_b(z) = 3\Delta R(z)a^{(1)}(z)$. However, since the relationship $R(z) \approx b_b(z)/3a(z)$ is not precise, the revised estimate for b_b is taken to be

$$b_b^{(1)}(z) = b_b^{(0)}(z) + \epsilon \Delta b_b(z)$$

where $\epsilon < 1$. This has the property that it pushes b_b in the right direction, but with $\epsilon \approx 0.5$, there is little possibility of overshoot. These are then averaged over depth as before and $b_b^{(1)}$ is combined with $\tilde{b}_b$ to provide $b^{(1)}$. The revised IOPs are then inserted into the RTE and its solution provides the quantities required for the next step in the iteration: $E_u^{(1)}(z)$, $E_d^{(1)}(z)$, and $E_0^{(1)}(z)$. This is then repeated many times. The algorithm is stopped when the residual error after n iterations, defined as

$$\delta^{(n)} \stackrel{\text{def}}{=} \frac{1}{N}\sum_{i=1}^{N} |\ell n[E_d^{(n)}(z_i)] - \ell n[E_d(z_i)]| + \frac{1}{N}\sum_{i=1}^{N} |\ell n[E_u^{(n)}(z_i)] - \ell n[E_u(z_i)]|,$$

where the superscripted irradiances are those computed in the n^{th} iteration and z_i are the depths at which the irradiance data are given, reaches a minimum. The radiative transfer in the algorithm is determined by a coupled ocean-atmosphere model and the RTE is solved by Monte Carlo methods.

Gordon & Boynton (1997) tested the inversion using simulated data and showed that the retrieved a and b_b values were only weakly dependent on the assumed particle phase function. For example, when the correct phase function ($\tilde{b}_b = 0.036$) was used in the inversion of simulated data the errors in a and b_b were $< 1\%$; however, when an incorrect phase function ($\tilde{b}_b = 0.011$) was used to invert the same data, the error in a was still $\leq 1\%$, and the error in b_b was $< 11\%$. Thus a factor of 3 error in $\tilde{b}_b$ did not lead to an unmanageably large error in b_b. Gordon & Boynton (1997) also inverted

Tyler's Lake Pend Oreille data (Tyler & Preisendorfer 1962) and retrieved excellent values of a compared to measurements.

Gordon & Boynton (1997) applied a similar algorithm to measurements of $L_u(z)$ and $E_d(z)$. This was effected by estimating and updating the 'Q-factor,' $Q = E_u/L_u$ at each iteration, and at the n^{th} iteration using $Q^{(n)}(z)$ to estimate $E_u^{(n)}(z) = Q^{(n)}(z)L_u(z)$. This $E_u^{(n)}(z)$ is combined with measured $E_d(z)$ and used as in the earlier E_u and E_d algorithm. The performance of the $L_u(z)$ and $E_d(z)$ is only slightly degraded compared to the $E_u(z)$ and $E_d(z)$ algorithm.

When applied to a finite depth medium with bottom albedo A, the algorithm functions as before, except the initial value of b is taken to be equal to $a^{(0)}$ because the initial estimate of b_b from $R(z)$ is likely to be strongly influenced by the presence of the bottom. Also, the radiative transfer code now includes the bottom reflection with the correct albedo placed at the correct depth. Tests of the algorithm using simulated data show that the error in the retrieved a, although remaining small, is larger than the infinitely deep ocean. The error in b_b can be very large, particularly when b_b is small and the bottom albedo is large, i.e., ~ 1. If the incorrect bottom albedo is used, the resulting $L_u(z)$ or $E_u(z)$ from the RTE provides a poor fit to the measured profiles.

Gordon & Boynton (1998) applied these ideas to a vertically stratified medium. In a medium in which the IOPs change with depth, Gordon (1980) showed that $K_d(z)$ (and therefore $K_1(z)$) depended mostly on the IOPs at depth z. Since $\overline{\mu}$ is not as strong a function of depth as K_d even in the presence of stratification, Gershun's law is still useful for estimating $a(z)$. In contrast to the simple $R(0) \approx b_b/3a$ for a homogeneous water body, in a stratified water body, Gordon & Clark (1980) showed that $R(0)$ depends on a depth-weighted average of b_b/a over the water column, i.e.,

$$R(0) \approx \frac{\langle X(0) \rangle}{3},$$

with

$$\begin{aligned} \langle X(0) \rangle &\stackrel{\text{def}}{=} \frac{\int_0^{z_{90}} X(z)\, g(z)\, dz}{\int_0^{z_{90}} g(z)\, dz}, \\ g(z) &\stackrel{\text{def}}{=} [E_d(z)/E_d(0)]^2, \\ X(z) &\stackrel{\text{def}}{=} b_b(z)/a(z), \end{aligned}$$

and z_{90} is the depth over which the downwelling irradiance falls to $1/e$ of its value at the surface. In the same manner as assuming $R(z) \approx b_b/3a$ in the homogeneous case, Gordon & Boynton (1998) assumed

$$R(z) \approx \frac{\langle X(z) \rangle}{3}, \tag{20}$$

with

$$\langle X(z)\rangle \stackrel{\text{def}}{=} \frac{\int_z^{z'_{90}} X(z')g(z,z')\,dz'}{\int_z^{z'_{90}} g(z,z')\,dz'},$$

$$g(z,z') \stackrel{\text{def}}{=} [E_d(z')/E_d(z)]^2,$$

$z' \geq z$, and z'_{90} is the depth over which $E_d(z')$ falls to $1/e$ of its value at $z = z'$. To simplify the numerical computations, they extended the integration to the maximum depth at which irradiance data is obtained (z_{Max}). The equation for $R(z)$ can then be inverted for $X(z)$ given the $R(z)$ profile:

$$X(z) \approx 3\left[R(z) - \frac{dR(z)}{dz}\int_z^{z_{\text{Max}}} dz' \left[\frac{E_d(z')}{E_d(z)}\right]^2\right]. \tag{21}$$

This provides an avenue for obtaining $b_b(z)/a(z)$ from the irradiance profiles.

In the stratified case, the algorithm proceeds as before. In going from the n^{th} to $(n+1)^{\text{th}}$ iteration, $a(z)$ and $b_b(z)$ are changed according to

$$a^{(n+1)}(z) = \overline{\mu}^{(n)}(z)K_1(z),$$

and

$$b_b^{(n+1)}(z) = b_b^{(n)}(z) + \epsilon\Delta b_b^{(n)}(z),$$

where

$$\Delta b_b^{(n)}(z) = \Delta X^{(n)}(z)a^{(n+1)}(z),$$

and

$$\Delta X^{(n)}(z) = X(z) - X^{(n)}(z),$$

with $X^{(n)}(z)$ the profile of $X(z)$ computed from $R^{(n)}(z)$, the computed reflectance profile after the n^{th} iteration. Thus, the new absorption coefficient profile is always determined by the previous estimate of the average cosine, and the new backscattering profile by the new absorption coefficient and reflectance profiles. The only real difference between the homogeneous and stratified algorithms is the dR/dz term in $X(z)$. In a manner completely analogous to the homogeneous case, the algorithm can be structured to operate with $L_u(z)$ and $E_d(z)$ rather than $E_u(z)$ and $E_d(z)$. Gordon & Boynton (1998) thoroughly tested the algorithm using simulated data and found that it was capable of resolving vertical structure in the IOPs to the extent that K_d could be accurately computed. When the derivatives of E_u and E_d could be computed accurately, the algorithm performance was similar to the homogeneous case. The weak dependence of the retrievals on the assumed scattering phase function was also similar to the earlier algorithm.

The Gordon & Boynton (1998) algorithm has the attribute that it provides IOPs that *exactly* reproduce the AOPs; however, if the physics

used to relate the AOPs and IOPs is incomplete, the retrieved IOPs will be incorrect although the reconstructed irradiances will be essentially perfect. As Raman scattering is important, particularly at longer wavelengths, it cannot be ignored, so Boynton & Gordon (2000) developed a version of the Gordon & Boynton (1998) algorithm that included Raman scattering. In their algorithm, they proposed using measurements of the light field at the excitation wavelength to estimate the Raman source function $J_r(z, \theta, \lambda)$ at the wavelength of interest, λ. Their procedure is straightforward: the Raman contribution to the irradiances at λ are estimated and removed leaving the elastic contribution. The irradiance profiles resulting from elastic scattering are then inserted into the Gordon & Boynton (1998) algorithm for inversion.

Evaluation of $J_r(z, \theta, \lambda)$ is relatively simple. The inversion algorithm is applied to the irradiance data at λ_e to retrieve the IOPs along with the profiles of $E_0(z, \lambda_e)$ and $E_2(z, \lambda_e)$ that are required for J_r. In this procedure it is assumed that the Raman correction is not required at λ_e (if it is required, then the full Raman algorithm we are describing must be used at λ_e as well). The main difficulty is in computing the Raman generated light field at λ because it depends on the *unknown* IOPs at λ as well as on J_r. This is overcome by first assuming IOP profiles for $a(z)$ and $b_b(z)$ at λ and computing the Raman light field. The Raman contribution is then subtracted, and the Gordon & Boynton (1998) algorithm (henceforth called the 'elastic algorithm') is used to provide new estimates for the IOPs at λ. The new IOP estimates are used recompute the Raman light field, which is subtracted from the measurements, and the elastic portion is inverted to give new IOPs etc., i.e.,

$$\cdots J_r + \mathrm{IOPs}^{(n)} \rightarrow \mathrm{RLF} \rightarrow \mathrm{ELF} \rightarrow \mathrm{IOPs}^{(n+1)} \rightarrow J_r + \mathrm{IOPs}^{(n+1)} \rightarrow \mathrm{RLF} \cdots,$$

where RLF and ELF refer to the Raman light field and elastic light field, respectively.

Boynton & Gordon (2000) studied the efficacy of this algorithm and presented an example for a stratified water body in which the error in $a(z)$ and $b_b(z)$ reached 20% and a factor of 10, respectively, before the Raman correction, and 2% and 10%, respectively, after the Raman correction. It should be mentioned that in the absence of measurements of the light field at λ_e, a method similar to that used by Loisel & Stramski (2000) to remove Raman effects could be employed; however, the Boynton & Gordon (2000) procedure is preferable because no additional assumptions are required (e.g., relationships between the chlorophyll concentration and the IOPs), although it does require the light field at λ_e.

Finally, in trying to apply the Gordon & Boynton (1998) algorithm to irradiance data measured in very clear water it was found that occasionally

the retrieved b_b was less than that of pure sea water (b_{bw}) in the blue. Although the error in b_b was not excessive ($\sim 20\%$), it was large enough to render $b_b(z) < b_{bw}$ for some depths. This problem was traced to the fact that the retrievals become more dependent on the phase function as the water clarity increases. In the Gordon-Boynton algorithms, the retrievals were made using either Henyey-Greenstein phase functions ($g = 0.85$ or 0.90) or the Petzold (1972) turbid water phase function. These are realistic for most waters, but under very clear conditions, they are a poor approximation in the backscattering direction. Boynton & Gordon (2002) resolved this difficulty by using a two component phase function identical to Morel & Loisel (1998) and Loisel & Stramski (2000), i.e., eq. (18). The particle component assumes a particular $P_p(\Theta)$ (e.g., Henyey-Greenstein or Petzold), and the fraction of water scattering $\eta(z)$ is treated as a variable. (Note that if η is fixed at some value, we have a fixed phase function for the medium, which is exactly the Gordon & Boynton (1998) assumption.) The algorithm works as follows: (1) a profile of $\eta(z)$ is assumed, and the IOPs are estimated by an algorithm similar to the elastic algorithm (e.g., Gordon & Boynton 1998); (2) the resulting $b_p(z)$ is used to estimate $\eta(z)$, and if the $\eta(z)$ profile differs significantly from that assumed, $\eta(z)$ is updated, etc., i.e.,

$$\cdots\ \eta^{(n)}(z) \rightarrow \text{elastic algorithm} \rightarrow \text{IOPs}^{(n)} \rightarrow \eta^{(n+1)}(z) \cdots$$

This algorithm considerably improves the retrievals in very clear waters, and is essentially the same as Gordon & Boynton (1998) in more turbid waters. It should be noted that the correct $b(z)$ profile can only be obtained if the particle phase function is correct; in essence only $a(z)$ and $b_b(z)$ can be retrieved in general.

4. Inversion of fluorescent light fields

The fact that the Raman scattering cross section is known allowed inclusion of this inelastic process in the inversion algorithms. The other inelastic process of importance in natural waters is fluorescence. There are at present only two ways to assess directly the importance of fluorescence in the in-water light field. In the first, the fluorescence has a spectral character that allows it to be distinguished from the elastic scattering. An example is the natural fluorescence of phytoplanktonic chlorophyll, which has a spectrally narrow emission peak at 683 nm (Gordon 1979). The second is to measure the in-water light field with sufficient spectral resolution ($\Delta\lambda \lesssim 0.1$ nm) that the solar Fraunhofer lines can be resolved. Solar Fraunhofer absorption lines will become shallower (less absorption) due to light generated by inelastic processes (Kattawar & Xu 1992, Ge et al. 1993, Waters 1995, Hu & Voss 1997). By measuring the 'depth' of the

lines, the light field can be portioned between elastic and inelastic scattering. Unfortunately, there are few instruments with sufficient spectral resolution for the latter, and there are fluorescence processes that are not manifest in narrow easily-identifiable spectral features. Thus, it is of interest to try to understand how fluorescent light fields might fit into the inverse methods of radiative transfer. Preisendorfer & Mobley (1988) have presented a theory of fluorescent light fields based on the two-flow model; however, their inversion method suffers from the same defect as the Preisendorfer & Mobley (1984) inversion method for elastic processes. The Tao et al. (1994) algorithm can operate in the presence of fluorescence, but in its present formulation can only be used to estimate the total contribution of all natural internal sources (from all excitation wavelengths) at a given wavelength. It cannot separate the contribution from individual spectral regions, although it could likely be reformulated to do so. Here I briefly discuss a new approach for inversion in the presence of inelastic processes which can provide a partial decomposition of b_{in}.

4.1. Estimation of a and b_{in}

Central to all of the inversion algorithms is Gershun's law, which in the presence of inelastic processes can be written

$$\frac{dE_1(z,\lambda)}{dz} = -a(z,\lambda)E_0(z,\lambda) + \int b_{in}(z,\lambda_e \to \lambda)E_0(z,\lambda_e)\,d\lambda_e.$$

We will assume that the fluorescence emission and excitation are both broad band, e.g., as with the fluorescence of CDOM (Hawes et al. 1992). Following Preisendorfer & Mobley (1988), it will be useful to divide the excitation spectrum into a large number (N) of spectral intervals, the i^{th} being denoted as $\Delta\lambda_i$ centered at λ_i. Then, we write for a particular emission wavelength λ_j

$$\int b_{in}(z,\lambda_e \to \lambda_j)E_0(z,\lambda_e)\,d\lambda_e = \sum_{i=1}^{N'} b_{in}(z,\lambda_i \to \lambda_j)E_0(z,\lambda_i)\Delta\lambda_i,$$

where $N' < N$ is the number of intervals required to fill the spectrum between λ_e and λ_j. Then we can rewrite Gershun's law as

$$\sum_{i=1}^{i<j} b_{in}(z,\lambda_i \to \lambda_j)E_0(z,\lambda_i)\Delta\lambda_i = \frac{dE_1(z,\lambda_j)}{dz} + a(z,\lambda_j)E_0(z,\lambda_j).$$

Assume for the moment that both $E_1(z,\lambda)$ and $E_0(z,\lambda)$ are measured for all λ, so all of the irradiances in Gershun's law are known. For a given z, assuming that $b_{in}(z,\lambda_j \to \lambda_j) = 0$, this equation has $j-1$ unknown b_{in}'s and one unknown a for a total of j unknowns. For example, for $j = 1$, $a(z,\lambda_1)$ is unknown, for $j = 2$, $b_{in}(z,\lambda_1 \to \lambda_2)$ and $a(z,\lambda_2)$ are unknown, etc. Thus, even when the light field is measured at all wavelengths and depths, there

are always more unknowns than the single Gershun equation at each depth. Some way is needed to restrict the number of unknowns.

The simplest restriction on the number of unknowns is to assume that IOPs are depth independent, i.e., we restrict ourselves to homogeneous media. Then, writing $b_{in}(z,\lambda_i \rightarrow \lambda_j)\Delta\lambda_i$ as $B(i,j)$, $E_0(z,\lambda_i)$ as $E_0(z,i)$, and $a(z,\lambda_j)$ as $-B(j,j)$, we have

$$\sum_i^{i\le j} E_0(z,i)B(i,j) = \frac{dE_1(z,j)}{dz}.$$

By using measurements of the light field at j depths, in principle we can find a solution for the IOPs. Writing the unknowns $B(i,j)$ as a column vector with rows labeled λ_i, i.e.,

$$\mathbf{B} = \begin{pmatrix} B(1,j) \\ B(2,j) \\ \vdots \\ B(j,j) \end{pmatrix},$$

and $E_0(z_k,i)$, where $k = 1, \cdots j$, as a square matrix,

$$\mathbf{E}_0 = \begin{pmatrix} E_0(z_1,1) & E_0(z_1,2) & \cdots & E_0(z_1,j) \\ E_0(z_2,1) & E_0(z_2,2) & \cdots & E_0(z_2,j) \\ \vdots & \vdots & \ddots & \vdots \\ E_0(z_j,1) & E_0(z_j,2) & \cdots & E_0(z_j,j) \end{pmatrix},$$

and $E_1(z_k,j)$ as a column vector

$$\mathbf{E}_1 = \begin{pmatrix} E_1(z_1,j) \\ E_1(z_2,j) \\ \vdots \\ E_1(z_j,j) \end{pmatrix},$$

we have

$$\mathbf{E}_0\mathbf{B} = \frac{d\mathbf{E}_1}{dz}.$$

The solution is of course

$$\mathbf{B} = \mathbf{E}_0^{-1}\frac{d\mathbf{E}_1}{dz}.$$

One should note that the columns of $\mathbf{E}_0$ are just the scalar irradiance profiles for each waveband. These are similar in that they all display essentially exponential decay. This means that the matrix may be nearly singular (i.e., ill-conditioned) in which case one may not be able to find an accurate inverse.

It is important to understand the source of ill-conditioned situations and how to deal with them. Consider a medium for which $E_0(z,k_1) = E_0(z,k_2)$, i.e., two wavelength intervals have the same $E_0(z)$. Clearly, $\mathbf{E}_0$ is singular; however, from Gershun's law we see that it is impossible to separate the individual contributions from $\Delta\lambda_{k_1}$ and $\Delta\lambda_{k_2}$ to J_{in}. One can only determine the contribution of $\Delta\lambda_{k_1} \cup \Delta\lambda_{k_2}$, i.e., $b_{in}(k_1 \to j)\Delta\lambda_{k_1} + b_{in}(k_2 \to j)\Delta\lambda_{k_2}$. Thus, $\Delta\lambda_{k_1}$ and $\Delta\lambda_{k_2}$ must be considered together as a single (disjoint) spectral interval, removing the singularity from $\mathbf{E}_0$.

4.2. Estimation of b_b

There is no way to use Gershun's law to estimate the backscattering coefficient. For this we need to solve the inverse problem completely. However, given $\mathbf{E}_1$ and $\mathbf{E}_0$, this is possible assuming that the medium is homogeneous. From the Gershun equations and the procedure described above, we already have $a(\lambda_j)$ and $b_{in}(\lambda_i \to \lambda_j)$ for all $\lambda_i < \lambda_j$. To determine $b_b(\lambda_j)$, we could start with an initial estimate $b_b(\lambda_j) = 3R(0,\lambda_j)/a(\lambda_j)$. This should be a good initial estimate for situations where the fluorescence is weak at the surface. Next, choose either $P(\Theta)$ or $P_p(\Theta)$ and solve the RTE *at* λ_j using the inelastic source functions determined from $b_{in}(\lambda_i \to \lambda_j)$. This gives estimated profiles of $E_1(z,\lambda_1)$ and $E_0(z,\lambda_1)$ that can be compared with the measured data. Based on the results of the comparison, an improved estimate of $b_b(\lambda_j)$ can be made as in Gordon & Boynton (1997). It is important to note that in this case ($\mathbf{E}_1$ and $\mathbf{E}_0$ measured in a homogeneous medium) the estimate of $b_b(\lambda_j)$ requires solving the RTE *only* at λ_j. This procedure is identical to the inversion in the presence of Raman scattering (Boynton & Gordon 2000), i.e., the inelastic cross sections are already known at the start of the b_b inversion process.

4.3. Inversion when only $\mathbf{E}_1$ is measured

The immediate question now is, what if only $E_u(z,\lambda)$ and $E_d(z,\lambda)$ are measured as in the Gordon and Boynton algorithms? In this case, we write $\mathbf{E}_0$ in terms of $\mathbf{E}_1$, i.e.,

$$\mathbf{E}_0 = \begin{pmatrix} \overline{\mu}(z_1,1)^{-1}E_1(z_1,1) & \overline{\mu}(z_1,2)^{-1}E_1(z_1,2) & \cdots & \overline{\mu}(z_1,j)^{-1}E_1(z_1,j) \\ \overline{\mu}(z_2,1)^{-1}E_1(z_2,1) & \overline{\mu}(z_2,2)^{-1}E_1(z_2,2) & \cdots & \overline{\mu}(z_2,j)^{-1}E_1(z_2,j) \\ \vdots & \vdots & \ddots & \vdots \\ \overline{\mu}(z_j,1)^{-1}E_1(z_j,1) & \overline{\mu}(z_j,2)^{-1}E_1(z_j,2) & \cdots & \overline{\mu}(z_j,j)^{-1}E_1(z_j,j) \end{pmatrix}.$$

Now, assume that we have by some means completed the inversion for wave bands up through $j-1$ and are looking for the solution in the j^{th} waveband. The $j-1$ inversions provided estimates of $\overline{\mu}(z,\lambda_i)$ with $i = 1$ to $j-1$. Thus, in the above equation, only $\overline{\mu}(z,\lambda_j)$ is unknown. As in

Boynton & Gordon (2000), we consider an iterative set of solutions to the RTE in which after the k^{th} iteration, the $\overline{\mu}$'s are labeled $\overline{\mu}^{(k)}$. (Note: the $\overline{\mu}^{(k)}$ required here is for the *entire* light field — elastic *plus* inelastic.) Then we estimate $\mathbf{E}_0$ as

$$\mathbf{E}_0^{(k)}=\begin{pmatrix} \overline{\mu}(z_1,1)^{-1}E_1(z_1,1) & \overline{\mu}(z_1,2)^{-1}E_1(z_1,2) & \cdots & \overline{\mu}^{(k)}(z_1,j)^{-1}E_1(z_1,j) \\ \overline{\mu}(z_2,1)^{-1}E_1(z_2,1) & \overline{\mu}(z_2,2)^{-1}E_1(z_2,2) & \cdots & \overline{\mu}^{(k)}(z_2,j)^{-1}E_1(z_2,j) \\ \vdots & \vdots & \ddots & \vdots \\ \overline{\mu}(z_j,1)^{-1}E_1(z_j,1) & \overline{\mu}(z_j,2)^{-1}E_1(z_j,2) & \cdots & \overline{\mu}^{(k)}(z_j,j)^{-1}E_1(z_j,j) \end{pmatrix},$$

and use this to obtain a new estimate ($\mathbf{B}^{(k)}$) of the absorption coefficient at j and the inelastic scattering coefficients from i into j,

$$\mathbf{B}^{(k)} = [\mathbf{E}_0^{(k)}]^{-1}\frac{d\mathbf{E}_1}{dz}.$$

This allows us to obtain a new estimate of $b_b(\lambda_j)$ in the manner described above. This iterative procedure continues until the measured and computed $E_u(z,\lambda)$ and $E_d(z,\lambda)$ agree. Schematically,

$$\cdots J_{in} + \text{IOPs}^{(n)} \rightarrow \text{ILF} \rightarrow \text{ELF} \rightarrow \text{IOPs}^{(n+1)} \rightarrow J_{in} + \text{IOPs}^{(n+1)} \rightarrow \text{ILF} \cdots,$$

where ILF refers to the inelastically-induced light field, and the IOPs include $b_{in}(\lambda_i,\lambda_j)$. Note that the only difference between the procedure when only $\mathbf{E}_1$ is provided, compared to the procedure when both $\mathbf{E}_1$ and $\mathbf{E}_0$ are provided, is that in the former inelastic scattering-absorption vector $\mathbf{B}$ (and thus the inelastic source functions) is reevaluated at each iteration, while in the latter these quantities are computed only once. The solution for $i < j$ must have been carried out first; however, that can be effected in the same manner as the solution presented above for $i = j$. Thus, to effect a complete solution, one sequentially solves the inverse problem within each wave band from $i = 1$ to $i = N$. The result is $a(j)$, $b_b(j)$, and $b_{in}(i \rightarrow j)$ (with $i < j$), $j = 1$, to N.

We note also that, in a homogeneous medium such as we have been discussing, it is straightforward to include the Raman scattering as well as fluorescence into the procedure. All that is required is that the inverse problem has been solved at the Raman excitation wavelength, which is already a necessity in the fluorescence problem. That solution would then be used to provide an additional source function (J_r) along with J_f in the RTE at λ_j. Thus, in principle a complete solution to the inverse problem in the presence of inelastic processes can be effected in a *homogeneous* water body.

One obvious avenue for including vertical structure in the analysis is to approximate the vertical structure by a set of homogeneous layers. The above analysis could then be carried out separately for each layer. A possible

difficulty is that it may not be clear how to assign the position of layers based on the irradiance profiles alone, because the principal absorber may not be responsible for, or related to, the fluorescence. Another difficulty is that irradiance measurements must be carried out at a sufficient number of depths in each layer to provide the necessary number of equations to carry out the inversion.

5. Discussion

It is important to keep in mind a few relevant facts. First, in the absence of inelastic processes, given the irradiance quartet, it is a relatively simple matter to estimate a (Gershun's law). However, as E_0 is only rarely measured, a can be determined only if $\overline{\mu}$ can be estimated. From the analysis provided by Morel & Prieur (1975b) the range of variation in $1/\overline{\mu}_d$ (1.069-1.265) is only $\sim 20\%$. This means that estimating $1/\overline{\mu}_d$ by ~ 1.16 will result in $\sim \pm 10\%$ uncertainty in the retrieval of a. Therefore, given E_1, estimation of a within $\pm 10\%$ is not difficult even in the presence of vertical stratification. The addition of the difficult E_0 measurement to the measurement suite would only reduce the uncertainty below 10%. Second, given a, estimation of b_b from equations like eqs. (11) and (12) is straightforward; however, errors due to stratification could be important. Putting this in perspective, to be more useful than the crudest estimates, algorithms must retrieve a with an uncertainty significantly less that 10% and be able to address stratification. Third, E_d data are extremely noisy near the surface due to wave-induced focusing of the solar beam (Dera & Olszewski 1967, Dera & Gordon 1968, Stramski 1986, Stramski & Dera 1988), which Zaneveld et al. (2001) show can be generated even in 'calm' seas. This means that accurate E_d data can be obtained only below some depth, e.g., $\sim 10 - 20$ m, that is dependent on the sea state. Fourth, thin ($\sim$ few cm) persistent layers are sometimes observed in the IOPs (e.g., see Cowles et al. (1998) and other papers in the same issue of *Oceanography*). The presence of such layers could be easily missed or be considered to be noise in the AOP measurements. Thus, the first two observations suggest that inversion is not too difficult, while the last two suggest that the environment itself presents significant challenges to inversion. The relevant question is, how do the various algorithms described earlier perform considering these observations?

As we have described, AOP inversion algorithms are based on either explicit or implicit schemes that fit the observed irradiances to solutions of the RTE, either carried out earlier (explicit) or developed during the inversion process using trial IOPs (implicit). In either type of scheme, one aspect of AOP inversion that should be clear is that the only quantities

Table 1. Comparison of several inverse methods in oceanic optics

	Gordon (1991)	Kirk (1994)	Gordon & Boynton (1998, 1999, 2000)	Leathers et al. (1999)	Loisel & Stramski (2000)
Input Data	$R(0,-)$ and $\langle K_d \rangle$	$R(0,-)$ and $\langle K_d \rangle$	$L_u(z)$ & $E_d(z)$ or $E_u(z)$ & $E_d(z)$	$L_u(z)$ & $E_d(z)$ or $E_u(z)$ & $E_d(z)$	$R(0,-)$ and $\langle K_d \rangle$
Assumptions					
General[1]	1-d Scalar RT	1-d Scalar RT	1-d Scalar RT	1-d Scalar RT	1-d Scalar RT
Atmosphere[2]	Clear sky (coupled) or overcast	None	Clear sky (coupled) or overcast	NA	Clear sky (Hydrolight) or coupled
Water[3]	Homogeneous	Homogeneous $P(\Theta)$	None $P(\Theta)$ or $P_p(\Theta)$	Asymptotic $P(\Theta)$	Homogeneous $P_p(\Theta)$
Surface[4]	Smooth and rough (C & M)	Smooth	Smooth	Smooth	Smooth and rough (C & M)
Inelastic Processes	None	None	Raman through measurement at λ_e	None	Raman through a bio-optical model
Bottom Reflection	No	No	Yes	No (but can be included)	No
Recovered Quantities	Mean a and b_b	Mean a and b_b	$a(z)$ and $b_b(z)$	$a(z)$ and $b_b(z)$	Mean a and b_b
Retrieves Vertical Structure	No	No	Yes	Yes	No

[1]'1-d Scalar RT' means that the IOPs are assumed to be independent of horizontal position (they depend only on depth) and the polarization of the radiation is ignored. [2]'Coupled' refers to a coupled ocean-atmosphere model. In contrast, 'Hydrolight' means that the standard Hydrolight atmospheric input is assumed. Leathers et al. (1999) use asymptotic theory, so the atmosphere and sea surface do not enter into the computation ('NA' means not applicable). [3]'Homogeneous' means that the IOPs are independent of depth. '$P(\Theta)$' means that a phase function is assumed for the medium, etc. [4]'C & M' means that the surface roughness follows that developed in Cox & Munk (1954).

that one can expect to accurately retrieve at a given λ are $a(\lambda)$ and $b_b(\lambda)$, and $b_{in}(\lambda' \rightarrow \lambda)$. Any inversion algorithm that purports to retrieve $b(\lambda)$ or $c(\lambda)$ solely from irradiance measurements must have made the retrieval based on assuming a phase function for the medium (or at least for the particle component of the medium), and the retrieved values will depend directly (and strongly) on the assumed phase function. In contrast, in most inversion schemes the retrieval of b_b is only weakly dependent on the assumed phase function. Table 1 compares several of the algorithms described in the text, providing their assumptions regarding the atmosphere, the water surface, vertical structure, inelastic processes, etc. I have excluded from Table 1 the algorithm of Tao et al. (1994), as it requires the seldom-measured irradiance quartet, and the algorithm of Stramska et al. (2000) because it requires *both* E_u and L_u, which are rarely measured simultaneously. All of the algorithms in Table 1 (as well as the excluded Tao et al. (1994) and Stramska et al. (2000)) perform well within the limitations set by the assumptions used in their development (e.g., asymptotic theory, homogeneous water bodies, etc.).

In comparing the various inversion algorithms in Table 1, it is useful to divide the algorithms into two classes: a structure-resolving class consisting of those algorithms that either can, or purport to be able to, perform well in retrieving vertical structure in the absorption and scattering and a structure-averaging class consisting of those that attempt to retrieve only average quantities over a defined surface layer from the surface to some prescribed depth. All of the structure-averaging algorithms are essentially the same, differing only in the details of developing the empirical relationships, and in the scope of the radiative transfer computations used in deriving them. For example, Gordon (1991) uses $\tilde{b}_b$ to characterize the influence of the phase function on K_d, Kirk (1994b) uses μ_s, and Loisel & Stramski (2000) use η. Clearly, the Loisel & Stramski (2000) algorithm is preferred over the other two because it is based on a much larger simulation set and because it includes Raman scattering. The structure-resolving algorithms differ significantly even in their basic assumptions.

As mentioned above, given accurate irradiance measurements, all of the algorithms perform reasonably well within the range of validity of the assumptions used in the derivation. However, given that surface waves prevent accurate measurements, does this limit the validity of any algorithm? The answer is to a certain extent no. Several of the algorithms use a mean K_d (or K_1) from the surface to some depth z_d, along with the reflectance just beneath the surface $R(0)$. As long as z_d is below the region of significant wave-induced irradiance fluctuations, and the surface E_d is measured *above* the surface to avoid fluctuations (and then propagated

through the surface to form the appropriate mean K_d and $R(0)$), such algorithms should perform well as long as there is little vertical structure between the surface and z_d. However, in the presence of highly absorbing thin layers between the surface and z_d these algorithms will overestimate K_d over most of the depth range and, as such, overestimate a and b_b. Examples of the effect of vertical structure on the Loisel & Stramski (2000) algorithm are provided in Loisel et al. (2001). They show that large errors in both a (10-15%) and b_b (as much as 40%) are sometimes possible with realistic profiles of IOPs in the surface layer. Concerning the structure-resolving algorithms, the Gordon and Boynton algorithms will work in the same manner as the structure-averaging algorithms, because they implicitly assume the absence of vertical structure between the surface and the first depth at which E_d data become useful. The Leathers et al. (1999) algorithm, based on asymptotic theory, will yield a realistic a because $\overline{\mu}$ is never too far from the asymptotic value, but could display large error in b_b because of the possibility of significant differences between $R(0)$ and R_∞. Thus, both classes of algorithms should produce realistic retrievals as long as the water is clear enough that their working depth is below the level significantly influenced by fluctuations, and as long as there is little vertical structure between that depth and the surface; however, the Leathers et al. (1999) will likely yield poor estimates for b_b.

Considering the structure-resolving algorithms in the region free of fluctuations, the Gordon and Boynton algorithms must be superior as they represent essentially an exact solution to the RTE and can adequately deal with vertical structure. Gordon & Boynton (1998) show that the principal source of error in $a(z)$ is the error in the determination of $K_1(z)$ from the experimental data, i.e., if a thin absorbing layer were not adequately sampled in E_d and E_u significant error would result, so the limitation of their algorithm is adequate irradiance sampling. Similar comments apply to the estimate of a using asymptotic methods, as K_1 must be computed in these as well. In cases where there is little variation in ω_0 with depth, there should be little difference between the exact solution and one based on asymptotic theory, particularly if the McCormick (1996) method (eq. (17)) is used to estimate the asymptotic values. One must be aware, however, that as the depth increases, the inelastic processes can become relatively more important, and thus must be included in order to retrieve realistic IOPs. Boynton & Gordon (2000) explicitly includes Raman scattering; however, it requires measurements of the AOPs at the Raman excitation wavelength as well. Fluorescence can be included as well, as described in Section 4, but requires spectral measurements (and inversion) of the AOPs for all wavelengths less than λ.

Some of the modern inversion algorithms that I have reviewed have been applied to AOP data for which the IOPs were directly measured (Leathers et al. 1999, Stramska et al. 2000, Loisel et al. 2001). To assess the agreement between the inversion-derived (IOP_{inv}) and the directly measured (IOP_{meas}) the authors performed the following regression:

$$IOP_{inv} = S \times IOP_{meas} + I,$$

where the IOPs were a (Leathers et al. 1999, Stramska et al. 2000), $a - a_w$ (Loisel et al. 2001), b_b (Stramska et al. 2000), and $b_b - b_{bw}$ (Loisel et al. 2001). The values of S and I along with the r^2 for the regressions are provided in Table 2. The data range for each of the studies was $0.02 \leq a \leq 0.16$ m^{-1} for Stramska et al. (2000), $0.1 \leq a \leq 0.7$ m^{-1} for Leathers et al. (1999), and $0.002 \leq a - a_w \leq 0.8$ m^{-1} for Loisel et al. (2001). The results generally show good agreement between the measured and retrieved IOPs. Interestingly, of the three, the model I consider to be the best (Loisel & Stramski 2000) shows the largest deviation in S from unity. The general nearness of S to unity suggests that the sampling scale mismatch between inverted and measured IOPs may not be as serious as it could be. However, the small slope ($S \approx 0.9$) observed by Loisel et al. (2001) is confusing, because one would expect $a - a_w$ measured at large scale to be greater than that measured at the smaller scale ($S > 1$) because the small scale measurement will leave some large particles unsampled. Similar comments apply to $b_b - b_{bw}$.

Table 2. Comparison between inverse and measured a and b_b (I is in m^{-1})

IOP		Leathers et al. (1999)	Stramska et al. (2000)	Loisel et al. (2001)
a	S	1.03	0.99	0.903
or	I	0.007	–0.0046	0.008
$a - a_w$	r^2	0.98	0.94	0.98
b_b	S	–	0.97	0.87
or	I	–	0.0005	0.00015
$b_b - b_{bw}$	r^2	–	0.86	0.87

6. Concluding remarks

We have reviewed several methods for inverting natural in-water light field measurements (providing AOPs) to yield the IOPs $a(z, \lambda)$, $b_b(z, \lambda)$ and $b_{in}(z, \lambda)$. The review has been limited by omitting two-flow estimates as well as those employing artificial internal sources. In addition, methods

for retrieving bio-optical parameters from above the sea surface using reflectance models (Bricaud & Morel 1987, Gordon et al. 1988, Lee et al. 1996, Garver & Siegel 1997), although extremely important in remote sensing, have been omitted as well.

The history shows a systematic progression in the development of explicit algorithms culminating with Loisel & Stramski (2000). Truly implicit algorithms are rather new, the first being that of Gordon & Boynton (1997). The Loisel and Stramski algorithm seeks to estimate the mean $a(\lambda)$ and $b_b(\lambda)$ over a depth $1/K_d(\lambda)$ from measurement of $R(0)$ and $\langle K_d \rangle_1$ at λ, while the Gordon and Boynton algorithms (Gordon & Boynton 1998, Boynton & Gordon 2000, 2002) seek vertical profiles for $a(\lambda)$ and $b_b(\lambda)$, given irradiance profiles, and therefore is significantly more computationally intense. The interference of Raman scattering is handled differently in the two algorithms: Loisel and Stramski correct the irradiances for Raman scattering by estimating its contribution using a bio-optical model that relates the IOPs to the chlorophyll concentration; Boynton & Gordon (2000) require AOP measurements in the Raman excitation band to estimate the Raman correction. In the absence of significant wave-induced light field fluctuations, both algorithms achieve their goals well. Their performance is similarly degraded in the fluctuation zone. Fluorescence can be added to the Gordon and Boynton algorithm in a straightforward manner as described in Section 4; however, as the fluorescence-induced component of the light field is usually weak (except possibly at great depth), it remains to be seen whether such a formulation will be useful in the presence of environmental and sensor noise.

It is now possible to make $a(z)$ and $c(z)$ measurements simultaneously with the AOPs (Zaneveld & Bartz 1984, Zaneveld et al. 1990, 1992), and direct a measurements show good agreement with AOP-a retrievals. This suggests that the scale mismatch between the AOP retrievals and IOP measurements may not be as serious as one could imagine. Thus, one must ask what, if any, additional information can result from inversion, given measurement of $c(z)$, at least at a single wavelength. The answer is that, given $c(z, \lambda)$, it would be possible to compute $b(z, \lambda)$, from which $\tilde{b}_b(z, \lambda)$ could be determined after retrieving b_b. This would provide some limited information on the scattering phase function. In addition, direct measurement of $a(z, \lambda)$ would provide an indication of the strength of the inelastic contribution (particularly fluorescence) to the light field at λ using Gershun's law. Also, such measurements (a and/or c) even at a single wavelength would provide a direct measure of the stratification of the IOPs, and this would be helpful in effecting an AOP inversion in the wave-induced fluctuation zone.

In this writer's opinion, the greatest shortcoming of the inverse methods described here is that only the total a, b_b, and b_{in} can be estimated. No information is obtained concerning the decomposition of any of the IOPs into their component parts.

References

Aas E., 1987, *Two stream irradiance model for deep waters*, Appl. Opt., 26, 2095–2101.

Austin R. W., Petzold T. J., 1981, *Remote sensing of the diffuse attenuation coefficient of sea water using the Coastal Zone Color Scanner*, [in:] *Oceanography from space*, J. R. F. Gower (ed.), Plenum Press, New York, 239–256.

Beardsley G. F., Zaneveld J. R. V., 1969, *Theoretical dependence of the near-asymptotic apparent optical properties on the inherent optical properties of sea water*, J. Opt. Soc. Am., 59, 373–377.

Boynton G. C., Gordon H. R., 2000, *Irradiance inversion algorithm for estimating the absorption and backscattering coefficients of natural waters: Raman scattering effects*, Appl. Opt., 39, 3012–3022.

Boynton G. C., Gordon H. R., 2002, *An irradiance inversion algorithm for absorption and backscattering profiles in natural waters: improvement for very clear waters*, Appl. Opt., 41, (in press).

Bricaud A., Morel A., 1987, *Atmospheric corrections and interpretation of marine radiances in CZCS imagery: use of a reflectance model*, Oceanol. Acta, 7, 33–50.

Cattrall C., 2001, *Retrieval of the columnar aerosol phase function and single-scattering albedo from sky radiance over the ocean: measurement of African dust*, Ph. D. dissertation, University of South Florida, 75 pp.

Cowles T. J., Desiderio R. A., Carr M.-E., 1998, *Small-scale planktonic structure: persistence and trophic consequences*, Oceanography, 11, 4–9.

Cox C., Munk W., 1954, *Measurements of the roughness of the sea surface from photographs of the sun's glitter*, J. Opt. Soc. Am., 44, 838–850.

Dera J., Gordon H. R., 1968, *Light field fluctuations in the photic zone*, Limnol. Oceanogr., 13, 697–699.

Dera J., Olszewski J., 1967, *On the natural irradiance fluctuations affecting photosynthesis in the sea*, Acta Geophys. Polon., 15, 351–364.

Garver S. A., Siegel D. A., 1997, *Inherent optical property inversion of ocean color spectra and its biogeochemical interpretation: 1 time series from the Sargasso Sea*, J. Geophys. Res., 102C, 18607–18625.

Ge Y., Gordon H. R., Voss K. J., 1993, *Simulations of inelastic scattering contributions to the irradiance fields in the ocean: variation in Fraunhofer line depths*, Appl. Opt., 32, 4028–4036.

Gershun A., *The light field*, 1939, J. Math. Phys., 18, 51–151.

Gordon H. R., 1973, *Simple calculation of the diffuse reflectance of the ocean*, Appl. Opt., 12, 2803–2804.

Gordon H. R., 1979, *The diffuse reflectance of the ocean: the theory of its augmentation by chlorophyll a fluorescence at 685 nm*, Appl. Opt., 18, 1161–1166.

Gordon H. R., 1980, *Irradiance attenuation coefficient in a stratified ocean: a local property of the medium*, Appl. Opt., 19, 2092–2094.

Gordon H. R., 1989a, *Dependence of the diffuse reflectance of natural waters on the Sun angle*, Limnol. Oceanogr., 34, 1484–1489.

Gordon H. R., 1989b, *Can the Lambert-Beer law be applied to the diffuse attenuation coefficient of ocean water?*, Limnol. Oceanogr., 34, 1389–1409.

Gordon H. R., 1991, *Absorption and scattering estimates from irradiance measurements: Monte Carlo simulations*, Limnol. Oceanogr., 36, 769–777.

Gordon H. R., 1993, *The sensitivity of radiative transfer to small-angle scattering in the ocean: a quantitative assessment*, Appl. Opt., 32, 7505–7511.

Gordon H. R., 1999, *Contribution of Raman scattering to water-leaving radiance: a reexamination*, Appl. Opt., 38, 3166–3174.

Gordon H. R., Boynton G. C., 1997, *A radiance – irradiance inversion algorithm for estimating the absorption and backscattering coefficients of natural waters: homogeneous waters*, Appl. Opt., 36, 2636–2641.

Gordon H. R., Boynton G. C., 1998, *A radiance – irradiance inversion algorithm for estimating the absorption and backscattering coefficients of natural waters: vertically stratified water bodies*, Appl. Opt., 37, 3886–3896.

Gordon H. R., Brown O. B., 1973, *Irradiance reflectivity of a flat ocean as a function of its optical properties*, Appl. Opt., 12, 1549–1551.

Gordon H. R., Brown O. B., Evans R. H., Brown J. W., Smith R. C., Baker K. S., Clark D. K., 1988, *A semi-analytic radiance model of ocean color*, J. Geophys. Res., 93D, 10909–10924.

Gordon H. R., Brown O. B., Jacobs M. M., 1975, *Computed relationships between the inherent and apparent optical properties of a flat homogeneous ocean*, Appl. Opt., 14, 417–427.

Gordon H. R., Clark D. K., 1980, *Remote sensing optical properties of a stratified ocean: an improved interpretation*, Appl. Opt., 19, 3428–3430.

Gordon H. R., Ding K., Gong W., 1993, *Radiative transfer in the ocean: computations relating to the asymptotic and near-asymptotic daylight field*, Appl. Opt., 32, 1606–1619.

Gordon H. R., Morel A. Y., 1983, *Remote assessment of ocean color for interpretation of satellite visible imagery: a review*, Springer-Verlag, New York, 114 pp.

Gordon H. R., Xu X., 1996, *Marine asymptotic daylight field: effects of inelastic processes*, Appl. Opt., 35, 4194–4205.

Gordon H. R., Zhang T., 1995, *Columnar aerosol properties over oceans by combining surface and aircraft measurements: simulations*, Appl. Opt., 34, 5552–5555.

Hawes S. K., Carder K. L., Harvey G. R., 1992, *Quantum fluorescence efficiencies of fulvic and humic acids: effects on ocean color and fluormetric determination*, Society of Photo-Optical Instrumentation Engineers, Ocean Optics XI, 1750, 212–223.

Højerslev N. K., 1973, *Inherent and apparent optical properties of the western Mediterranean and the Hardangerfjord*, Københavns Universitet, Inst. Fys. Oceanogr., Copenhagen, Report No. 21, 1–26.

Højerslev N. K., 1975, *A spectral light absorption meter for measurements in the sea*, Limnol. Oceanogr., 20, 1025–1034.

Højerslev N. K., 1996, *Optical properties of sea water*, [in:] *Landolt-Bornstein, numerical data and functional relationships in science and technology, New Series V/3a, Group V: Geophysics and Space Research*, J. Sündermann (ed.), Springer-Verlag, Berlin, 383–462.

Højerslev N. K., Zaneveld J. R. V., 1977, *A theoretical proof of the existence of the submarine asymptotic daylight field*, Københavns Universitet, Inst. Fys. Oceanogr., Copenhagen, Report No. 34, 16 pp.

Holl L. J., McCormick N. J., 1995, *Ocean optical-property estimation with the Zaneveld-Wells algorithm*, Appl. Opt., 34, 5433–5441.

Hu C., Voss K. J., 1997, *In situ measurements of Raman scattering in clear ocean water*, Appl. Opt., 36, 6962–6967.

Kattawar G. W., 1975, *A three-parameter analytic phase function for multiple scattering calculations*, J. Quant. Spectrosc. Radiat. Transfer, 15, 839–849.

Kattawar G. W., Xu X., 1992, *Filling-in of Fraunhofer lines in the ocean by Raman scattering*, Appl. Opt., 31, 6491–6500.

Kirk J. T. O., 1981a, *Estimation of the scattering coefficient of natural waters using underwater irradiance measurements*, Aust. J. Mar. Freshw. Res., 32, 533–539.

Kirk J. T. O., 1981b, *Monte Carlo study of the nature of the underwater light field in, and the relationships between optical properties of, turbid yellow waters*, Aust. J. Mar. Freshw. Res., 32, 517–532.

Kirk J. T. O., 1983, *Light and photosynthesis in aquatic ecosystems*, Cambridge University Press, Cambridge, 401 pp.

Kirk J. T. O., 1984, *Dependence of relationship between inherent and apparent optical properties of water on solar altitude*, Limnol. Oceanogr., 29, 350–356.

Kirk J. T. O., 1991, *Volume scattering function, average cosines, and the underwater light field*, Limnol. Oceanogr., 36, 455–467.

Kirk J. T. O., 1994a, *The relationship between inherent and apparent optical properties of surface waters and its dependence on the shape of the volume scattering function*, [in:] *Ocean optics*, R. W. Spinrad, K. L. Carder & M. J. Perry (eds.), Oxford University Press, New York, 40–58.

Kirk J. T. O., 1994b, *Estimation of the absorption and scattering coefficients of natural waters by the use of underwater irradiance measurements*, Appl. Opt., 33, 3276–3278.

Kishino M., Ishizaka J., Satoh H., Usaka K., Saitoh S., Miyio T., Kawasaki K., 1996, *Optical characteristics of sea water in the north Pacific Ocean*, Society of Photo-Optical Instrumentation Engineers, Ocean Optics XIII, 2963, 173–178.

Leathers R. A., McCormick N. J., 1997, *Ocean inherent optical property estimation from irradiances*, Appl. Opt., 36, 8685–8698.

Leathers R. A., Roesler C. S., McCormick N. J., 1999, *Ocean inherent property determination from in-water light field measurements*, Appl. Opt., 38, 5096–5103.

Lee Z. P., Carder K. L., Hawes S. K., Steward R. G., Peacock T. G., Davis C. O., 1996, *Method to derive ocean absorption coefficients from remote sensing reflectance*, Appl. Opt., 35, 453–462.

Loisel H., Stramski D., 2000, *Estimation of inherent optical properties of natural waters from the irradiance attenuation coefficient and reflectance in the presence of Raman scattering*, Appl. Opt., 39, 3001–3011.

Loisel H., Stramski D., Mitchell B. G., Fell F., Fournier-Sicre V., Lemasle B., Babin M., 2001, *Comparison of the ocean inherent optical properties obtained from measurements and inverse modeling*, Appl. Opt., 40, 2384–2397.

Maffione R. A., Voss K. J., Honey R. C., 1993, *Measurement of the spectral absorption coefficient in the ocean with an isotropic point source*, Appl. Opt., 32, 3273–3279.

Marshall B. R., Smith R. C., 1990, *Raman scattering and in-water ocean optical properties*, Appl. Opt., 29, 71–84.

McCormick N. J., 1992, *Asymptotic optical attenuation*, Limnol. Oceanogr., 37, 1507–1578.

McCormick N. J., 1995, *Mathematical models for the mean cosine of irradiance and the diffuse attenuation coefficient*, Limnol. Oceanogr., 40, 1013–1018.

McCormick N. J., 1996, *Analytical transport theory applications in optical oceanography*, Ann. Nucl. Energy, 23, 381–395.

Mobley C. D., 1994, *Light and water; radiative transfer in natural waters*, Academic Press, New York, 592 pp.

Mobley C. D., Gentili B., Gordon H. R., Jin Z., Kattawar G. W., Morel A., Reinersman P., Stamnes K., Stavn R. H., 1993, *Comparison of numerical models for computing underwater light fields*, Appl. Opt., 32, 7484–7504.

Morel A., 1974, *Optical properties of pure water and pure sea water*, [in:] *Optical aspects of oceanography*, N. G. Jerlov & E. S. Nielsen (eds.), Academic Press, New York, NY, 1–24.

Morel A., 1988, *Optical modeling of the upper ocean in relation to its biogenous matter content (Case I Waters)*, J. Geophys. Res., 93C, 10,749–10,768.

Morel A., Gentili B., 1991, *Diffuse reflectance of oceanic waters: its dependence on Sun angle as influenced by the molecular scattering contribution*, Appl. Opt., 30, 4427–4438.

Morel A., Loisel H., 1998, *Apparent optical properties of oceanic waters: dependence on the molecular scattering contribution*, Appl. Opt., 37, 4765–4776.

Morel A., Prieur L., 1975a, *Relations théoriques entre le facteur de réflexion diffuse de l'eau mer, à diverses profondeurs, et les caractéristiques optiques*, UGGI, XVI Assembly, Grenoble.

Morel A., Prieur L., 1975b, *Analyse spectrale des coefficients d'attenuation diffuse, de retrodiffusion pour diverses regions marines*, Rapport No. 17, Centre Rech. Océanogr. de Villefranche-sur-Mer, Final Report Contract No. M0–A01–78–00–4092, Juillet 1975.

Mueller J. L., Trees C., 1997, *SeaWiFS Technical Report Series: Volume 41, Revised SeaWiFS prelaunch algorithm for diffuse attenuation coefficient K(490)*, NASA, Greenbelt, MD, Technical Memorandum 104566.

Pegau W. S., Cleveland J. S., Doss W., Kennedy C. D., Maffione R. A., Mueller J. L., Stone R., Trees C. C., Weidemann A. D., Wells W. H., Zaneveld J. R. V., 1995, *A comparison of methods for the measurement of the absorption coeffcicent in natural waters*, J. Geophys. Res., 100C, 13,201–13,220.

Petzold T. J., 1972, *Volume scattering functions for selected natural waters*, Scripps Inst. Oceanogr., Visibility Laboratory, San Diego, CA. 92152, SIO Ref. 72–78.

Preisendorfer R. W., 1959, *On the existence of characteristic diffuse light in natural sea waters*, J. Mar. Res., 18, 1–9.

Preisendorfer R. W., 1961, *Application of radiative transfer theory to light measurements in the sea*, Union Géodésique et Géophysique Internationale, 10, 11–30.

Preisendorfer R. W., Mobley C. D., 1984, *Direct and inverse irradiance models in hydrologic optics*, Limnol. Oceanogr., 29, 903–929.

Preisendorfer R. W., Mobley C. D., 1988, *Theory of fluorescent irradiance fields in natural waters*, J. Geophys. Res., 93D, 10,831–10,855.

Press W. H., Flannery B. P., Teukolsky S. A., Vetterling T., 1992, *Numerical recipes in FORTRAN*, Cambridge University Press, Cambridge, 963 pp.

Prieur L., Morel A., 1971, *Étude théorique du régime asymptotique: relations entre charactéristiques optiques et coefficient d'extinction relatif à la pénétration de la lumière du jour*, Cahiers Océanogr., 23, 35–48.

Prieur L., Sathyendranath S., 1981, *An optical classification of coastal and oceanic waters based on the specific absorption curves of phytoplankton pigments, dissolved organic matter, and other particulate materials*, Limnol. Oceanogr., 26, 671–689.

Stavn R. H., 1990, *Raman scattering effects at the shorter visible wavelengths in clear ocean water*, Society of Photo-Optical Instrumentation Engineers, Ocean Optics X, 1302, 94–100.

Stavn R. H., Weidemann A., D., 1988, *Optical modeling of clear ocean light fields: Raman scattering effects*, Appl. Opt., 27, 4002–4011.

Stavn R. H., Weidemann A. D., 1989, *Shape factors, two-flow models, and the problem of irradiance inversion in estimating optical parameters*, Limnol. Oceanogr., 34, 1426–1441.

Stramska M., Stramski D., Mitchell B. G., Mobley C. D., 2000, *Estimation of the absorption and backscattering coefficients from in-water radiometric measurements*, Limnol. Oceanogr., 45, 628–641.

Stramski D., 1986, *Fluctuation of solar irradiance induced by surface waves in the Baltic*, Bull. Polish. Acad. Sci. Earth Sci., 34, 333–344.

Stramski D., Dera J., 1988, *On the mechanism for producing flashing light under a wind-disturbed water surface*, Oceanologia, 25, 5–21.

Sugihara S., Kishino M., Okami N., 1984, *Contribution of Raman scattering to upward irradiance in the sea*, J. Oceanogr. Soc. Japan, 40, 397–404.

Tao Z., McCormick N. J., Sanchez R., 1994, *Ocean source and optical property estimation from explicit and implicit algorithms*, Appl. Opt., 33, 3265–3275.

Tyler J. E., 1960, *Radiance distribution as a function of depth in an underwater environment*, Bull. Scripps Inst. Oceanogr., 7, 363–411.

Tyler J. E., Preisendorfer R. W., 1962, *Transmission of energy within the sea: light*, [in:] *The sea*, M. N. Hill (ed.), Interscience, New York, 1962. 397–451.

Voss K. J., 1989, *Use of the radiance distribution to measure the optical absorption coefficient in the ocean*, Limnol. Oceanogr., 34, 1614–1622.

Waters K. J., 1995, *Effects of Raman scattering on water-leaving radiance*, J. Geophys. Res., 100C, 13151–13161.

Weidemann A. D., Stavn R. H., Zaneveld J. R. V., Wilcox M. R., 1995, *Error in predicting hydrosol backscattering from remotely sensed reflectance*, J. Geophys. Res., 100, 163–177.

Zaneveld J. R. V., 1974, *New developments of the theory of radiative transfer in the oceans*, [in:] *Optical aspects of oceanography*, N. G. Jerlov & E. S. Nielsen (eds.), Academic Press, New York, NY, 121–134.

Zaneveld J. R. V., 1989, *An asymptotic closure theory for irradiance in the sea and its inversion to obtain the inherent optical properties*, Limnol. Oceanogr., 34, 1442–1452.

Zaneveld J. R. V., Bartz R., 1984, *Beam attenuation and absorption meters*, Society of Photo-Optical Instrumentation Engineers, Ocean Optics VII, 489, 318–324.

Zaneveld J. R. V., Bartz R., Kitchen J. C., 1990, *A reflective-tube absorption meter*, Society of Photo-Optical Instrumentation Engineers, Ocean Optics X, 1302, 124–136.

Zaneveld J. R. V., Boss E., Barnard A., 2001, *Influence of surface waves on measured and modeled irradiance profiles*, Appl. Opt., 40, 1442–1449.

Zaneveld J. R. V., Kitchen J. C., Bricaud A., Moore C., 1992, *Analysis of in situ spectral absorption meter data*, Society of Photo-Optical Instrumentation Engineers, Ocean Optics XI, 1750, 187–200.

Zhang T., Gordon H. R., 1997, *Retrieval of elements of the columnar aerosol scattering phase matrix from polarized sky radiance over the ocean: simulations*, Appl. Opt., 36, 7948–7959.

Appendix 1
List of acronyms

Acronym	Meaning
AOP	apparent optical property
ELF	elastic light field
ILF	inelastic light field
IOP	inherent optical property
RLF	Raman light field
RT	radiative transfer
RTE	radiative transfer equation
TOA	top of the atmosphere

Appendix 2

List of frequently used symbols*

Symbol	Name
a	total absorption coefficient
b	total elastic scattering coefficient
$b_{in}(\lambda' \rightarrow \lambda)$	total inelastic scattering coefficient from λ' to λ
b_b	total elastic backscattering coefficient
$\mathbf{B}$	column vector of $b_{in}(\lambda_e \rightarrow \lambda)\Delta\lambda_e$ and $a(\lambda)$ for a given depth
$\tilde{b}_b$	total elastic backscattering probability
$\tilde{b}_f$	total elastic forward scattering probability $(1 - \tilde{b}_b)$
b_p	particle scattering coefficient
b_w	water elastic scattering coefficient
β	total volume scattering
β_p	particle volume scattering function
β_w	water elastic volume scattering function
$\beta_{in}(\lambda' \rightarrow \lambda)$	inelastic volume scattering function from λ' to λ
$\beta^{(0)}$, $\beta_{in}^{(0)}$	azimuthly averaged β and β_{in}
c	total attenuation coefficient $(a + b + \int b_{in}(\lambda \rightarrow \lambda')\, d\lambda')$
E	irradiance
E_d	downwelling irradiance
E_u	upwelling irradiance
E_0	scalar irradiance
E_{0d}	downwelling scalar irradiance
E_{0u}	upwelling scalar irradiance
E_1	vector (or net) irradiance $(E_d - E_u)$
E_n	n^{th} moment of $L^{(0)}$(Section 2.1.2)
$\mathbf{E}_0$	matrix of E_0 (rows, wavelength; columns, depth)
$\mathbf{E}_1$	matrix of E_1 (rows, wavelength; columns, depth)
$\mathbf{E}_0^{-1}$	inverse of $\mathbf{E}_0$
ϵ_n	expansion coefficient of $\beta_{in}^{(0)}$ (Section 2.1.2)
η	b_w/b
θ	propagation polar angle
θ_0	solar zenith angle
θ_{w0}	refracted (or in-water) solar zenith angle
Θ	scattering angle
I	radiant intensity

List of frequently used symbols* (continued)

Symbol	Name
J_f	source function for fluorescence (eq. 3)
J_r	source function for Raman scattering (eq. 4)
J_{in}	general inelastic source function
K_x	$-d\ell n(E_x)/dz$, where $x = d$, u, 0, 1, etc.
K_L	$-d\ell n(L_u)/dz$
K_∞	asymptotic value of K_d, K_u, K_0, etc.
$\langle K_d \rangle$	mean K_d from the surface to z_{10}
$\langle K_d \rangle_e$	mean K_d from the surface to z_1
$\langle K_d \rangle_1$	mean K_d from the surface to z_e
L	radiance
$L^{(0)}$	azimuthly averaged radiance
L_u	radiance measured by a nadir-viewing radiometer
λ	wavelength
λ_e	exicitation wavelength for inelastic scattering
$\overline{\mu}$	average cosine of the radiance (E_1/E_0)
$\overline{\mu}_d$	average cosine of the downwelling radiance (E_d/E_{0d})
$\overline{\mu}_u$	average cosine of the upwelling radiance (E_u/E_{0u})
$\overline{\mu}_0$	average cosine of the radiance when $b = b_{in} = 0$
$\overline{\mu}_s$	average cosine of β
μ_w	$\cos\theta_{0w}$
ν_1	largest eigenvalue of the source-free RTE
$\hat{\xi}$	direction of propagation of radiation
ϖ_n	expansion coefficient of $\beta^{(0)}$ (Section 2.1.2)
P	elastic scattering phase function (β/b); radiant power
P_p	particle scattering phase function (β_p/b_p)
P_w	water elastic scattering phase function (β_w/b_w)
$\vec{r}$	position vector of a point in space
R	irradiance reflectance (E_u/E_d)
$R_{\mu_w=1}$	R when the sun is at the zenith
R_{μ_w}	R for a general solar position
R_∞	asymptotic value of R for given IOPs
R_L	radiance factor (L_u/E_d)
τ	optical depth ($\tau = \int c(z)\,dz$)

List of frequently used symbols* (continued)

Symbol	Name
ϕ	propagation azimuth angle
$\phi(\cdot)$	eigenfunction of the source-free RTE
X	b_b/a
ω_0	single scattering albedo (b/c)
Ω	solid angle
z	depth
z_{10}	depth at 10% of surface irradiance
z_1	depth at 1% of surface irradiance
z_e	depth at $1/e$ of surface irradiance
$\approx$	approximately equal to
$\stackrel{\text{def}}{=}$	definition, e.g., $\omega_0 \stackrel{\text{def}}{=} b/c$
$\cong$	approximate equality in a relationship developed through curve fitting, e.g., least-squares
$\sim$	of the order of
$\lesssim$	less than approximately
$\gtrsim$	greater than approximately

*Many of these quantities depend on depth, wavelength, direction, etc. Such dependencies are included here only as required for clarity, e.g., $b_{in}(\lambda' \rightarrow \lambda)$.