4. TITLE AND SUBTITLE
Towards Development of an Improved Technique for Remote Retrieval of Water Quality Components: An Approach Based on Gordon's Parameter Spectral Ratio

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14. ABSTRACT
Radiative transfer modeling is used to compare the performance of two spectral reflectance ratios ($\Omega_R$ and $\Omega_L$), and these against of the Gordon spectral ratio ($\Omega_g$)'s performance. All of these ratios are used to extract water quality parameters (WQP) from the ocean. Inputs to the model are: five different scattering phase functions with particulate backscattering probability $B_p$ (from 0.009 to 0.156), fourteen values of solar zenith angle in the water $\theta$, (from 0° to 46°), and seven values of $\pi$ (from 0.125 to 0.5). The results indicate that $\Omega_R$ is more accurate than $\Omega_L$ because it's less sensitive to different solar and atmospheric parameters. The Gordon's spectral ratio, $\Omega_g$, is more accurate than any of the reflectance ratios $\Omega_R$ and $\Omega_L$ for any natural waters because it is totally independent on solar and atmospheric conditions. It is recommended that it always be used to extract WQP in extremely clear or turbid natural waters.

15. SUBJECT TERMS
reflectance ratios, Gordon parameter, retrieval water quality parameters, radiative transfer

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Towards Development of an Improved Technique for Remote Retrieval of Water Quality Components:
An Approach Based on the Gordon's Parameter Spectral Ratio

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INTRODUCTION

Remote-sensing retrieval of water quality components (WQCs) such as chlorophyll-\(a\), suspended solids concentration, or dissolved organic matter absorption is based on relationships between the WQCs and underwater spectral radiances or reflectances. The use of spectral radiance ratios or spectral reflectance ratios largely decreases errors caused by the angular scattering features of water particles, geometrical conditions of illumination and observation, and bottom effect. Additionally, it flattens the non-linear behavior of reflectance as a function of Gordon’s parameter \(G = b_v/(a + b_b)\) (\(a\) and \(b_b\) are the absorption and backscattering coefficients, respectively). Numerous successful examples of this approach may be found in Dekker and Peters (1993), O’Reilly et al. (1998), Kalio et al. (2001), Doxaran et al. (2002), Brezonik et al. (2005), Dall’Olmo and Gitelson (2005), Ouillon et al. (2008), Lunetta et al. (2009), Morel and Gentili (2009). However, these ratios are not free from uncertainties caused primarily by lighting geometry, particulate scattering phase function \(p(\theta)\), and contribution \(d_E\) of the diffuse downwelling irradiance to the total (direct+diffuse) downwelling irradiance \(E_d\). To overcome these uncertainties in remote-sensing, the use of the Gordon’s parameter spectral ratio is recommended over the application of spectral reflectance ratios. In this paper, the above inaccuracies taking place under using the spectral reflectance ratios of two different types of underwater reflectances (irradiance reflectance \(R\) and remote-sensing reflectance \(r_n\)) are examined and compared to the \(G(\lambda)\) ratios.

CONCISE DESCRIPTION OF THE MAIN CALCULATIONS

The \(R\) and \(r_n\) may be defined in terms of physical (optical) quantities as follows (Haltrin, 1998; Sokoletsky, 2005; Sokoletsky et al., 2009a):

\[
R = d_E SA + (1 - d_E) PA ,
\]

and

\[
r_n = \frac{1}{\pi} \left[ d_E SA + (1 - d_E) RF \right],
\]

where SA, PA, and RF are the spherical albedo, plane albedo, and reflectance factor, respectively. Determinations of these quantities are given, for instance, in Hulst (1974), Nicodemus et al. (1977), Hapke (1993), Kokhanovsky and Sokoletsky (2006), and briefly repeated below. The reflectance factor is defined as the ratio of the intensity of light reflected from a given layer to the intensity of light reflected from the Lambertian absolutely white surface. The plane albedo is defined as the integral of the reflectance factor \(RF(\mu_t, \mu_v, \varphi)\):

\[
PA(\mu_t) = \frac{1}{\pi} \int_0^{2\pi} \int_0^{\infty} RF(\mu_t, \mu_v, \varphi) \mu_t d\mu_t d\varphi ,
\]
and the spherical albedo is defined as the integral of the plane albedo:

\[
SA = 2 \int_0^1 PA(\mu_i) \mu_i d\mu_i ,
\]

(4)

where \(\mu_i\) is the cosine of the incidence angle \(\theta_i\) in the medium (water), \(\mu_v\) is the cosine of the viewing angle \(\theta_v\) in the medium, and \(\varphi\) is the azimuthal angle between the incident and scattered beam directions. Note that it follows from the conservation energy law: \(SA = 1\) and also \(PA(\mu_i) = 1\) at any \(\mu_i\) for nonabsorbing semi-infinite media (Sobolev, 1975; Kokhanovsky, 2004), although \(RF(\mu_i, \mu_v, \varphi)\) may be > 1 at \(\omega_b = 1\), where \(\omega_b\) is the single-scattering albedo. The \(d_E\) may vary approximately from 1/8 to 1/2 in the visible range for different atmospheric and geometrical conditions \((\theta_i < 45^\circ)\) (Haltrin, 1997; Rigollier et al., 2000; Hojerslev, 2004).

Calculations of \(RF\) were performed following an algorithm and FORTRAN code developed by Mishchenko et al. (1999) for the numerical solution of the radiative transfer equation (invariant imbedding method). \(PA\) and \(SA\) were derived by numerical integration following Eqs. (3) and (4). Input parameters for calculation \(RF, PA, SA, R\) and \(r_e\) were: the given scattering phase function \(p(\theta)\) (with the known backscattering probability \(B = b/b_i\), where \(b\) is the total scattering coefficient), \(\omega_b\) and \(\theta_i\). The viewing angle \(\theta_v\) was accepted as 0° relative to the zenith direction for all simulations; in this particular case a dependence of \(RF\) (and, hence, \(r_e\)) on azimuth \(\varphi\) disappears.

5 different \(p(\theta)\) were selected for simulations (Kokhanovsky and Sokoletsy, 2006; Sokoletsy et al., 2009b) so that maximally to cover possible situations in natural waters – from the very clear oceanic to completely turbid inland waters (Table 1, Fig. 1):

**Table 1. Scattering phase functions used for the study simulations.**

<table>
<thead>
<tr>
<th>#</th>
<th>(r_{ef}, \mu m)</th>
<th>(n)</th>
<th>(k)</th>
<th>(B)</th>
<th>(g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>1.2</td>
<td>0.01</td>
<td>0.0087</td>
<td>0.9583</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>1.2</td>
<td>0.01</td>
<td>0.0163</td>
<td>0.9377</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>1.25</td>
<td>0.001</td>
<td>0.0229</td>
<td>0.9062</td>
</tr>
<tr>
<td>4</td>
<td>0.175</td>
<td>1.25</td>
<td>0.001</td>
<td>0.0588</td>
<td>0.6963</td>
</tr>
<tr>
<td>5</td>
<td>0.116</td>
<td>1.25</td>
<td>0.001</td>
<td>0.1559</td>
<td>0.5033</td>
</tr>
</tbody>
</table>

Table 1 shows input parameters used for simulation of different \(p(\theta)\): effective radius \(r_{ef}\) of the gamma particle size distribution and refractive indices \(m = n - ik\); asymmetry parameter \(g\) and backscattering probability \(B\) for the derived \(p(\theta)\) are also shown. Note that the phase function \#2 is a quasi-Fournier-Forand-Mobley \(p(\theta)\) is not directly connected with \(r_{ef}\) and \(m\); this \(p(\theta)\) has been described separately by Sokoletsy et al. (2009b).
IRRADIANCE REFLECTANCE AND REMOTE-SENSING REFLECTANCE SIMULATIONS

Simulations of $R$ and $r_{rs}$ as a function of $G = \omega_0 B/[1 - \omega_0 (1 - B)]$ performed for 5 selected phase functions, listed in the Table 1, two incidence angles $\theta_i$ in the water (0° and 46°) and two values of $d_E$ (1/8 and 1/2) are shown in Figs. 2 and 3. As it seems from these figures, the curves may be well presented by the linear dependence in the double logarithmic scales, hence, $R$ and $r_{rs}$ may be written as power dependences on $G$:

$$R(G, p(\theta), \theta_i, d_E) = \alpha_R(p(\theta), \theta_i, d_E)G^{\beta_R(p(\theta), \theta_i, d_E)}$$  \hspace{1cm} (5)\]

$$r_{rs}(G, p(\theta), \theta_i, \theta_v, \phi, d_E) = \alpha_{r_{rs}}(p(\theta), \theta_i, \theta_v, \phi, d_E)G^{\beta_{r_{rs}}(p(\theta), \theta_i, \theta_v, \phi, d_E)}$$  \hspace{1cm} (6)

It is important to stress that irradiance reflectance depends on lesser number of parameters than remote-sensing reflectance. Further simplifications may be made by applying the spectral reflectance ratios:
Fig. 2. Irradiance reflectance calculated for the given $p(\theta)$ taken from the Table 1 (the first number in parentheses), $\theta_l$ (the second number, in degrees) and $d_E$ (the third number).

Fig. 3. The same as Fig. 2, but for remote-sensing reflectance.
\[ \Omega_R = \frac{R(G(\lambda_1), p(\theta), \theta_i, d_E)}{R(G(\lambda_2), p(\theta), \theta_i, d_E)} \approx \left[ \frac{G(\lambda_1)}{G(\lambda_2)} \right]^{\beta_R(p(\theta), \theta_i, d_E)} = \Omega_G^{\beta_R(p(\theta), \theta_i, d_E)} = \Omega_R^{\beta_R(p(\theta), \theta_i, d_E)}, \] (7)

\[ \Omega_r = \frac{r_{rs}(G(\lambda_1), p(\theta), \theta_i, \theta_v, \varphi, d_E)}{r_{rs}(G(\lambda_2), p(\theta), \theta_i, \theta_v, \varphi, d_E)} \approx \left[ \frac{G(\lambda_1)}{G(\lambda_2)} \right]^{\beta_r(p(\theta), \theta_i, \theta_v, \varphi, d_E)} = \Omega_G^{\beta_r(p(\theta), \theta_i, \theta_v, \varphi, d_E)}. \] (8)

As it can be seen from Eqs. (7) and (8), only Gordon's parameter spectral ratios \( \Omega_G \) and exponents \( \beta_R \) and \( \beta_r \) are included in the spectral reflectance ratio computations. The spectral differences for \( p(\theta), \theta_i, \theta_v, \) and \( d_E \) parameters, generally very small, were excluded. The values of \( \beta_R \) and \( \beta_r \) estimated by the least-squares method for different \( p(\theta), G < 0.6, \theta_v = 0°, \) and \( d_E = 1/8 \) and \( d_E = 1/2 \) are shown as functions of \( \theta_i \) in Figs. 4 and 5, respectively. The \( G \) values used include all known natural waters (Haltrin and Gallegos, 2003). As expected, from the optical behavior of RF, PA and SA, variability of exponents with \( \theta_i \) for \( \Omega_r \) is less than for \( \Omega(R) \), especially for small \( \theta_i \). Simulations performed for all \( 5 \) \( p(\theta) \) described above, \( 14 \) angles \( \theta_i \in [0°; 48°] \), and \( 7 \) values of \( d_E \in [1/8; 1/2] \), yielded values of \( \beta_R = 1.04\pm0.02 \) and \( \beta_r = 1.05\pm0.04 \).

Variability of \( \Omega_R \) \( [\text{Var}(\Omega_R)] \) and \( \Omega_r \) \( [\text{Var}(\Omega_r)] \) with the above parameters was estimated as the standard deviation divided by the average values of \( \Omega_R \) and \( \Omega_r \), respectively, versus \( \Omega_G \) and \( d_E \) using Eqs. (7) and (8). Plots of this variability (Fig. 6) show that \( \text{Var}(\Omega_R) < \text{Var}(\Omega_r) \); the variability is lesser for larger values of \( d_E \). In any case, the figure demonstrates that inaccuracies resulting from the different \( p(\theta) \) and \( \theta_i \) are rather small. It explains the success of the remote-sensing methods based on spectral reflectance ratios. This modeling has shown that uncertainties lie in the range of \( [0%; 4.1%] \) and \( [0%; 11.3%] \) for \( \Omega_R \) and \( \Omega_r \), respectively, if the \( \Omega_G \in [0.1; 10] \). However, within the more realistic range of \( \Omega_G \in [0.5; 2] \), the same uncertainties are significantly smaller: \( [0%; 1.3%] \) and \( [0%; 3.1%] \).

It is important to stress that the Gordon’s parameter spectral ratios \( \Omega_G \) (over of the spectral reflectance ratios considered in the study) do not depend completely on illumination/observation and atmospheric conditions and, hence, their using is more preferable than \( \Omega_R \) and \( \Omega_r \). The spectral values of \( G(\lambda) \) can be directly derived from the inherent optical measurements of ocean optics sensors such as WetLabs ac-9 or ac-s spectrophotometers.

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Fig. 4. Irradiance reflectance exponent calculated for the given $p(\theta)$ taken from the Table I (the first number in parentheses) and $d_E$ (the second number).

Fig. 5. The same as Fig. 4, but for the remote-sensing reflectance exponent.
Fig. 6. Variations of irradiance reflectance (solid lines) and remote-sensing reflectance (dotted lines) spectral ratios as a function of the Gordon’s parameter spectral ratio and $d_E$ (legend).

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