Ocean inherent optical property estimation from irradiances

Robert A. Leathers and Norman J. McCormick

A method is evaluated for estimating the absorption coefficient \( a \) and the backscattering coefficient \( b_b \) from measurements of the upward and downward irradiances \( E_u(z) \) and \( E_d(z) \). With this method, the reflectance ratio \( R(z) \) and the downward diffuse attenuation coefficient \( K_d(z) \) obtained from \( E_u(z) \) and \( E_d(z) \) are used to estimate the inherent optical properties \( R_* \) and \( K_* \) that are the asymptotic values of \( R(z) \) and \( K_d(z) \), respectively. For an assumed scattering phase function \( \beta \), there are unique correlations between the values of \( R_* \) and \( K_* \) and those of \( a \) and \( b_b \) that can be derived from the radiative transfer equation. Good estimates of \( a \) and the Gordon parameter \( G = b_b/(a + b_b) \) can be obtained from \( R_* \) and \( K_* \) if the true scattering phase function is not greatly different from the assumed function. The method works best in deep, homogeneous waters, but can be applied to some cases of stratified waters. To improve performance in shallow waters where bottom effects are important, the deep- and shallow-measurement reflectance models also are developed. © 1997 Optical Society of America

**Key words:** Ocean optics, radiative transfer, optical properties, inverse problem.

1. Introduction

Determination of the beam absorption, scattering, and backscattering coefficients \( a, b, \) and \( b_b \) of natural waters is a primary goal of optical oceanographers. These inherent optical properties (IOP's) affect the ocean surface color, the transfer of heat to the upper ocean, the transmission of photosynthetically available radiation through the water column, and underwater visibility. The value of \( a \) is also used in models that predict phytoplankton growth rate and ocean primary production, and *in situ* measurements of \( a \) and \( b_b \) are necessary to validate remote sensing algorithms designed to monitor IOP's on a global scale.

A common method for determining \( a \) is spectrophotometric analysis of discrete water samples. However, this method is time-consuming, has a limited sampling rate, and is subject to errors. Alternatively, \( a \) can be determined from *in situ* natural light measurements. Most simply, \( a \) can be determined from simultaneous *in situ* monochromatic irradiance and monochromatic scalar irradiance measurements with the Gershun law; however, monochromatic scalar irradiance detectors are not yet readily available. Instead, estimates of \( a \) have been made from near-surface irradiance measurements in conjunction with measurements of remote sensing reflectance or estimates of the downward mean cosine of the radiance distribution. However, the former requires additional above-surface measurements and accurate empirical correlations, whereas the latter assumes the downward mean cosine does not change significantly within the surface layer, and both methods are susceptible to wave-induced fluctuations and to ship shadow.

Reflecting-tube instruments make it possible to obtain small-volume *in situ* estimates of \( a \) and \( c = a + b_b \) where the beam attenuation coefficient \( c \) is the inverse of the mean free path of a photon. Because reflecting-tube instruments are subject to scattering errors, they use a small sampling volume to minimize these errors, and as a result these instruments can break up or fail to collect large optically active aggregates (marine snow), can give high readings that are due to rare events of large particles entering the sensing area, and can have difficulty detecting low constituent concentrations.

In contrast, IOP estimation from natural irradiances can be obtained from large-volume measurements, and therefore small concentrations of constituents, both large and small, can be detected. Another advantage of calculating IOP's from irradiance measurements is that it enables one to obtain
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**Abstract:**
This report discusses the estimation of ocean inherent optical properties from irradiances. The methodology involves the use of remote sensing data to infer optical properties such as attenuation and backscattering coefficients. The approach aims to improve understanding of oceanic optical characteristics, which are crucial for various applications including remote sensing, marine biology, and climate studies.
the water properties and light field from the same instrument. At the very least, large-volume measurements can be correlated with small-volume measurements to improve the confidence in these estimates. Perhaps the primary advantage of the large-volume methods is that much irradiance data have already been collected and archived that can be reanalyzed with new algorithms for the estimation of $a$ and $b_b$.

Here we evaluate the estimation of $a$ and $b_b$ from only in situ profiles of the upward and downward irradiances $E_u(z)$ and $E_d(z)$ at geometric depths $z$. We note that Gordon and Boynton\(^9\) demonstrated that good estimates of $b$ are not possible from only irradiance measurements, and for this reason we focus on estimating $a$ and $b_b$. Our approach is to determine $a$ and $b_b$ through the determination of the reflectance $R(z)$ and the downward diffuse attenuation coefficient $K_d(z)$. The values of $R(z)$ and $K_d(z)$ are used to estimate the IOP’s $R_\infty$ and $K_\infty$, which are the values far from the surface of $R(z)$ and $K_d(z)$, respectively. Given a specific scattering phase function $\beta$, there are unique correlations between the values of $R_\infty$ and $K_\infty$ and those of $a$ and $b_b$, that can be derived from the radiative transfer equation.

The relevant equations of radiative transfer are introduced in Section 2. Estimation of $R_\infty$ and $K_\infty$ in deep, homogeneous waters is considered in Section 3, and the method of calculating $a$ and $b_b$ from $K_\infty$ and $R_\infty$ is presented in Sections 4 and 5. The importance of selecting an appropriate scattering phase function is investigated in Section 6, and a simplified algorithm that is independent of the scattering phase function is evaluated in Section 7. In Sections 8 and 9 we consider cases in which the water is optically shallow and inhomogeneous, respectively.

2. Basic Equations

The integrodifferential transfer equation for waters with homogeneous optical properties and no internal sources is

$$\mu \partial L(z, \mu)/\partial z + cL(z, \mu) = b \int_{-1}^{1} \tilde{\beta}(\mu, \mu')L(z, \mu')d\mu',$$

where $L(z, \mu)$ is the radiance integrated over all azimuthal directions for polar angle $\cos^{-1} \mu$ with respect to the depth $z$. All quantities in Eq. (1) are implicitly a function of wavelength. The azimuthally integrated scattering phase function $\tilde{\beta}(\mu, \mu')$ is normalized such that its expansion in Legendre polynomials has the form

$$\tilde{\beta}(\mu, \mu') = \frac{1}{2} \sum_{n=0}^{M} (2n + 1) f_n P_n(\mu) P_n(\mu'), \quad f_0 = 1,$$

where $f_n$ are the expansion coefficients, $P_n(\mu)$ are the Legendre polynomials, and $M$ is the degree of scattering anisotropy. The coefficient $f_1 = g$ is the scattering asymmetry factor. The backscattering coefficient,

$$b_b = b \int_{-1}^{0} \tilde{\beta}(\mu, 1)d\mu,$$

can be calculated from\(^1^0\)

$$\tilde{b}_b = b_b/b = (1/2) \left[ 1 - \sum_{n \text{ odd}} (2n + 1) f_n \int_{0}^{1} P_n(\mu)d\mu \right]$$

once the $f_n$ coefficients are specified. The integral factors in Eq. (4) can be calculated numerically from the recursion relationship $(n + 1) \int_{0}^{1} P_n(\mu)d\mu = -(n - 2) \int_{0}^{1} P_{n-2}(\mu)d\mu$, starting with $\int_{0}^{1} P_1(\mu)d\mu = 0.5$.

The irradiance reflectance $R(z)$ is

$$R(z) = E_u(z)/E_d(z),$$

where $E_u(z)$ and $E_d(z)$ are the upward and downward irradiances:

$$E_u(z) = \int_{-1}^{0} |\mu| L(z, \mu)d\mu,$$

$$E_d(z) = \int_{0}^{1} \mu L(z, \mu)d\mu.$$  

The downward diffuse irradiance attenuation coefficient $K_d$ is defined by

$$K_d(z) = -\frac{1}{E_d(z)} \frac{dE_d(z)}{dz} = -\frac{d \ln[E_d(z)]}{dz}.$$  

Although the magnitudes of $R(z)$ and $K_d(z)$ near the surface depend on the surface illumination, at large depths in deep homogeneous waters with no internal sources the values of $R(z)$ and $K_d(z)$ approach asymptotic values $R_\infty$ and $K_\infty$, respectively, that are IOP’s. To evaluate $R_\infty$ and $K_\infty$, we separate the spatial and angular dependencies in Eq. (1) with the eigenmodes:

$$L(z, \mu) = \phi(\pm v_j, \mu) \exp(\mp cz/v_j)$$

and use Eq. (2) to find that the discrete eigenfunctions $\phi(\pm v_j, \mu)$ satisfy

$$\phi(\pm v_j, \mu) = \frac{\omega_0 v_j}{2(v_j + \mu)} \times \sum_{n=0}^{M} (2n + 1) f_n g_n(\pm v_j) P_n(\mu), \quad v_j > 1,$$

where $\omega_0$ is the single-scattering albedo $\omega_0 = b/c$. The Chandrasekhar polynomials\(^1^1\) $g_n$ satisfy the recursion formula

$$ng_n(v_j) = h_{n-1} v_j g_{n-1}(v_j) - (n - 1) g_{n-2}(v_j),$$

where $g_0(v_j) = 1$ and $g_1(v_j) = v_j$.
starting with \( g_{-1} = 0 \) and \( g_0 = 1 \), where \( h_n = (2n + 1)(1 - \omega_0^2) \). From the spherical harmonics \( (P_N) \) method\(^\text{12} \) with \( N \) odd and arbitrarily large, the positive eigenvalues \( v_j \) are approximately the roots of

\[
g_{N+1}(v_j) = 0. \tag{12}
\]

With this formalism, the procedure in Appendix A shows that, for deep homogeneous waters, \( R_\infty \) and \( K_\infty \) satisfy\(^\text{13} \)

\[
R_\infty = \frac{\int_0^1 \phi(-v_1, \mu) \mu d\mu}{\int_0^1 \phi(+v_1, \mu) \mu d\mu}, \tag{13}
\]

\[
K_\infty = c/v_1, \tag{14}
\]

where \( v_1 \) is the largest positive eigenvalue. Thus \( R_\infty \) can be computed directly from only \( \beta \) and \( \omega_0 \), whereas \( K_\infty \) can be determined from the values of \( \beta \), \( \omega_0 \), and \( c \). We can avoid the numerical integration in Eq. (13) by utilizing equations for computing the numerator and denominator of Eq. (13) that are given in Ref. 14 [Eq. (22)].

3. Estimation of \( R_\infty \) and \( K_\infty \) in Deep, Locally Homogeneous Waters

Given the upward and downward irradiance measurements at arbitrary depths \( z \), \( R(z) \) is calculated directly from Eq. (5). Values of \( K_d(z) \) are calculated from finite differences of \( \ln[E_d(z)] \) with respect to \( z \), an approximation that is exact at large depths where \( \ln[E_d(z)] \) varies linearly with \( z \). Thus the calculation of \( R(z) \) at a specified depth requires the measurement or interpolation of \( E_u(z) \) and \( E_d(z) \) at that depth, whereas that of \( K_d(z) \) requires at least the measurement of \( E_d(z) \) at two depths.

In optically deep, source-free, and homogeneous waters, the vertical profiles of \( R(z) \) and \( K_d(z) \) approach the asymptotic values \( R_\infty \) and \( K_\infty \) that we seek. The simplest approach to estimate \( R_\infty \) and \( K_\infty \) is to calculate \( R(z) \) and \( K_d(z) \), preferably at large depths, and take \( R_\infty = R(z) \) and \( K_\infty = K_d(z) \). We refer to this as the asymptotic method (AM) since the approximation is exact in the asymptotic regime. The accuracy of this method depends on the degree to which the light field differs from the asymptotic field and on the noise in the irradiance measurements.

If measurement noise were negligible, the AM would be essentially exact at sufficiently large depths. For illustration, consider the case in which the incident radiation is composed of 70% direct beam and 30% diffuse skylight and the cosine of the angle of the direct beam is \( \mu_0 = 0.866 \). The corresponding upper-boundary condition just above the sea surface can be modeled as a superposition of direct sunlight, defined with a Dirac delta function, and diffuse skylight:

\[
L(0^\circ, \mu) = 0.7\delta(\mu - 0.866) + 0.3, \quad 0 \leq \mu \leq 1. \tag{15}
\]

Let \( \omega_0 = 0.7 \) and let the scattering be characterized by the Henyey–Greenstein scattering phase function\(^\text{15} \) \( \bar{P}_{\text{HG}} \), for which \( f_n = g^n \), with the scattering asymmetry factor \( g = 0.85 \). We take the 200th-order scattering anisotropy \( (M = 200) \) and an index of refraction of 1.34. From Eqs. (13) and (14), we calculate \( R_\infty = 0.04119 \) and \( K_\infty/c = 0.4707 \). The value of \( K_\infty \) is normalized by \( c \) so that the result depends only on \( \omega_0 \) and the \( f_n \) values. Let the vertical distance be measured in optical depths \( \tau = cz \) and take the water to be very deep (50 optical depths) with a purely absorbing bottom. As shown in Fig. 1, the profiles of \( R(\tau) \) and \( K_d(\tau)/c \) converge to their asymptotic values. The profiles shown in Fig. 1 were computed with the discrete ordinates radiative transfer code DISORT\(^\text{16,17} \) which takes into account the index of refraction mismatch at the surface. The magnitudes of \( R(\tau) \) and \( K_d(\tau)/c \) below \( \tau = 2 \) each vary over a range of approximately 6% and below \( \tau = 4 \) vary by less than 3%. This small range of \( R(\tau) \) and \( K_d(\tau) \) values away from the surface is typical and aids in the estimation of \( K_\infty/c \) and \( R_\infty \). Table 1 shows the error in values of \( R_\infty \) and \( K_\infty \) predicted by the AM from the simulated data shown in Fig. 1. Irradiance values at 1 optical depth vertical spacing were used to calculate \( K_d(\tau) \). The errors in the predictions decrease monotonically with depth. However, note that predictions from measurements below 4 optical depths are accurate to within a few percent. This indicates that even

![Fig. 1. Diffuse attenuation coefficient and irradiance reflectance profiles from simulated irradiance data (\( \omega_0 = 0.7, g = 0.85 \)). The values of \( R \) are multiplied by 10.](image)

Table 1. Predictions of \( K_\infty \) and \( R_\infty \) from the Simulated \( K_d(\tau) \) and \( R(\tau) \)

<table>
<thead>
<tr>
<th>( \tau )</th>
<th>( R_\infty )</th>
<th>( K_d(\tau)/c )</th>
<th>( R_\infty )</th>
<th>( K_d(\tau)/c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>4.0</td>
<td>4.5</td>
<td>0.78</td>
<td>1.3</td>
</tr>
<tr>
<td>4</td>
<td>2.5</td>
<td>2.8</td>
<td>0.32</td>
<td>0.48</td>
</tr>
<tr>
<td>5</td>
<td>1.6</td>
<td>1.8</td>
<td>0.12</td>
<td>0.19</td>
</tr>
<tr>
<td>7</td>
<td>0.68</td>
<td>0.75</td>
<td>0.012</td>
<td>0.018</td>
</tr>
</tbody>
</table>

\(^\text{a Estimates are made from the deepest values of } R(\tau) \text{ and } K_d(\tau) \text{ (AM) and from extrapolation with an exponential model (EM) for } K_d(\tau) \text{ and } R(\tau). \)

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though the AM is only theoretically exact at large depths, it can produce good estimates from relatively shallow measurements. In practice, irradiance measurements contain noise. Consider random noise \( r \) in the irradiance measurements that is proportional to the irradiance magnitude. The measured reflectance \( R_m(z) \) is

\[
R_m(z) = \left(1 + \frac{r_u - r_d}{1 + r_d}\right) R(z),
\]

where \( R(z) \) is the true reflectance and \( r_u \) and \( r_d \) are the uncorrelated random noise in the upward and downward irradiance measurements, respectively, after any smoothing or averaging of the data. The measured downward diffuse attenuation coefficient is

\[
K_d^m(z) = K_d(z) - d[\ln(1 + r_d)]/dz.
\]

When the AM is used, the relative error of \( R_m \) is independent of \( R \) whereas that of \( K_m \) is proportional to \([\Delta z K_d(z)]^{-1}\), where \( \Delta z \) is the vertical spacing between \( K_d(z) \) values. For example, if the noise \( r_d \) and \( r_u \) is normally distributed, then the standard deviations of \( (r_u - r_d)/(1 + r_d) \) and \([\ln(1 + r_d) - \ln(1 + r_u)]\) are both approximately 1.4s if \( s \) is the standard deviation of both \( r_u \) and \( r_d \). In such a case, the relative errors in \( R_m \) and \( K_m \) at large depths are 1.4s and 1.4s/[\( K_d(z)\Delta z \)], respectively.

In addition to the AM for estimating \( R_m \) and \( K_m \), one can use analytical approximations to \( R(z) \) (Ref. 18) and \( K_d(z) \) (Ref. 19) given by

\[
R(z) \approx R_a + [R(z_r) - R_a] \exp[-\tilde{\Phi}(z - z_r)], \quad z > z_{r},
\]

(18)

\[
K_d(z) \approx K_a + [K_d(z_r) - K_a] \exp[-\tilde{\Phi}(z - z_r)], \quad z > z_{r},
\]

(19)

where \( z_r \) is some reference depth and the IOP \( \tilde{\Phi} \) can be calculated \(^{20}\) from \( \tilde{\Phi} = c(v_2 - v_1) \), where \( v_2 \) is the second largest positive eigenvalue from Eq. (12). Because values of \( R(z) \) and \( K_d(z) \) are predicted for depths below those of the measurements, we refer to this method as the extrapolation method (EM). At large depths the exponential term in Eqs. (18) and (19) becomes negligible and EM estimates become equal to those from the AM. From values of \( R(z) \) at depths \( z_0, z_1, \) and \( z_2 \), with \( z_1 = (z_0 + z_2)/2 \), \( R_m \) can be obtained from Eq. (18) as \(^{20}\)

\[
R_m = \frac{R(z_0) R(z_2) - R^2(z_1)}{R(z_0) + R(z_2) - 2R(z_1)}.
\]

(20)

An analogous equation \(^{19}\) holds for the determination of \( K_m \) from Eq. (19).

Estimates of \( R_m \) and \( K_m \) from the EM for the noise-free data in Fig. 1 are given in Table 1. Irradiance values at 1 optical depth vertical spacing were used, and the results are presented as a function of the depth of the deepest irradiance value used. All predictions are within 0.8% of the true value and, as expected, improve with increasing depth. This indicates that \( R_m \) and \( K_m \) can be estimated from relatively shallow measurements, at least when there is no simulated noise. For example, at \( \tau = 3 \), \( R_m \) calculated from the EM is within 0.78% of the true value, whereas \( R_m \) estimated by the AM is in error by 4%. Similarly, at \( \tau = 4 \), \( K_m \) calculated from the EM is within 0.48% of the true value, whereas \( K_m \) estimated by the AM is in error by 2.8%.

When noise is present, however, estimation of \( R_m \) and \( K_m \) from the EM can give improved results over the AM only if the noise in \( R(z) \) and \( K_d(z) \) is much smaller than the exponential terms in Eqs. (18) and (19) at the depths of the measurements. Thus the extrapolation method may be superior near the surface, but it is inferior to the AM at depths where the true \( R(z) \) and \( K_d(z) \) vary only slowly with depth. Because our emphasis is on deeper-water applications, the EM is not examined further.

4. Estimation of Fundamental IOP’s from \( R_m \) and \( K_m \)

The parameters \( a, b, \) and \( b_0 \) are fundamental IOP’s. In addition, Gordon \textit{et al.} \(^{21}\) showed that \( R(\tau) \) at the surface is nearly proportional to the ratio \( b_0/(a + b_0) \), and many remote sensing algorithms are designed to measure either \( b_0/a \) or \( b_0/(a + b_0) \). We choose to define the ratio \( G = b_0/(a + b_0) \) as the (dimensionless) Gordon parameter in view of his many contributions to the field of ocean optics and his observation of the importance of \( G \) in remote sensing applications.

If the scattering phase function \( \beta \) is assumed, then \( a \) and \( b_0 \) can be determined from measurements of \( R_m \) and \( K_m \). The first step in the solution of this inverse problem is to calculate \( \omega_0 \) from \( R_m \) and \( \beta \), or from \( R_m \) and \( g \) if the phase function \( \beta_{HG} \) is assumed. For example, Fig. 2 shows the interdependence of \( R_m, \omega_0, \) and \( g \) for the phase function \( \beta_{HG} \). Although in a typical forward calculation \( R_m \) depends on \( \omega_0 \) and \( g \), in this inverse problem \( R_m \) is a measured quantity. The value of \( \omega_0(R_m, g) \) can be found from an iterative solution of Eq. (13) with the help of Eqs. (10)–(12), and in the process the value of \( \nu_1 \) is calculated from Eq. (12). Next, \( c \) is calculated from \( \nu_1 \) and the measured value of \( K_m \) from Eq. (14). \( a \) and \( b \) are calculated from \( \omega_0 \) and \( c \), and \( b_0 \) is computed from Eq. (4) with use of \( \beta_n = g^n \) with the assumed \( g \). Finally, ratios such as \( b_0/a \) and \( b_0/(a + b_0) \) can be formed from \( a \) and \( b_0 \).
Table 2. Percent Errors in the Estimates of IOP's for Selected Values of Percent Errors in \( R_\alpha \) and \( K_\alpha \)

<table>
<thead>
<tr>
<th>( R_\alpha )</th>
<th>( K_\alpha )</th>
<th>( a )</th>
<th>( b ) and ( b_\alpha )</th>
<th>( b_\alpha/a )</th>
<th>( G )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0</td>
<td>-1.04</td>
<td>3.32</td>
<td>4.41</td>
<td>4.06</td>
</tr>
<tr>
<td>-5</td>
<td>0</td>
<td>1.08</td>
<td>-3.38</td>
<td>-4.41</td>
<td>-4.08</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>3.91</td>
<td>8.49</td>
<td>4.41</td>
<td>4.06</td>
</tr>
<tr>
<td>-5</td>
<td>5</td>
<td>6.14</td>
<td>1.45</td>
<td>-4.41</td>
<td>-4.08</td>
</tr>
<tr>
<td>5</td>
<td>-5</td>
<td>-5.99</td>
<td>-1.84</td>
<td>4.41</td>
<td>4.06</td>
</tr>
<tr>
<td>-5</td>
<td>-5</td>
<td>-3.97</td>
<td>-8.21</td>
<td>-4.41</td>
<td>-4.08</td>
</tr>
<tr>
<td>0</td>
<td>5</td>
<td>5.00</td>
<td>5.00</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 2 gives example calculations of the errors in the estimated values of \( a \), \( b \), \( b_\alpha/a \), and \( G \) obtained from various values of \( R_\alpha \) and \( K_\alpha \) when the true IOP's are \( \omega_0 = 0.7 \) and \( g = 0.85 \). These computations were performed with \( a = 0.15 \) and \( b = 0.35 \) and the correct phase function and by an iterative search for the optimal value of \( \omega_0 \). We achieved the search by minimizing the error in the calculated value of \( R_\alpha \) with respect to \( \omega_0 \) using Brent’s method, which is a combination of an inverse parabolic interpolation and a golden-section search. It can be seen that the errors in the calculations of the fundamental IOP’s are of the same order of magnitude as the errors in \( R_\alpha \) and \( K_\alpha \). Estimates of \( a \) are best when the errors in \( R_\alpha \) and \( K_\alpha \) have the same sign, whereas estimates of \( b \) are best when the errors in \( R_\alpha \) and \( K_\alpha \) have the opposite sign. As can be seen from Table 2, \( b_\alpha/a \) and \( G \) do not depend on \( K_\alpha \) since \( b_\alpha/a = \bar{b}_\alpha(1 - \omega_0)^{-1} \) and \( G = [1 + (1 - \omega_0)/(\omega_0\bar{b}_\alpha)]^{-1} \) and \( \omega_0 \) is independent of \( K_\alpha \).

In practice, \( \beta \) is not well known, and therefore estimates of \( \omega_0 \) and \( c \) (and of \( a \) and \( b \)) will contain errors that are due both to measurement errors in \( R_\alpha \) and \( K_\alpha \) and to the error in the assumed \( \beta \). Table 3 shows the percent errors in estimates of \( a \) and \( b \) calculated with the same iterative solution code as for Table 2 but with unknown \( g \) and for \( R_\alpha \) and \( K_\alpha \) that were computed for the indicated values of \( \omega_0 \) and \( g \). For the assumed \( g = 0.85 \), the values of \( a \) and \( b \) are underestimated when the true \( g < 0.85 \), are exact when \( g = 0.85 \), and are overestimated when \( g > 0.85 \). For this large range of \( g \), the worst estimate of \( a \) was in error by only 1.5%, whereas those for \( b \) were generally within 10%.

To assess more thoroughly the accuracy of predicting fundamental IOP’s from \( R_\alpha \) and \( K_\alpha \), in Section 5 we examine the sensitivity coefficients that quantify the extent to which errors in \( R_\alpha \), \( K_\alpha \), and \( g \) affect the estimates of the fundamental IOP’s.

5. Sensitivity Coefficients

Normalized sensitivity coefficients express the ratio of the relative error in an output (e.g., \( a \)) to a small relative error in an input (e.g., \( R_\alpha \)). In the development of equations for sensitivity coefficients in this section, it is assumed that the phase function can be expressed as a function of a single parameter, such as the scattering asymmetry factor \( g \) of the Heneyey-Greenstein phase function that is used for the numerical calculations.

A. Sensitivity Coefficients for \( \omega_0 \) and \( c \)

From the iterative search method discussed in Section 4, one can numerically solve for \( (R_\alpha/\omega_0)(\partial \omega_0/\partial R_\alpha) \) and \( (g/\omega_0)(\partial \omega_0/\partial g) \). These normalized sensitivity coefficients quantitatively express the sensitivity of the estimates of \( \omega_0 \) to errors in the measurement of \( R_\alpha \) and in the guess for \( g \), respectively. Furthermore, these coefficients are required to calculate the sensitivity coefficients for the other fundamental IOP’s. As shown in Appendix B, these sensitivity coefficients can also be expressed in terms of sensitivity coefficients for the forward problem. Because the forward problem is much easier to compute than the inverse problem, \( (R_\alpha/\omega_0)(\partial \omega_0/\partial R_\alpha) \) and \( (g/\omega_0)(\partial \omega_0/\partial g) \) were computed with Eqs. (B1) and (B2).

In Fig. 3, \( R_\alpha/\omega_0 \)(\( \partial \omega_0/\partial R_\alpha \)) is shown as a function of \( \omega_0 \). For \( 0.75 < g < 0.95 \), this normalized sensitivity coefficient varies roughly linearly from approximately 0.7 for \( \omega_0 = 0.2 \) to 0.05 for \( \omega_0 = 0.99 \). This indicates that estimates of \( \omega_0 \) from \( R_\alpha \) are moderately insensitive to small errors in \( R_\alpha \) and are least sensitive where the absorption relative to the beam attenuation is lowest. The sensitivity coefficient itself is

![Fig. 3. Normalized sensitivity coefficient of \( \omega_0 \) with respect to \( R_\alpha \) for \( g \) of \( \beta_{HG} \).](image-url)
only weakly dependent on \( g \) but is highest for small \( g \) when \( \omega_0 > 0.5 \) and for large \( g \) when \( \omega_0 \) is small. Unfortunately, as can be seen in Fig. 4, estimates of \( \omega_0 \) are much more sensitive to \( g \) than to \( R_\infty \). The sensitivity of \( \omega_0 \) to \( g \) is highly dependent on both \( g \) and \( \omega_0 \), and it is highest for large \( g \) and for small \( \omega_0 \). Thus the sensitivities of \( \omega_0 \) to errors in both \( g \) and \( R_\infty \) are lowest, and therefore estimates of \( \omega_0 \) will be best, when \( \omega_0 \) is high. For \( \omega_0 = 0.7 \) and \( g = 0.85 \), for example, a 10\% uncertainty in \( g \) can result in approximately an 18\% uncertainty in \( \omega_0 \), which would be unacceptably large. Much greater errors may result when \( g \) is very high (\( g > 0.9 \)), which is typical for the Petzold phase functions.\(^2\)\(^3\) Because we wish to implement this method of estimating IOP's without knowledge of \( g \), the high sensitivity of \( \omega_0 \) to \( g \) places a serious limitation on our ability to estimate \( \omega_0 \). However, some other IOP's calculated from \( \omega_0 \), in particular \( \alpha \), are far less sensitive to \( g \).

In the inverse problem, the largest eigenvalue \( \nu_1 \) is a function of \( \omega_0(R_\infty, g) \) and \( g \) and therefore can be written alternatively as a function of the independent variables \( R_\infty \) and \( g \). The beam attenuation coefficient is found from

\[
c = \nu_1(R_\infty, g)K_a,
\]

but henceforth the dependence of \( \nu_1 \) and \( \omega_0 \) on \( R_\infty \) and \( g \) will not be denoted explicitly. Note that \( K_a \) is a measured and therefore independent quantity. One can evaluate the normalized sensitivity coefficients for \( c \) from Eq. (21):

\[
\frac{K_a}{c} \frac{\partial c}{\partial K_a} = \frac{K_a}{c} \frac{\partial c}{\partial \nu_1} = \frac{K_a}{c} \frac{\partial c}{\partial R_\infty} = \frac{K_a}{c} \frac{\partial c}{\partial g} = \frac{g}{\nu_1} \frac{\partial \nu_1}{\partial g}.
\]

These are expressed in terms of normalized sensitivity coefficients \((R_\infty/\nu_1)(\partial \nu_1/\partial R_\infty)\) and \((g/\nu_1)(\partial \nu_1/\partial g)\), which must be computed either from an iterative solution method or, more easily, from Eqs. (B3) and (B4). The magnitude of \((R_\infty/c)(\partial c/\partial R_\infty)\), shown in Fig. 5, is typically less than unity, except for high \( \omega_0 \) and low \( g \), and is especially low when \( \omega_0 \) is low. However, the sensitivity of \( c \) to \( g \), shown in Fig. 6, is similar in magnitude to that of \( \omega_0 \) to \( g \), except that it is lowest for low values of \( \omega_0 \) and highest for high values of \( \omega_0 \).

B. Sensitivity Coefficients for \( a, b_0, b_0/a, \) and \( G \)

Because

\[
a = c(1 - \omega_0), \quad \frac{\partial \alpha}{\partial \omega_0} = -c, \quad \frac{\partial \alpha}{\partial c} = (1 - \omega_0),
\]

\[
b = c\omega_0, \quad \frac{\partial b}{\partial \omega_0} = \omega_0, \quad \frac{\partial b}{\partial c} = \omega_0,
\]
the normalized sensitivity coefficients for $a$ can be
determined directly from those for $\omega_0$ (Figs. 3 and 4)
and $c$ [Eqs. (22)–(24)]:

\[
\frac{K_a \partial a}{a \partial K_a} = \frac{K_a \partial a}{a \partial c} \frac{\partial c}{\partial K_a} = \frac{K_a}{a} (1 - \omega_0) \nu_1 = 1, \quad (27)
\]

\[
R_a \frac{\partial a}{a \partial R_a} = \frac{R_a \partial a}{a \partial b} \left[ \frac{R_a \partial c}{c \partial R_a} (R_a \frac{\partial c}{c \partial R_a}) + \frac{\partial a}{\partial c} \frac{\omega_0}{\partial a} \right] = \frac{R_a \partial c}{c \partial R_a} - \frac{\omega_0}{1 - \omega_0} \left( \frac{R_a}{\omega_0} \frac{\partial \omega_0}{\partial R_a} \right), \quad (28)
\]

\[
\frac{g \partial a}{a \partial g} = \frac{g \partial c}{c \partial g} + \frac{\partial a}{\partial c} \frac{g \partial \omega_0}{\partial \omega_0} \frac{g \partial \omega_0}{\partial g}.
\]

Similarly, the normalized sensitivity coefficients for $b$
are

\[
\frac{K_b \partial b}{b \partial K_b} = \frac{K_b \partial b}{b \partial a} \omega_0 \nu_1 = 1, \quad (30)
\]

\[
R_b \frac{\partial b}{b \partial R_b} = \frac{R_b \partial b}{b \partial c} \left[ \frac{R_b \partial c}{c \partial R_b} (R_b \frac{\partial c}{c \partial R_b}) + \frac{\partial b}{\partial c} \frac{\omega_0}{\partial b} \right] = \frac{R_b \partial c}{c \partial R_b} + \frac{\omega_0}{\partial b} \frac{\partial \omega_0}{\partial R_b}, \quad (31)
\]

\[
\frac{g \partial b}{b \partial g} = \frac{g \partial c}{c \partial g} + \frac{\partial b}{\partial c} \frac{g \partial \omega_0}{\partial \omega_0} \frac{g \partial \omega_0}{\partial g}.
\]

Thus, all else being equal, the percent error in $a$ and
$b$ that is due to an error in $K_a$ is equal to the percent
error in $K_b$. The normalized sensitivity coefficients for
$b$ to $R_a$ and $g$ are equal to the sum of those for $c$
and $\omega_0$ to $R_a$ and $g$, respectively, whereas the expres-
sions for the normalized sensitivity coefficients for $a$
to $R_a$ and $g$ are similar to those for $b$ except that for
$a$ the coefficients involving $\omega_0$ are scaled by
$\omega_0/(1 - \omega_0) = b/a$. Note that because
$c / \partial R_a$ and $\partial \omega_0 / \partial R_a$ have the same sign, the sensitivity coefficients for $a$
are less than those for $b$, which is consistent with the
observation in Section 4.

The coefficient $(g/a)(\partial a / \partial g)$ is shown in Fig. 7.
The absolute value of the magnitude of the coefficient is
very low (<0.16) for $\omega_0 < 0.99$. It is highly depen-
dent on $\omega_0$, with the largest magnitude corresponding
to moderate values of $\omega_0$. The coefficient $(R_a / a)(\partial a / \partial R_a)$ is shown in Fig. 8. This coefficient also is
relatively small, with typical values ranging from $-0.1$
to $-0.6$ for $\omega_0 < 0.9$. Therefore, even though $a$
is calculated from $\omega_0$ and $c$, each of which are poorly
estimated from $R_a$ and $K_a$, $a$ can be calculated quite
well. As expected, the sensitivity of $b$ to $g$ as calcu-
lated from Eq. (32) is very large, especially for large
values of $g$, and therefore reasonable estimates of $b$
when $\beta$ is not known are not possible.

The normalized sensitivity coefficient of $b_h$ to $g$ is
the sum of those of $b$ to $g$ and $b_h$ to $g$:

\[
\frac{g \partial b_h}{b_h \partial g} = \frac{g \partial b}{b \partial g} + \frac{g \partial b_h}{b_h \partial g}.
\]

This introduces a fifth sensitivity coefficient $(g / b_h)(\partial b_h / \partial g)$ that must be computed numerically. A
plot of $(g \partial b_h)/(b_h \partial g)$ is shown in Fig. 9. The terms
$(g/b)(\partial b / \partial g)$ and $(g/b_h)(\partial b_h / \partial g)$ tend to cancel out
because the signs are different, so estimates of $b_h$
are moderately insensitive to $g$ [0.4 < $(g \partial b_h)/(b_h \partial g)$ <
0.9], indicating that estimates of $b_h$ will be reasonable
even if $g$ is not well known. Because $b_h = b \bar{b}$, the
normalized sensitivity coefficient of $b_h$ to $K_a$ is unity,
wheras that of $b_h$ to $R_a$ is identical to that for $b$
given in Eq. (31) and is shown in Fig. 10.
Recall that both $b_y/a$ and $G$ are independent of $K_v$. The normalized sensitivity coefficient of $b_y/a$ to $g$ is

$$\frac{g}{(b_y/a)} \frac{\partial (b_y/a)}{\partial g} = \frac{g}{b_y} \frac{\partial b_y}{\partial g} - \frac{g}{a} \frac{\partial a}{\partial g} = \frac{g}{b_y} \frac{\partial b_y}{\partial g} + \frac{1}{(1 - \omega_v) \omega_v} \frac{g}{\partial \omega_v} \partial \omega_v,$$  

(34)

and the sensitivity coefficient of $G$ to $g$ is proportional to that of $(b_y/a)$ to $g$:

$$\frac{g}{G} \frac{\partial G}{\partial g} = \frac{a}{a + b_y} \left[ \frac{g}{(b_y/a)} \frac{\partial (b_y/a)}{\partial g} \right].$$  

(35)

Because $\partial b_y/\partial g$ and $\partial a/\partial g$ have the same sign and $|(g \partial b_y)/(b_y \partial g)| > |(g \partial a)/(a \partial g)|$, then from Eq. (34) the magnitude of the sensitivity of $b_y/a$ to $g$ is less than that of $b_y$, and because $a/(a + b_y) < 1$, then from Eq. (35) $G$ is even less sensitive to $g$ than is $b_y/a$, especially for large $\omega_v$. The normalized sensitivity coefficients of $b_y/a$ and $G$ to $R_\infty$ are in the same form as those to $g$:

$$\frac{R_\infty}{(b_y/a)} \frac{\partial (b_y/a)}{\partial R_\infty} = \frac{R_\infty}{b_y} \frac{\partial b_y}{\partial R_\infty} - \frac{1}{(1 - \omega_v) \omega_v} \frac{R_\infty}{\partial \omega_v} \partial \omega_v,$$  

(36)

$$\frac{R_\infty}{G} \frac{\partial G}{\partial R_\infty} = \frac{a}{a + b_y} \left[ \frac{R_\infty}{(b_y/a)} \frac{\partial (b_y/a)}{\partial R_\infty} \right].$$  

(37)

The sensitivities of $G$ are shown in Figs. 11 and 12.

6. Choice of the Phase Function Model

Equations (29) and (32) hold for any model of the phase function $\tilde{\beta}$ that can be specified by a single parameter $g$. In Figs. 7 and 9 the one-term Henyey–Greenstein function was used because of its simplicity. Other models could be used, however. For example, phase functions obtained by a combination of the pure seawater phase function and the Petzold particle phase function$^{24}$ can also be specified by the
value of \( g \) or, more commonly, the chlorophyll concentration.

Even if the single parameter defining the phase function model is known, errors may be introduced into the estimates of \( a \) and \( b_b \) if the shape of the true phase function differs from that predicted by the model. For example, Fig. 13 shows four phase functions that are all characterized by \( g = 0.85 \) but that have very different shapes in the backscattering directions. These were generated from the two-term Henyey–Greenstein model, which is a linear combination of two one-term Henyey–Greenstein functions:

\[
\bar{\beta}(g_1, g_2, \alpha) = \alpha \beta(g_1) + (1 - \alpha) \beta(g_2),
\]

with parameters \( g_1, g_2, \) and \( \alpha \) for \( 0 \leq \alpha \leq 1 \). Selection of a negative \( g_2 \), for example, yields an enhanced backscattering effect. Shown are \( a \), the one-term function \((g_1 = 0.85, \alpha = 0) \); \( b \), a monotonic function with more backscattering \((g_1 = 0.88, g_2 = -0.062, \alpha = 0.97) \); \( c \), the function whose first three moments match those of the water–Petzold particle mixture model \((g_1 = 0.90, g_2 = -0.26, \alpha = 0.96) \); and \( d \), a case with extremely high backscattering \((g_1 = 0.90, g_2 = -0.64, \alpha = 0.97) \). These results show that, to obtain good estimates of \( b_b \), it is not sufficient for the assumed phase function to be characterized by an appropriate value of \( g \); the amount of backscattering is also important. In particular, the one-term Henyey–Greenstein function model should not be used in the estimation of \( b_b \) in natural waters; the Petzold phase function or a two-term Henyey–Greenstein function similar to \( c \) would be better.

### Table 4.

<table>
<thead>
<tr>
<th>Assumed ( \beta ) Phase Function</th>
<th>Assumed ( \beta ) Phase Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a )</td>
<td>( b_b )</td>
</tr>
<tr>
<td>a</td>
<td>0.0</td>
</tr>
<tr>
<td>b</td>
<td>-2.5</td>
</tr>
<tr>
<td>c</td>
<td>-5.3</td>
</tr>
<tr>
<td>d</td>
<td>-6.9</td>
</tr>
</tbody>
</table>

\( a \) is the one-term phase function \( a \) \((a = 0) \) and \( b \) the two-term function \( c \) \((g_1 = 0.90, g_2 = -0.26, \alpha = 0.96) \). The true phase functions used in the forward calculation of \( R_\alpha \) and \( K_\alpha \) are functions \( a, c, b, \) and \( d \) \((g_1 = 0.88, g_2 = -0.062, \alpha = 0.97) \). and \( d \) \((g_1 = 0.90, g_2 = -0.64, \alpha = 0.97) \). The phase functions in Fig. 13 were used to determine the effect of the amount of backscattering in the assumed phase function on the estimates of the IOP’s. Values of \( R_\alpha \) and \( K_\alpha \) were first calculated from the forward problem for each of the four phase functions. Then the values of \( a \) and \( b_b \) were estimated from the \( R_\alpha \) and \( K_\alpha \) with the approach in Section 4 assuming either phase function \( a \) or \( c \). Table 4 shows the percent errors in the estimated IOP’s. Estimates of \( b_b \) were several times more sensitive to the assumed \( \beta \) than were those of \( a \). Because phase functions \( a \) and \( b \) are decreasing monotonically in the backscattering direction, estimates of \( b_b \) assuming phase function \( a \) were in error by as much as 30% when the true \( \beta \) exhibits the enhanced backscatter-

7. **Phase-Function-Independent Algorithm**

Haltrin recognized that a simple model for an approximate phase function \( \beta(\mu, \mu’) = 2b_b + 2(1 - 2b_b)\delta(\mu - \mu’) \) conveys much of the information needed to describe highly forward scattering. For this \( \beta \) he derived equations for \( R_\alpha \) and \( K_\alpha/c \) from a carefully derived two-flux theory:

\[
a/b_b = \frac{(1 - \sqrt{R_\alpha})^2(1 + 4\sqrt{R_\alpha} + R_\alpha)}{4R_\alpha},
\]

\[
K_\alpha/c = (1 - \omega_\alpha)\left\{1 + G\left[1 + 2G - [G(4 + 5G)]^{1/2}\right]\right\}^{1/2}.
\]

Equation (39) can be used to estimate \( a/b_b \) from \( R_\alpha \) and \( G \) can be calculated from \( G = (1 + a/b_b)^{-1} \). Then \( a \) can be estimated from a rearrangement of Eq. (40):

\[
a = K_\alpha\left\{1 + G\left[1 + 2G - [G(4 + 5G)]^{1/2}\right]\right\}^{-1/2},
\]

which enables one to also obtain \( b_b \). The primary difference between Haltrin’s model and that proposed in Section 4 is that in Haltrin’s model only two closed-
form analytical equations are needed and no assumption about the phase function is required, whereas in the method proposed in Section 4 an assumed phase function must be incorporated into the iterative solution of Eqs. (10)–(13). Although Eqs. (39) and (41) have the significant advantage in that they are easier to implement in practice, they are less flexible since they do not admit a priori information about the phase function.

Table 5 shows the percent errors in estimates of a and b_\text{b} obtained from Eqs. (39) and (41) for the one-term Henyey–Greenstein phase function with 0.75 ≤ g ≤ 0.95 and 0.5 ≤ \omega_0 ≤ 0.9. As for Table 3, the values of R_∞ and K_\infty were computed for the given values of \omega_0 and g. The calculations were performed for c = 1; however, the percent errors in a and b_\text{b} were found to be insensitive to the value of c. The errors in the estimates of a range from 1.4% to 5.2%, whereas those in the estimates of b_\text{b} range from 32% to 100%. The errors in a are roughly twice those in Table 3 obtained with the approach described in Section 4, whereas the errors in b_\text{b} are many times larger. Similar results were obtained with the San Diego Petzold water phase function for a case of 10-mg/l chlorophyll concentration and 685-nm light; for \omega_0 = 0.5, 0.7, and 0.9 the percent errors in a were 1.8, 2.6, and 1.9, respectively, and the percent errors in b_\text{b} were 44, 61, and 81, respectively.

The large errors in b_\text{b} should be expected because of the high sensitivity of b_\text{b} to the shape of the backscattering portion of \beta demonstrated in Section 6. The degree to which the \beta-dependent approach of Section 4 outperforms Haltrin’s approach depends on how well the assumed \beta matches the actual scattering phase function of the water.

8. IOP Estimation in Shallow Waters

In shallow water where the entire water column is in the euphotic zone, profiles R(z) and K_d(z) are affected by the interaction of light with the bottom. Although the effects of the bottom usually do not reach as far into the water column as do surface conditions, bottom effects can cause errors in IOP estimation. If the water is so shallow that significant surface and bottom effects overlap, then R(z) and K_d(z) never reach R_∞ and K_∞, respectively. However, estimates of R_∞ and K_∞ can still be made in water of at least a few optical depths. In this case, R(z) and K_d(z) near the surface tend toward R_∞ and K_∞ with increasing depth and near the bottom deviate away from R_∞ and K_∞. The asymptotic method for estimating R_∞, for example, can be applied by taking R_∞ = R(z_m) at a mid-water-column depth z_m where R(z) is a maximum or minimum or is at an inflection point.

Figure 14 shows R(\tau) for water of 5 optical depths with a purely absorbing bottom (R_b = 0). Shown are R_∞ from Eq. (13), the local irradiance ratio R(\tau) that forms the asymptotic model (AM), and the depth-dependent estimates of R_∞ from the deep-measurement reflectance model (DMRM) and the shallow-measurement reflectance model (SMRM).
and evaluate the differences at the two depths. The estimated value of \( R_\infty \) follows from

\[
\left( \frac{1 - R_\infty}{1 + R_\infty} \right)^2 = \frac{[E_d(z) - E_u(z)]^2}{[E_d(z) + E_u(z)]^2} \tag{42}
\]

Note that this technique for estimating \( R_\infty \) can be especially useful for \( z \) near the bottom because it incorporates the growing eigenmode \( g_1(z) = v_1 \exp(c z) \) (see Appendix C) that is needed to account for the asymptotic contribution of the bottom boundary condition. An advantage of the DMRM is that the bottom albedo \( R_b \) need not be known, but a disadvantage is that differences of noisy irradiance measurements potentially can lead to large errors.

For the SMRM one needs to know the bottom albedo \( R_b \) and the depth of the water column \( z_b \). From measurements of \( R(z) \) at arbitrary geometric depth \( z \), \( R_\infty \) can be predicted from

\[
R_\infty = \{ R(z) - R_b \exp(-2K_d(z)(z_b - z)) \} / \{ 1 - \exp(-2K_d(z)(z_b - z)) \}. \tag{43}
\]

The values of \( R_\infty \) predicted by the AM, where \( R_\infty = R(z) \), the DMRM, and the SMRM are shown as a function of depth in Figs. 14 and 15. Estimates of \( R_\infty \) from the SMRM require an estimate of \( K_c \); however, it was found that these estimates are not very sensitive to \( K_c \), and the approximation \( K_c = K_d(\tau) \) was used in Figs. 14 and 15. It can be seen that the DMRM method does poorly compared with the AM near the surface but yields much better estimates than the AM below mid-depth. The SMRM method performs better than the DMRM near the surface, but performs worse than the DMRM near the bottom. Both the DMRM and the SMRM give the best estimates of \( R_\infty \) at mid-depths, away from both boundaries.

Estimates of \( R_\infty(\tau) \) from the DMRM method are more susceptible to noise in the irradiance measurements than are those from the SMRM or AM. However, smoothing of \( R_\infty(\tau) \) was found to be effective in reducing this noise in simulated data, making good estimates of \( R_\infty \) from the DMRM possible.

Profiles of \( K_d(z) \) tend to be less influenced by the bottom depth and albedo than are \( R(z) \), especially if the bottom is highly absorbing. Similar to \( R(z) \), \( K(\tau) \) tends to be closest to \( K_c \) at its minimum, maximum, or inflection point. Unfortunately, a shallow-water method such as those for \( R_\infty \) could not be developed for \( K_\infty \).

9. IOP Estimation in Inhomogeneous Waters

For inhomogeneous waters, \( R_\infty \) and \( K_\infty \) as computed from Eqs. (13) and (14) now depend on the local IOP’s at \( z \), so that \( R_\infty(z) \) and \( K_\infty(z) \) are a function of depth. If the optical properties vary only gradually with depth, then \( R(z) \approx R_\infty(z) \) and \( K_d(z) \approx K_\infty(z) \) below the depths where the surface illumination dominates. On the other hand, if the optical properties are highly variable with depth, some type of weighted average of the IOP’s can be estimated, but the fine structure cannot be determined accurately.

Figure 16 shows a simulated example of three distinct water layers. For all three layers \( g = 0.85 \), but \( \omega_0 = 0.7, 0.65, \) and 0.60, from top to bottom. Shown are \( R_\infty \) from Eq. (13), the local irradiance ratio \( R(\tau) \), and the estimate of \( R_\infty(\tau) \) from the DMRM. The AM for estimating \( R_\infty(\tau) \) in the three layers could be applied by one taking the maximum \( R(\tau) \) in the upper layer, the inflection point in the middle layer, and the asymptotic value in the deep bottom layer. Because the top two layers in this case are both affected by a distinctly different layer below them, estimates of \( R_\infty \) from the DMRM are more accurate than those from the AM just above the interfaces, but are less accurate just below the interfaces. Both methods do a good job of identifying the location of the interfaces.

10. Summary

We have tested numerically an inverse radiative transfer method for estimating two inherent optical
properties from the irradiance ratio \( R(z) \) and the downward diffuse attenuation coefficient \( K_d(z) \) computed from upward and downward irradiance measurements. The method involves two steps. First, the IOP’s \( R_\infty \) and \( K_\infty \) are estimated from \( R(z) \) and \( K_d(z) \). Second, IOP's such as \( a \) and \( b_0 \) are calculated from the analytical equations in (13) and (14) for \( R_\infty \) and \( K_\infty \).

The simplest approach to the first step is to use the AM, where it is assumed \( R_\infty = R(z) \) and \( K_\infty = K_d(z) \). In deep waters, the exponential method of Eqs. (18) and (19) can yield better results than the AM if only shallow irradiance measurements are available. On the other hand, in shallow waters the DMRM and SMRM reflectance models of Eqs. (42) and (43) yield better estimates for \( R_\infty \) than the AM, but we were unable to develop a deep- or shallow-measurement diffuse attenuation coefficient model.

In the second step, a scattering phase function is assumed, and \( \omega_0 \) is estimated from \( R_\infty \) with an iterative search. The values of \( a \) and \( b_0 \) are then calculated from \( \omega_0 \) and \( K_\infty \). This approach was compared with Haltrin’s model that relates \( a \) and \( b_0 \) to \( R_\infty \) and \( K_\infty \) through two closed-form equations (39) and (41). Although Haltrin’s model is easier to implement, it is generally less accurate because no a priori information about the scattering phase function can be incorporated.

Example numerical calculations and a sensitivity analysis have shown that the absorption coefficient and the Gordon parameter \( G = b_0/(a + b_0) \) can be estimated quite well even if the scattering asymmetry factor is unknown. However, it was shown with use of the two-term Heneyy–Greenstein phase function that, because \( b_0 \) is sensitive to the backscattering portion of the phase function, it is important to use a realistic scattering phase model, such as a Petzold phase function, in the inverse solution.

**Appendix A: Deep-Water Asymptotic Irradiance Ratio and Diffuse Attenuation Coefficient**

The radiance for a source-free (i.e., no fluorescence or Raman scattering effects) homogeneous medium can be expressed as a superposition of eigenmodes of Eq. (9). The downward irradiance \( E_d(z) = E_d(z) \) and the upward irradiance \( E_u(z) = E_u(z) \) are obtained from an integration of the radiance over \( \mu \) with Eqs. (6) and (7):

\[
E_\pm(z) = \sum_{j=1}^J [C(\nu_j) g_\pm(\pm \nu_j) \exp(-cz/\nu_j)] + C(-\nu_j) g_\pm(\pm \nu_j) \exp(\nu_j/\nu_j), \tag{A1}
\]

where

\[
g_\pm(\nu_j) = \int_{\mu_0}^1 \phi(\nu_j, \mu) d\mu, \tag{A2}
\]

and the expansion coefficients \( C(\nu) \) depend on the IOP's and the surface illumination and bottom albedo boundary conditions. Beyond a couple of optical depths from either of the boundaries, the eigenvalues \( \nu_j \) make the dominant contributions so Eq. (A1) can be approximated by

\[
E_\pm(z) \approx [\nu_j(1 \pm R_\infty)]C(\nu_j) \exp(-cz/\nu_j)
+ C(-\nu_j) \exp(\nu_j/\nu_j), \tag{A3}
\]

and for deep waters where there are no bottom effects, \( C(-\nu_j) \to 0 \) and

\[
R_\infty = g_\pm(\nu_j)/g_\pm(\nu_j), \tag{A4}
\]

which is Eq. (13). In a similar manner, use of Eq. (A3) with \( C(-\nu_j) = 0 \) and Eq. (8) yields \( K_\infty \) of Eq. (14).

**Appendix B: Relationship between the Sensitivity Coefficients of the Forward and Inverse Problems**

The sensitivity coefficients for the inverse problem (the computation of \( \omega_0 \) and \( \nu_j \) from \( R_\infty \) and \( g \)) can be computed more easily when they are expressed in terms of partial derivatives of the forward problem (the computation of \( R_\infty \) and \( \nu_j \) from \( \omega_0 \) and \( g \)). Let the superscript \( f \) denote forward-problem variables, which depend on \( \omega_0 \) and \( g \), and unmarked variables denote inverse-problem variables. If we make a transformation of variables and use the Jacobian of the transformation, it follows that

\[
\frac{\partial \omega_0}{\partial R_\infty} = \frac{1}{\partial R_\infty^{\prime}/\partial \omega_0}, \tag{B1}
\]

\[
\frac{\partial \omega_0}{\partial g} = -\frac{1}{\partial R_\infty^{\prime}/\partial \omega_0} \frac{\partial R_\infty^{\prime}/\partial g}, \tag{B2}
\]

where \( R_\infty^{\prime} \) is computed directly from Eq. (13). These results are consistent with those of Fig. 2. Furthermore, from the chain rule and the previous two equations,

\[
\frac{\partial \nu_j}{\partial R_\infty} = \frac{\partial \nu_j}{\partial \omega_0} \frac{\partial \omega_0}{\partial R_\infty} = \frac{\partial \nu_j}{\partial \omega_0} \frac{1}{\partial \omega_0^{\prime}/\partial \omega_0}, \tag{B3}
\]

\[
\frac{\partial \nu_j}{\partial g} = \frac{\partial \nu_j}{\partial \omega_0} \frac{\partial \omega_0}{\partial g} = \frac{\partial \nu_j}{\partial \omega_0} \frac{\partial \nu_j^{\prime}/\partial \nu_j}{\partial \omega_0} \frac{1}{\partial \omega_0^{\prime}/\partial \omega_0}, \tag{B4}
\]

**Appendix C: Estimation of the Asymptotic Irradiance Ratio Near the Bottom**

1. Derivation of the DMRM

From Eqs. (A3) and (A4),

\[
E_\pm(z) \approx g_\pm(\nu_j)(1 \pm R_\infty)[C(\nu_j) \exp(-cz/\nu_j)
+ C(-\nu_j) \exp(\nu_j/\nu_j)]. \tag{C1}
\]
After squaring the last equation we can see that
\[
[E_+(z) \pm E_-(z)]^2 \approx g(Cv_1)(1 \pm R_c)[C^2(v_1) \\
\times \exp(-2cz/v_1) + C^2(-v_1) \\
\times \exp(2cz/v_1) \pm 2C(v_1)C(-v_1)].
\] (C2)

Equation (42) follows after we evaluate this equation at two depths \(z_1\) and \(z_2\) and take the difference of the results.

2. Derivation of the SMRM

From Eqs. (A3) and (A4),
\[
R(z) = \frac{E_+(z)}{E_-(z)} = \frac{R_c + C(-v_1)\exp(2cz/v_1)/C(v_1)}{1 + C(-v_1)R_c \exp(2cz/v_1)/C(v_1)},
\] (C3)
so it follows that
\[
R(z) - R_c = \frac{C(-v_1)(1 - R_c)\exp(2cz/v_1)/C(v_1)}{1 + R_cC(-v_1)\exp(2cz/v_1)/C(v_1)}.
\] (C4)

For \(z\) in Eq. (C4) just below the surface,
\[
R(0^+) - R_c = \frac{C(-v_1)(1 - R_c)/C(v_1)}{1 + R_cC(-v_1)/C(v_1)},
\] (C5)
whereas for \(z\) in Eq. (C4) at the bottom, \(z = z_b\), the reflectance equals the bottom albedo \(R_b\), and
\[
R_b - R_c = \frac{C(-v_1)(1 - R_c)\exp(2cz_b/v_1)/C(v_1)}{1 + R_cC(-v_1)\exp(2cz_b/v_1)/C(v_1)}.
\] (C6)

From Eqs. (C5) and (C6),
\[
(R_b - R_c)\exp(-2cz_b/v_1) = \frac{[R(0^+) - R_c][1 + C(-v_1)R_c/C(v_1)]}{1 + R_cC(-v_1)\exp(2cz_b/v_1)/C(v_1)}.
\] (C7)

If \(R_cC(-v_1)/C(v_1) \approx 1\), then
\[
(R_b - R_c)\exp(-2cz_b/v_1) \approx R(0^+) - R_c.
\] (C8)

It follows that if the bottom albedo is known and \(K_c \approx c/v_1\) is estimated from \(E_d(z)\), then \(R_c\) can be estimated from \(R(0^+)\):
\[
R_c = [R(0^+) - R_c \exp(-2K_cz_b)]/[1 - \exp(-2K_cz_b)].
\] (C9)

This equation has been used by others, e.g., Ref. 27. Equation (43) is a generalization away from \(z = 0^+\) and uses either the local \(K_d(z)\) or the best estimate of \(K_c\).

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