Comparative analysis of selected radiative transfer approaches for aquatic environments

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A comparative analysis is presented of simple approaches to radiative transfer in plane-parallel layers, such as the self-consistent Haltrin approach, the Chandrasekhar–Klier exact solution for isotropic scatters, an extended version of two-flux radiative Kubelka–Munk theory, the neutron-diffuse Gate–Brinkworth theory, and different versions of the $\delta$-Eddington theory. It is shown that the Haltrin approach is preferable to others and can be used for the solution of an inverse optical problem of the estimation of absorption and backscattering coefficients of aquatic environments from measured apparent optical properties. Two different methods of transformation from measured irradiance reflectance at combined illumination to irradiance reflectance induced by diffuse illumination only are developed. An analysis of the use of the different models for estimation of the effect of the bottom albedo is also presented. © 2005 Optical Society of America

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1. Introduction

Inherent optical properties (IOP's), such as the average cosine of scattering $\bar{\mu}$, the volume coefficients of absorption $a$, scattering $b$, and backscattering $b_b$, and the volume beam-attenuation coefficient $c$, are potentially expedient variables for the characterization of aquatic environments. The independence of IOP's on Sun position and weaker spatial (horizontal and vertical) variability of IOP's in comparison with apparent optical properties (AOP's), such as the average cosine of the underwater light field $\bar{\mu}$, the diffuse attenuation coefficient $k$, and the reflectance coefficient $\bar{R}$, suggest the use of these properties as the output of inverse optical models, whereas measured AOP's serve as the input of such models.

The majority of existing practical methods for the estimation of IOP's in natural waters is based on semianalytic inverse optical models. In turn, these models are derived from the radiative-transfer consideration with the application of such tools as the Snell, the Fresnel, and the Gershun laws, the Mie and the Hulst theories, Monte Carlo simulations, algebraic nonlinear optimization, principal component analysis, and the neural network approach. In addition to the above-mentioned simulations, Haltrin and colleagues developed in recent years a simple two-flux approach to the solution of the light transfer problem for irradiance in waters with arbitrary turbidity, depth, and surface illumination. The basis of this approach is the presentation of the underwater light field with irradiance traveling in two directions: downward and upward. The distinctive features of such an approach are as follows: (1) the system of equations used is equivalent to the original radiative transfer equation, yielding the same values of irradiances; (2) the scattering phase function is chosen to obtain an analytical solution that relates IOP's to AOP's; and (3) the diminution of the loss of accuracy is achieved by use of empirical relations between the average cosine for downward irradiance $\bar{\mu}_d$ and the total average cosine $\bar{\mu}$.

Verification of the self-consistent Haltrin approach for the reflectance coefficient in a semi-infinite medium illuminated by diffuse light was carried out by comparison with some other approaches and demonstrated excellent agreement with the experimental results of Timofeeva and the semianalytical model of Gordon et al. It is clear, however, that, in real aquatic environments, the reflectance coefficient depends on two constituents of incoming irradiance: direct solar and diffuse sky. Thus, for the solution of the radiative transfer problem under natural conditions, at least two additional parameters should be taken into consideration, namely, the parameter rep-
representing the relation between direct and diffuse incoming radiation and the parameter describing the Sun’s position.

We consider two different approaches for the solution of the problem of estimation of the reflectance coefficient of a plane-parallel semi-infinite layer illuminated by diffuse light \( R_{\text{dir}} \). This coefficient is derived from the easily measured reflectance coefficient \( R_{s} \) of such a layer when it is illuminated by natural (direct and diffuse) light, the solar zenith angle \( \theta_0 \), and the direct-to-diffuse incoming irradiance ratio \( s \). Two other problems are connected with the first problem and to each other; they also are considered in this paper: (2) an estimation of the diffuse reflectance coefficient and to each other; they also are considered in this paper: (2) an estimation of the diffuse reflectance coefficient \( R_{\text{diff}} \) at any distance to the bottom \( \Delta Z = Z_B - Z \) (where \( Z_B \) is the bottom depth and \( Z \) is the current depth) from \( R_{s} \), the diffuse attenuation coefficient in the asymptotic light regime \( k_{\text{a}} \) and the bottom albedo \( A_{\text{b}} \), and (3) an estimation of the absorption and the scattering properties [the diffuse absorption coefficient \( K \) and the diffuse scattering coefficient \( S \) of the Kubelka–Munk (KM) theory, and the volume absorption coefficient \( a \) and the volume backscattering coefficient \( b_{\text{h}} \) of other theories and approaches] in finite and semi-infinite layers from \( \Delta Z \), \( R_{s} \), and \( k_{\text{a}} \).

The main tool for the solution of the above-mentioned problems is the self-consistent Haltrin approach. In addition, this study includes an analysis of other theories and approaches, such as Monte Carlo simulations by Kirk and by Morel and Gentili, the exact solution of Chandrasekhar’s radiative transfer equation obtained by Klier for isotropic scattering, the extended version of the two-flux radiative KM theory, the neutron diffuse Gate–Brinkworth theory, different versions of the \( \bar{\alpha} \)-Eddington theory, and some other approaches.

2. Reflectance Models

A. Haltrin Model

We represent the total irradiance reflectance within any plane-parallel layer \( R = E_u/E_d \) (where \( E_u \) is the total upward irradiance and \( E_d \) the total downward irradiance) as a superposition of the diffuse reflectance coefficient owing to direct illumination \( R_{\text{dir}} \) and the diffuse reflectance coefficient owing to diffuse illumination \( R_{\text{diff}} \), as follows:

\[
R = \frac{E_{u,d} + E_{u,d}^{\text{dir}}}{E_{d,d} + E_{d,d}^{\text{dir}}} = \frac{R_{\text{dir}} E_{d,d}^{\text{dir}} + R_{\text{diff}} E_{d,d}^{\text{diff}}}{E_{d,d}^{\text{dir}} + E_{d,d}^{\text{diff}}} = \frac{s R_{\text{dir}}^{\text{dir}} + R_{\text{diff}}^{\text{diff}}}{1 + s}, \quad s = \frac{E_{u,d}^{\text{dir}}}{E_{d,d}^{\text{dir}}},
\]

where \( E_{u,d}^{\text{dir}} \) and \( E_{d,d}^{\text{diff}} \) are the direct and the diffuse parts of the downward irradiance, respectively, and \( E_{u,d}^{\text{diff}} \) and \( E_{d,d}^{\text{diff}} \) are parts of the diffuse upward irradiance that are caused by direct and diffuse illumination, respectively.

In accord with the Haltrin model, the values of reflectance constituents and hence the reflectance coefficient itself, are assumed to be the same throughout the water column far away from the colored bottom layer. For an optically semi-infinite plane-parallel layer with a scattering isotropic phase function in the backward hemisphere, the reflectance coefficient of the surface illuminated by direct sunlight \( R_{\text{dir}} \) expressed as a function of the cosine of the refracted solar zenith angle just below the surface \( \mu_w \) and the average cosine of the asymptotic light field (i.e., when optical properties are assumed to be invariant with depth) \( \mu_{\text{as}} \) is as follows:

\[
R_{\text{dir}} = \frac{(1 - \mu_{\text{as}}^2)}{1 + \mu_{\text{as}}(4 - \mu_{\text{as}}^2)}.
\]

The reflectance coefficient of an optically semi-infinite plane-parallel layer that is illuminated by diffuse skylight \( R_{\text{diff}} \) with the transport approximation to the scattering phase function and far away from the bottom was related with \( \mu_{\text{as}} \) by the following simple formula:

\[
R_{\text{as}} = \frac{(1 - \mu_{\text{as}}^2)}{1 + \mu_{\text{as}}}.
\]
partly collimated, regardless of the angle of solar incidence.\textsuperscript{27} Thus, we can assume that at sufficiently deep layers the approximated equalities \( R_{\text{dir}}(Z) = R_{\text{dif}}(Z) = R(Z) \) hold. Note that the equality of \( R_{\text{dif}} \) to \( R_{\text{dir}} \) for case 1 waters (see Table 1) [with \( R \in [0.001, 0.1] \), see, e.g., Refs. 3 and 12] is achieved at lower solar zenith angles than for case 2 waters (for which the range \( R \in [0.01, 0.3] \) was assumed). A more rigorous analysis of Eqs. (2) and (3) shows that the relations \( 0 < R_{\text{dif}} = R_{\text{dir}} - R_{\text{dif}} < 1/9 \) holds at values of \( \mu_{w} \), satisfying the following conditions: \( 2/3 < \mu_{w} = [3R_{e} + 2(R_{e} - 1)^{1/2}]/(9R_{e} - 1) = 1/(2 - \mu_{e}) < 1 \). In a more general case for any \( \mu_{w} \in [0.666, 1] \), \( R_{\text{dif}} \) is not equal to \( R_{\text{dir}} \) and \( R_{\text{dif}} \) from measured \( \mu_{w} \) and \( R_{e} \) by approximated formulas. Below, a formula constructed for \( R_{\text{dif}} \) is presented that is more suitable than \( R_{\text{dir}} \) for the purposes of the present study:

\[
R_{\text{dif}} = R_{e}(1 + 2R_{e}[\mu_{w}(1 - R_{e})]^{2}).
\]  

(4)

The accuracy of Eq. (4) for the model’s complete parameter set of \( \mu_{w} \in [0.666, 1] \), \( \mu_{e} \in [0, 1] \), and \( s \in [0, \infty) \) was estimated; further, \( \mu_{e} \) was calculated by analytical inversion of Eq. (3) and then also estimated. Calculations show that, for the total natural range of variability of parameter \( s \) (\( s \in [1, 7] \)), see Ref. 40) the error, expressed in this paper by means of the normalized root-mean-square error, (NRMSE), for \( R_{\text{dif}} \) and \( \mu_{e} \) did not exceed 8.6% and 2.0%, respectively (see Table 1).

Equation (2) was derived under the assumption of an isotropic phase function in the backward hemisphere. However, it may be not valid in real, especially turbid, aquatic environments for either case 1 or 2 waters. Besides, experimental data from different authors contradict this formula and demonstrate a stronger dependence of \( R_{\text{dif}} \) on the solar zenith angle. A more detailed consideration of this issue and an alternative approach to the estimation of \( R_{\text{dif}} \) from \( R_{e} \) are proposed in Section 4 of this paper.

Now let us consider the reflectance \( R_{\text{dif}} \) from a homogeneous shallow layer with a bottom depth \( Z_{b} \) and a Lambertian bottom albedo \( A_{B} \). In accord with the Haltrin model, \( R_{\text{dif}} \) at depth \( Z \) can be expressed as \textsuperscript{17,18}

\[
R_{\text{dif}}(Z) = \frac{R_{e}(\mu_{e}(Z)Z_{B} - 7 + 2\mu_{e} - 2)}{1 - R_{e}[A_{B}]} \exp\left[\frac{Z_{B} - Z}{3}\right],
\]  

(5)

where \( k_{s} \) is the diffuse attenuation coefficient in the asymptotic light regime.

Equations (3) and (5)–(7) permit the prediction of vertical variations in \( R_{\text{dif}}(Z) \) if \( R_{e} \) and \( k_{s}(Z_{B} - Z) \) are known or estimated. The physical sense of the last product follows from the Lambert–Beer law for irradiance transmittance \( T_{b} \) of a layer with a perfectly black bottom (i.e., at \( A_{B} = 0 \)) from a current depth \( Z \) to the bottom depth \( Z_{b} \) in the asymptotic regime with a radiance distribution symmetrical about the vertical axis\textsuperscript{42}:

\[
T_{b} = \frac{E_{0}(Z_{B})}{E_{0}(Z)} = \exp\left[\frac{-a}{\bar{\mu}_{e}(Z_{B} - Z)}\right]
\]  

(8)

where \( E_{0}(Z) \) and \( E_{0}(Z_{B}) \) are scalar irradiances at depths of \( Z \) and \( Z_{B} \), respectively.

It is important to note that, in real aquatic environments, a quality \( k_{s} \) can be replaced with high accuracy by the attenuation coefficient for downward irradiance in the asymptotic light regime.\textsuperscript{38,43–47} Following the authors of Refs. 45, 48, and 49, we call a quality \( k_{s}\Delta Z \) (\( \Delta Z \) is the thickness of any plane-parallel layer, in particular, \( \Delta Z = Z_{b} - Z \)) an optical depth for the diffuse attenuation coefficient, denoted by \( \tau_{b} \).

Numerical simulations of the vertical variability of \( R_{\text{dif}}(Z) \) with \( \tau_{b} \) near the bottom were carried out for values of \( R_{\text{dif}}(2\%, 10\%, \text{and } 20\%) \) typical for natural waters\textsuperscript{12} and \( A_{B} (0\%, 20\%, \text{and } 60\%) \) typical for dif-

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Table 1. Estimated Accuracy (NRMSE) for the Estimation of \( R_{\text{dif}} \) and \( \mu_{e} \) by Use of Eqs. (4) and (3), Respectively

<table>
<thead>
<tr>
<th>Estimated Parameter</th>
<th>Water-Type Case</th>
<th>( s = 0 )</th>
<th>( s = 1 )</th>
<th>( s = 2 )</th>
<th>( s = 3 )</th>
<th>( s = 4 )</th>
<th>( s = 5 )</th>
<th>( s = 6 )</th>
<th>( s = 7 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R_{\text{dif}} )</td>
<td>1</td>
<td>5.2</td>
<td>3.9</td>
<td>5.9</td>
<td>7.0</td>
<td>7.7</td>
<td>8.1</td>
<td>8.4</td>
<td>8.6</td>
</tr>
<tr>
<td>( R_{\text{dif}} )</td>
<td>2</td>
<td>13.7</td>
<td>4.9</td>
<td>2.2</td>
<td>1.5</td>
<td>1.9</td>
<td>2.3</td>
<td>2.6</td>
<td>2.9</td>
</tr>
<tr>
<td>( R_{\text{dif}} )</td>
<td>1 and 2</td>
<td>16.7</td>
<td>6.0</td>
<td>2.7</td>
<td>2.0</td>
<td>4.0</td>
<td>2.9</td>
<td>3.2</td>
<td>3.6</td>
</tr>
<tr>
<td>( \bar{\mu}_{e} )</td>
<td>1</td>
<td>0.4</td>
<td>0.5</td>
<td>0.7</td>
<td>0.8</td>
<td>0.8</td>
<td>0.9</td>
<td>0.9</td>
<td>0.9</td>
</tr>
<tr>
<td>( \bar{\mu}_{e} )</td>
<td>2</td>
<td>5.4</td>
<td>2.0</td>
<td>1.1</td>
<td>1.1</td>
<td>1.4</td>
<td>1.5</td>
<td>1.7</td>
<td>1.8</td>
</tr>
<tr>
<td>( \bar{\mu}_{e} )</td>
<td>1 and 2</td>
<td>3.0</td>
<td>1.2</td>
<td>0.8</td>
<td>1.0</td>
<td>1.1</td>
<td>1.2</td>
<td>1.3</td>
<td>1.3</td>
</tr>
</tbody>
</table>

In percent.

\[
\bar{R}_{\text{dif}}(Z) = \frac{R_{e}(\mu_{e}(Z)Z_{B} - 7 + 2\mu_{e} - 2)}{1 - R_{e}[A_{B}]} \exp\left[\frac{Z_{B} - Z}{3}\right].
\]  

(6)

\[
\xi(Z) = A_{B} - R_{e} \exp\left[-\frac{Z_{B} - Z}{3}\right].
\]  

(7)

\[
\xi(Z) = A_{B} - R_{e} \exp\left[-\frac{Z_{B} - Z}{3}\right].
\]  

(7)
ifferent bottom substrates [Fig. 2(a)]. The results clearly demonstrate that, at any value of $R_{\text{diff}}/H$ and $AB$, $R_{\text{diff}}/H$ approaches $R_{\text{diff}}$ and becomes invariant to the impact of the bottom when $\tau_k > 2–3$.

B. Kubelka–Munk Model

The basis of another popular two-flux radiative theory for turbid plane-parallel layers with isotropic scattering (the Kubelka–Munk (KM) theory) was formulated in the beginning of the twentieth century. This theory has essentially been expanded and further developed throughout the following years. For the reflectance coefficient of a layer illuminated by diffuse light $R_{\text{diff}}$ the extended KM theory yields

$$R_{\text{diff}} = \frac{2A R_b A_B - R_b - A_B}{R_b A_B - 1}, \quad (9)$$

where the reflectance coefficient for the layer with a perfectly black bottom $R_b$ is determined as

$$R_b = 1 + \frac{K / S - [K / S (K / S + 2) + T_b^2]}{T_b} \exp(-\tau_k). \quad (10)$$

In Eq. (10) parameter $A$ and the ratio of the diffuse absorption coefficient $K$ to the diffuse scattering coefficient $S$ (the so-called remission function) are the functions of $R_{\text{diff}}$ as follows:

Fig. 2. Dependence of the reflectance coefficient for a plane-parallel layer illuminated by diffuse light $R_{\text{diff}}$ on the optical depth for the diffuse attenuation coefficient $\tau_k$ at selected values of the diffuse reflectance coefficient for an infinite layer $R_{\text{diff}}$ (solid curves, squares, and triangles for 2%, 10%, and 20%, respectively) and the bottom albedo $A_B$ (solid, long-dashed, and short-dashed curves for 0%, 20%, and 60%, respectively): (a) Haltrin model, (b) KM model, (c) CK model, (d) Lyzenda model, and (e) Albert–Mobley model.
A = 0.5(R_\text{e, dif} + 1/R_\text{e, dif}) \quad (11)
\frac{K}{S} = A - 1 = 0.5(R_\text{e, dif} - 1)^2 / R_\text{e, dif} \quad . \quad (12)

Note that Eq. (9) can also be expressed in the equivalent form

\[ R_\text{dif} = \frac{1 - A_B[A - B \coth(BS\Delta Z)]}{A + B \coth(BS\Delta Z) - A_B} \quad , \quad (13) \]

where

\[ BS\Delta Z = \arcoth \left( \frac{1 - AR_\text{b}}{BR_\text{b}} \right) \quad , \quad (14) \]

\[ B = (A^2 - 1)^{1/2} = 0.5(R_\text{e, dif} - 1/R_\text{e, dif}) \quad . \quad (15) \]

The vertical variations of \( R_\text{dif}(\tau_b) \) were plotted for the same parameters of \( R_\text{e, dif} \) and \( A_B \) as for the Haltrin model [Fig. 2(b)] and demonstrated a similar behavior but with one small difference: The optical depth value, for which \( R_\text{dif}(\tau_b) \) becomes indistinguishable from \( R_\text{e, dif} \), is greater than that for the Haltrin model (beginning from \( \tau_b \approx 3-4 \)).

C. Chandrasekhar–Klier Model

In 1960, Chandrasekhar formulated the radiative transfer equation,\(^{25}\) and, in 1972, Klier\(^{24}\) developed its exact solution for isotropic distribution of scattered photons. Below, we compare the solution of Klier for the reflectance \( R_\text{dif} \) with the less exact KM approximation. Taking into account that the parameter \( \phi \) of Klier can be expressed in the form \( \phi = -1/R_\text{e, dif} \) and changing designations in the Chandrasekhar–Klier (CK) model to designations that are more adequate for the present study, we get

\[ R_\text{dif} = \frac{1 - A_B(A - B \coth \tau_b)}{A + B \coth \tau_b - A_B} \quad , \quad (16) \]

where the parameters \( A \) and \( B \) are determined by Eqs. (11) and (15).

The above solution, in its general form, is numerically different from the KM solution [Eq. (13)], although Klier in his paper states (without a proof) that both solutions are formally identical. I believe that the identities of both approaches exist only in the case of infinite layers, and I prove this statement in Subsection 3.A, below. Now I wish only to note that the difference between the KM and the CK solutions increase with the increase of the layer reflectance and with the decrease of the optical depth. For aquatic environments with a reflectance of \( R_\text{e, dif} < 20\% \) the difference seems quite insignificant [compare Figs. 2(b) and 2(c) for both solutions]. Numerical analysis of Eqs. (13) and (16) carried out for \( \tau_b \in [0, 4] \) and the model values of parameters \( R_\text{e, dif}: 2\%, 10\%, 20\% \) and \( A_B: 0\%, 20\%, 60\% \) yields a NRMSE difference of approximately 1.4\% for the KM solution in comparison with the CK solution.

D. Lyzenda Model

The following model was proposed by Lyzenda\(^{50}\) for irradiance reflectance:

\[ R_\text{dif} = R_\text{e, dif}[1 - \exp(-2\tau_b)] + A_B \exp(-2\tau_b) \quad . \quad (17) \]

It is the simplest approach and yields results close to those of the KM and the CK models [Fig. 2(d)]. However, they were slightly different from those of the Haltrin model.

E. Albert–Mobley Model

The recent Albert–Mobley model\(^{51}\) represents an improved Lyzenda model with the following differences: the new model distinguishes between the downward and the upward attenuation coefficients and between radiation reflected in the water column and from that reflected from the bottom. In addition, the authors introduce two coefficients to fit their model to results derived from the radiative-transfer program Hydrolight Version 3.1.\(^{52}\) However, the results of their simulations\(^{51}\) demonstrate that, at concentrations of total suspended matter greater than 3 mg/l, a backscatter probability of \( b_s/b_{\text{ss}} = 0.019 \), and at some other assumptions, characteristic for case 2 waters, all three attenuation coefficients are close to one another. Taking these simplifications into account, one obtains from their model

\[ R_\text{dif} = R_\text{e, dif}[1 - 1.0546 \exp(-2\tau_b)] + 0.9755A_B \exp(-2\tau_b) \quad , \quad (18) \]

i.e., results that are close to the above-considered models [see Fig. 2(e)] and that show maximal, although insignificant, divergence from Haltrin model.

3. Inverse Optical Models

In this section, we consider an inverse optical problem of the estimation of scattering properties (such as parameters \( S \) and \( b_s \)) and absorption (such as parameters \( K \) and \( a \)) from the measured reflectance coefficient. The solution of the inverse optical problem is only the first step to the elucidation of an inverse physical problem, such as an estimation of the concentration of a disperse phase in a two-phase colloidal system or of phytoplankton cells in an aquatic environment, particle size or cell distribution, individual optical and structural characteristics of pigmented and other particles, error predictions for IOP retrievals, and so forth. However, optical properties obtained as a result of the solution of an inverse optical problem cannot be considered to be true, as they depend on the approach selected. Therefore, this study refers not only to various optical models but also to the formulas connecting optical characteristics derived by different approaches. For simplicity a diffuse scattering coefficient \( S \) and a diffuse absorption coefficient \( K \) of the KM theory are chosen as the basic optical properties.
A. Kubelka–Munk Model

The principal distinction of the extended KM theory from any other theory that considers nonasymptotic optical fields consists of two assumptions: (1) the parameters $K$ and $S$ vary along the vertical coordinate, and (2) the ratio $K/S$ is considered to be a constant that is independent of the vertical location for any given medium.30,31 According to this theory $S$ is considered to be a constant because of numerical errors arising from the calculation of $\mu_s$. Therefore, the calculation of $K_s$ at various $\tau_b$ results in the following expressions for $R_s$ and $S$: 

$$R_{b,s} = R_s^{\text{diff}} (1 - T_b^{2}) = R_s^{\text{diff}} [1 - \exp(-2\tau_b)], \quad (19)$$

$$p_{S,s} = \tau_b / B, \quad S_s = k_{s} / B. \quad (20)$$

Now, if we compare Eqs. (13) and (16) and take into account Eq. (20), it can be proved that the KM and the CK models are identical for the case of infinite layers. It should also be noted that, in the calculation of $p_{S,s}$ one encounters serious difficulties at large values of $\tau_b$ because of numerical errors arising from the calculation of $R_b$ by Eq. (10). Therefore, the calculation of $p_{S,s}$ at large $\tau_b$ (at approximately 10–20, depending on $R_s^{\text{diff}}$) could be carried out from the preliminarily established linear regression between $p_{S,s}$ and $\tau_b$. Note that, at $R_s^{\text{diff}} = 2^{1/2} - 1 = 0.414$, parameter $B = 1$; hence, $p_{S,s} \rightarrow \tau_b$ and $S \rightarrow k_s$. At large $\tau_b$:

$$K_s = k_s (1 - R_s^{\text{diff}}) / (1 + R_s^{\text{diff}}). \quad (21)$$

By analogy with a scattering power, a term, the absorption power $p_K = (\Delta Z)K$, is coined. The dependence of $p_K$ versus $\tau_b$ (Fig. 4) is similar to the dependence of $p_S$ versus $\tau_b$, with, however, an oppositely oriented dependence on $R_s^{\text{diff}}$. It is also interesting to note that, for a completely nonscattering medium when $S = 0$ and $R_s^{\text{diff}} = 0$, from Eq. (21) follows an expected equivalency between $K_s$ and $k_s$; hence, equivalency exists between $p_K$ and $\tau_b$.

B. Haltrin Model

The relation between the true or volume absorption coefficient $a$ and the input parameters $k_s$ and $R_s^{\text{diff}}$ can be established from Eq. (3) and the Gershun law.54

$$k_s = a / \bar{\mu}_s, \quad (22)$$

as follows:

$$a = k_s \frac{1 - (R_s^{\text{diff}})^{1/2}}{1 + (R_s^{\text{diff}})^{1/2}}. \quad (23)$$

The relation between the ratio $a/b_b$ and $R_s^{\text{diff}}$:

$$\frac{a}{b_b} = \frac{\left[1 - (R_s^{\text{diff}})^{1/2}\right]^2 \left[1 + 4(R_s^{\text{diff}})^{1/2} + R_s^{\text{diff}}\right]}{4R_s^{\text{diff}}}, \quad (24)$$

was derived by Haltrin13,17 within the framework of his self-consistent approach and exhibited a high degree of closeness14,17 to the well-known equation of Gordon et al.24 Solving Eqs. (23) and (24) together, we obtain a relation between the backscattering coefficients $b_b$, $k_s$, and $R_s^{\text{diff}}$:

$$b_b = \frac{4k_s}{(1 / R_s^{\text{diff}} - 1) \left[1 + 4(R_s^{\text{diff}})^{1/2} + R_s^{\text{diff}}\right]^2}. \quad (25)$$

Plots of the relations between $\bar{\mu}_s = a/k_s$, $a/b_b$, $b_b/k_s$, $R_s^{\text{diff}}$, and the input $R_s^{\text{diff}}$ are shown in Fig. 5.
in other words, we assume that $A_B = R_{\text{diff}}$ and $\tau_k \to \infty$.

Remembering that $\tau_k = (\Delta Z) k_z$ and taking into account Eqs. (14), (15), and (25), one can derive an expression relating the ratio $\sigma = S/b_b$ with the other optical parameters:

$$
\sigma^{(H)} = \frac{\text{arcoth}(1 - AR_b) / BR_b)}{1 + 4R_{\text{diff}}^{1/2} + R_{\text{diff}}},
$$

where the index H notes the Haltrin model. Similarly, from Eqs. (12), (14), (15), and (25), we derive an expression for $\kappa = K/a$:

$$
\kappa^{(H)} = \frac{\text{arcoth}(1 - AR_b) / BR_b)}{\tau_k} \frac{1 + 2R_{\text{diff}}^{1/2} + R_{\text{diff}}}{1 + R_{\text{diff}}^{1/2} + R_{\text{diff}}},
$$

Thus, Eqs. (10), (11), (15), (26), and (27) allow one to express the ratios $\sigma$ (Fig. 6) and $\kappa$ (Fig. 7) as functions of the input parameters $\tau_k$ and $R_{\text{diff}}$. The figure plots demonstrate a relatively weak dependence of $\sigma$ and $\kappa$ (and hence, of $S$ and $K$, respectively) on the optical depth at $R_{\text{diff}} < 0.3$; however, at increasing values of $R_{\text{diff}}$ this dependence is strengthened. At $\tau_k \to \infty$, taking into account Eqs. (20) and (21), we get the ratios $\sigma^{(H)} = S/b_b$ and $\kappa^{(H)} = K/a$ as functions of $R_{\text{diff}}$ (Fig. 8, below):

$$
\sigma^{(H)} = \frac{1 + 4R_{\text{diff}}^{1/2} + R_{\text{diff}}}{2(1 + R_{\text{diff}}^{1/2})},
$$

$$
\kappa^{(H)} = \frac{1 + 2R_{\text{diff}}^{1/2} + R_{\text{diff}}}{1 + R_{\text{diff}}^{1/2}},
$$

respectively. The limits of the coefficients $\sigma^{(H)}$ and $\kappa^{(H)}$ for small absorptions ($R_{\text{diff}} \to 0$) and for large absorptions ($R_{\text{diff}} \to 1$) are

$$
\lim_{R_{\text{diff}} \to 0}\sigma^{(H)} = 0.5, \quad \lim_{R_{\text{diff}} \to 0}\kappa^{(H)} = 1,
$$

$$
\lim_{R_{\text{diff}} \to 1}\sigma^{(H)} = 1.5, \quad \lim_{R_{\text{diff}} \to 1}\kappa^{(H)} = 2.
$$

Within the framework of the CK model the following expressions (in transformed form) for $\sigma_x$ and $\kappa_x$ were derived by Klier\textsuperscript{24} for isotropic scattering:

$$
\sigma_x^{(\text{CK})} = \frac{4\xi}{\omega_0(1/R_{\text{diff}} - R_{\text{diff}})},
$$

$$
\kappa_x^{(\text{CK})} = \frac{\xi(1 - R_{\text{diff}})}{(1 - \omega_0)(1 + R_{\text{diff}})},
$$

where the index (CK) denotes the CK model.
relations are also shown in Fig. 8. Here the eigenvalue of the radiative-transfer equation \( \xi = k_\alpha/c \) and the single-scattering albedo \( \omega_0 = b/c \) are related with the reflectance \( R_\infty \) by means of the following equations:

\[
\lim_{R_\infty \to 0} \sigma_\infty^{(CK)} = 2(1 - \ln 2) = 0.6137 \quad \lim_{R_\infty \to 0} \kappa_\infty^{(CK)} = 1 \quad \lim_{R_\infty \to 0} \omega_0^{(CK)} = 1.5 \quad \lim_{R_\infty \to 1} \omega_0^{(CK)} = 2
\]  

\[
R_\infty = \frac{\ln(1 + \xi) - \xi}{\ln(1 + \xi) + \xi}, \quad (33)
\]

\[
\omega_0 = \frac{2\xi}{\ln[(1 + \xi)/(1 - \xi)]}, \quad (34)
\]

Several other approaches that permit the prediction of \( \sigma_\infty \) and \( \kappa_\infty \) were also derived within the framework of the neutron diffuse theory by Gate and Brinkworth and of the \( \delta \)-Eddington approximation of the second-order and the fourth-order by Meador and Weaver. For isotropic scattering these approaches have the following forms:

\[
\sigma_\infty^{(GB)} = \frac{7\omega_0 - 4}{2\omega_0}, \quad \kappa_\infty^{(GB)} = 2, \quad \text{(40)}
\]

\[
\sigma_\infty^{(MW-2)} = \frac{4\omega_0 - 1}{2\omega_0}, \quad \kappa_\infty^{(MW-2)} = 2; \quad \text{(41)}
\]

\[
\sigma_\infty^{(MW-4)} = \frac{15 - (1 - \omega_0)k_\infty^{(MW-4)}(16 - 3k_\infty^{(MW-4)})}{\omega_0(16 - 3k_\infty^{(MW-4)})}, \quad \kappa_\infty^{(MW-4)} = \frac{224}{132 - 55\omega_0 + 35[1 + 2(1 - \omega_0)/35 + 121(1 - \omega_0)^2/49]^{1/2}}, \quad \text{(42)}
\]
where the indices (GB), (MW-2), and (MW-4) respectively denote the Gate–Brinkworth, the second-order δ-Eddington, and the fourth-order δ-Eddington models. To express the models through the parameter $R_d$, one combines them all with Eqs. (33) and (34). The most important conclusion to be drawn from this consideration is a strong variation of the ratio $\sigma_r$ with $R_d$ for all models (Fig. 8), especially in the range for which $R_d < 0.3$. An analogous conclusion for the ratio $\kappa_r$ holds for only several models (Haltrin, CK, and MW-4); these models show a monotonic increase of $\kappa_r$ from 1, 1, and 4/3, respectively, to 2, with an increase of $R_d$ from 0 to 1. For the GB and the MW-2 models an equality, $\kappa_r = 2$, is assumed. Monotonic behavior for $\sigma_r$ is yielded by only two models: the Haltrin and the CK. It is also interesting to note that linear relations between $\kappa_r$ and $\sigma_r$ are close for some sets of models:

$$\kappa_r^{(CM)} = \begin{cases} \sigma_r^{(CM)} + (0.449 \pm 0.027), & R_d \in (0, 0.3] \\ \sigma_r^{(CM)} + (0.464 \pm 0.031), & R_d \in (0, 1) \end{cases}$$

(43)

$$\kappa_r^{(MV-4)} = \begin{cases} \sigma_r^{(CM)} + (0.500 \pm 0.018), & R_d \in (0, 0.3] \\ \sigma_r^{(CM)} + (0.499 \pm 0.015), & R_d \in (0, 1) \end{cases}$$

(44)

$$\kappa_r^{(H)} = \sigma_r^{(H)} + 0.5, \quad \text{for any values of } R_d.$$  

(45)

The Haltrin model appears to be more attractive than other models owing to the fact that it deals with assumptions that are more adequate for aquatic environments, such as the conspicuously anisotropic phase-scattering function. It is also important to note that, from a comparison of the Haltrin and the CK models (Fig. 8), it is clear that the scattering anisotropy affects the measured reflectance coefficient. This influence is minimal at extreme values of the $\kappa_r/\sigma_r$ ratio (i.e., at extreme values of $R_d$), and it increases toward intermediate values. Therefore, the effect of selected scattering phase functions would be greater in the case of turbid, highly productive waters (when $\kappa_r/\sigma_r$ ratios vary from approximately 1.37 to approximately 1.72) than in the case of clear oceanic waters (when $\kappa_r/\sigma_r$ ratios vary from approximately 1.47 to approximately 2.00). This conclusion also corresponds to the findings of other experimental and theoretical investigations.

### 4. Alternative Approach to the Estimation of $R_d$ for Turbid, Highly Productive Waters

The dependence of the irradiance reflectance from the surface when illuminated by direct Sun rays $R_d$ on the solar zenith angle is stronger than is predicted by the Haltrin model, Eq. (2). For example, Morel and Gentili proposed a linear Morel–Gentili model (MGM) for the calculation of $R_d$ in semi-infinite oceanic layers at solar zenith angles of $\theta_0 < 70^\circ$ obtained by Monte Carlo simulation. Toward this aim, they used a forward-peaked, strongly asymmetric scattering phase function for particles adopted from a well-known Petzold function, with a constant backscattering particle probability (it was accepted as 0.0190). As a result, their model has the form of

$$R_d = [(0.6279 - 0.2227\eta_0 - 0.0513\eta_0^2) + (0.2465\eta_0 - 0.3119)\mu_0](b/\alpha), \quad (46)$$

where $\mu_0 = \cos \theta_0$ and $\eta_0$ is the ratio of the molecular water backscattering $b_w$ to the total (water plus particles) backscattering $b$. The result of the calculations of $R_d(\mu_0)$, normalized to $R_d$ for a zenith Sun, at selected values of the parameter $\eta_0$ is represented in Fig. 9(a). The corresponding values of $b/\alpha$, estimated from the Morel bio-optical model for case 1 waters are also shown in Fig. 9.

Another model was proposed by Kirk that was based on Monte Carlo simulations and on extensive experimental material obtained for a range of water types from clear oceanic to turbid harbor waters. Simulations were carried out for different phase functions (i.e., with varied $b_w/b$ ratios) but at a constant ratio of $b/\alpha = 2$. Taking Eqs. (20) and (24) of Kirk’s paper (Ref. 21) into account and generalizing formulas presented in his Table (3) (and using his data from Table 1 for water types 2 to 6), I derived the following dependence:

$$R_d = [0.31 + (2.181\mu_s - 1.654)(\mu_0^{-1} - 1)](b/\alpha), \quad (47)$$

where $\mu_s$ is the average cosine of scattering. Further, taking into account that $\mu_s$ is closely connected with $b_w/b$ by exponential dependence (as was derived by Sokolovskiy et al. based on the data of Kirk), and
most linearly with the decrease in $\mu_0$ and with the decrease in the $b_b/a$ ratio. The latter relation corresponds to the increase in water turbidity and the decrease in the parameter $\eta_0$. At solar zenith angles $\theta_0 > 70^\circ$ (i.e., at $\mu_0 < 0.34$) the KM, similarly to the MGM, shows an increasingly flat dependence of $R_s^{\text{dir}}$ on $\mu_0$.

Another important conclusion to be made from the comparison of these models is the existence of an upper limit of dependence of $R_s^{\text{dir}}$ on $\mu_0$ for turbid, highly productive aquatic environments. It seems that the upper enveloped curve can be derived from Eq. (46) at $\eta_0$ tending to 0 (as was also noted by Højerslev$^{60}$) as follows:

$$R_s^{\text{dir}} = (0.6279 - 0.3119\mu_0)(b_b/a).$$ (49)

This conclusion is also valid on a qualitative level for the self-consistent Haltrin model [Fig. 9(c)]; however, there is a much flatter $R_s^{\text{dir}}$ dependence than for the models considered above in this section. Calculations for the Haltrin model were carried out for selected values of $b_b/a$ (including values used in the MGM and the KM), based on Eq. (2) and the inversion of Eqs. (22)–(24) [or, identically, from Eq. (37) of Ref. 17]:

$$\bar{q} = \left[ \frac{a / b_b}{3 + a / b_b + [9 + 4(a / b_b)]^{1/2}} \right]^{1/2},$$ (50)

Taking into account that the Haltrin model is based on an idealized phase function with isotropic behavior in the backward direction, whereas the MGM and the KM (and also a model by Gordon$^{57}$ that is similar to both models) are based more on natural aquatic-based sources, we propose for the calculation of $R_s^{\text{dir}}$ versus $\mu_0$ and $b_b/a$ for highly turbid aquatic environments the use of Eq. (49) as an alternative to Eqs. (2) and (50).

Let us now show how the above findings can be used as an alternative to Eq. (4) in the estimation of $R_s^{\text{dir}}$ from $R_s$ in highly turbid waters. Fitting the relation between $b_b/a$ and $R_s^{\text{dir}}$, Eq. (24), for 0.001 $\leq R_s^{\text{dir}} \leq 0.3$ by a quadratic polynomial (with NRMSE = 2.4%)

$$b_b/a = 0.01439 + 2.279R_s^{\text{dir}} + 10.54(R_s^{\text{dir}})^2$$ (51)

and then introducing Eqs. (49) and (51) to Eq. (1), we obtain a quadratic equation relative to $R_s^{\text{dir}}$:

$$10.54q(R_s^{\text{dir}})^2 + (2.279q + 1)R_s^{\text{dir}}$$

$$+ [0.01439q - (1 + s)R_s^{\text{dir}}] = 0, \quad q = (0.6279 - 0.3119\mu_0)s,$$ (52)

a positive root of which is the required solution. The direct-to-diffuse incoming irradiance ratio $s$ can be estimated from the regional meteorological observations or with the help of different algorithms if the
5. Conclusion

Selected radiative transfer approaches have been compared and evaluated from the point of view of their applicability to natural aquatic environments. Primary attention has been paid to simple two-flux approaches: an extended KM theory and the self-consistent Haltrin approach. The KM theory is widely used in different technological applications, medical physics, and atmospheric optics owing to the easy evaluation from optical measurements of the absorption and the scattering properties of the medium. However, an application of the KM theory to aquatic environments is rather rare, apparently owing to the fact that scattering processes in such environments are anisotropic (although isotropic scattering is the basic assumption for the KM theory). From this point of view, the Haltrin model is more applicable to natural waters of different types because it does use the phase function as a sum of the isotropic and the anisotropic parts. Besides, the Haltrin model is completely equivalent to the original radiative-transfer equation.

The KM and the Haltrin approaches have been compared with each other and with additional approaches for the solution of optical problems, either directly (the estimation of the irradiance reflectance coefficient $R$) or inversely (the estimation of the volume absorption $a$ and the backscattering $b_s$ coefficients). The common feature of the models under consideration has underlined the effect of the bottom albedo $A_b$ on $R$. As has been shown, this influence is significant up to values of the optical depth for a diffuse attenuation coefficient $\tau$ less than 2 to 4, depending on the optical parameters of the medium and the selected model. This study has also shown that the KM model does not allow the transformation of the parameters of absorption and scattering to the IOP’s $a$ and $b_s$ without the addition of the parameters $R_{\text{dif}}$ and $b_s$ for shallow and $R_{\text{dif}}$ solely for optically deep waters. However, taking into account that within the frame of the Haltrin model $R_{\text{dif}}$ is a function of $b_s/a$ only [Eqs. (24) or (51)], i.e., an IOP, one can state that the KM model’s remission function $K/S$, calculated from $R_{\text{dif}}$ solely is also an IOP, independent of sun position or depth. That fact alone might explain the success of using the $K/S$ ratio for the solution of different bio-optical problems in several studies. Consistent with the KM theory, all the other radiative transfer approaches considered in the paper (the self-consistent Haltrin model, the CK radiative transfer solution, the neutron diffuse Gate–Brinkworth model, and different versions of the $\delta$-Eddington theory) permit one’s obtaining $b_s/a$ solely from $R_{\text{dif}}$. On the other hand, the above-mentioned theories not permit one’s obtaining $a$ or $b_s$ separately from only $R_{\text{dif}}$, requiring additional parameters such as $k_s$ or $\omega_0$ for such an assignment. Nevertheless, the self-consistent Haltrin model seems to be more preferable than other approaches, primarily owing to the use of the more realistic scattering phase function.

A transformation from a measured total irradiance reflectance of the semi-infinite layer $R_s$ to the part of the reflectance that depends on only the diffuse illumination $R_{\text{dif}}$ is, therefore, an important step of the solution of various optical and bio-optical tasks. Two different methods of such a transformation have been developed, and their analysis has been carried out. Several other problems, such as the estimation of the direct-to-diffuse incoming irradiance ratio $s$ and the transformation of the measured above-water irradiance reflectance to the measured subsurface irradiance reflectance are out of the scope of the current study and need special consideration.

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