Numerical Radiative Transfer Simulations to Examine Influence of Shape of Scattering Phase Function of Suspended Particles on the Ocean Colour Reflectance

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Abstract: Effects of shape of particle scattering phase function on the ocean colour reflectance are examined by means of radiative transfer simulations. The simulations suggest that different shape of particle phase function may cause 19% of discrepancy in the reflectance for oceanic waters, even if the backscattering probability of suspended particles does not change. The discrepancy can be even larger for absorbing waters in coastal zone.

Keywords: Ocean Colour Reflectance, Phase Function Effects, Numerical Simulations

1. Introduction

Numerical simulation of radiative transfer is a useful method to understand and predict variability of the ocean color reflectance from which biogeochemical properties of seawater may be exploited. When optically shallow waters and inelastic scattering (including Raman scattering and fluorescence) are not considered, the time-independent simulations for 1D space (depth) are equivalent to solving the Equation of Radiative Transfer (ERT):

$$\left[\cos \theta \frac{d}{d \tau} + 1 \right] L(\Omega, \tau) = \omega \int 4\pi L(\Omega', \tau) P(\Psi, \tau) d\Omega'$$

(1)

where $L$ and $d\Omega'$ represent the radiance and infinitesimal solid angle, respectively. $\omega$ is the single scattering albedo and $P(\Psi, \tau)$ is the scattering phase function of seawater. If $\omega$ and $P$ are given, the ERT can be solved with respect to $L$, provided initial and boundary conditions are given. From the solution of the ERT, the ocean colour reflectance can be obtained by $R_{rs}$.

$L_{rs} / \int_0^{\pi/2} L \cos \theta \ d\Omega = L_{rs} / E_{d}$ where $\theta$, $L_{rs}$ and $E_{d}$ are the viewing zenith angle, the upward radiance (i.e. $L(\theta, <90^\circ)$ and the downward irradiance, respectively. Due to difficulties in measuring $P$, the classic measurements of $P$ taken by PETZOLD (1972) have been assumed in the radiative transfer simulations for analysis of $R_{rs}$. Effects of this assumption should be evaluated prior to drawing final conclusions.

Only a few evaluations of the assumption exist. Plass et al. (1985) showed that shape of phase function can significantly affect $L_{rs}$. More recently however, Mooley et al. (2002) concluded that the exact shape of the phase function in backscattering directions is not critical if the backscattering probability is correct and a 10% of error is acceptable. Thus, results from the two groups do not agree well with each other, and re-examination is required. The objective of this paper is to re-evaluate the influence of the shape of $P$ on $R_{rs}$ by means of numerical simulations and to see whether the use of the single shape of $P$ (i.e. PETZOLD $P$) is valid for different water types.

2. Simulations

The numerical radiative transfer simulations are made by Hydrolight (Mooley, 1995) for $R_{rs}$,
The weighting function \( W (\equiv b_w / (b_w + b_s)) \) explains a contribution of the particle scattering to the total scattering. Variations in \( P \) are caused by variations of \( P_w \), \( P_s \) and \( W \). Since variations in \( P_w \) are relatively much less than these in \( P_s \) and \( W \), variations in \( P \) are determined by these in \( P_s \) and \( W \) in practice.

Due to the lack of sufficient measurements of \( P_w \), Lorentz-Mie computations were performed just to obtain an idea of variability in \( P_w \). In the Lorentz-Mie computations, particle size distribution \( N (D) \) was varied according to Junge distribution \( N (D) \sim D^{-\xi} \) where \( N \) and \( D \) represent number of particles and sphere-equivalent diameter of particles, respectively. Junge slope \( \xi \) was varied from 3.0 to 5.0. The complex refractive index \((n)\) was varied from 1.05 to 1.22 for the real part to consider algal particles and mineral particles, and 0.0 to 0.001 for the imaginary part \((k)\) to consider absorbing particles. The computations show that the shape of \( P_s \) is remarkably variable at small and large angles (Fig. 1). According to Gordon (1993) however, the scattering at the small scattering angles has little effect on the light field. Hence we focus on \( P_s \) at large angles, or backscattering angles. The \( P_s \) at backscattering angles predicted by Lorentz-Mie theory may be classified into three classes: (I) \( P_s \) with a peak at around 180° of scattering angle (Fig. 1a), (II) \( P_s \) with no such peak (Fig. 1c) and (III) the intermediate case (Fig. 1b). In order to examine possible maximum effects of phase function on the ocean colour reflectance, two boundary shapes of \( P_s \) (i.e. backward-peaked and non-backward-peaked phase functions) are considered.

### 2.2.1 Backward-peaked phase function of suspended particles

The backward-peaked \( P_s \) obtained from Lorenz-Mie computations (Fig. 1a) has a similar shape to that of Petzold phase function (shown as a bold curve in Fig. 2) which has a remarkable peak at backward direction. Because the aim of this paper is to examine effects of use of the Petzold \( P_s \) in ocean colour analysis, the Petzold \( P_s \) is used here as a reference phase function that represents the backward-peaked \( P_s \) at the same time.

### 2.1 Phase function, \( P \)

The phase function of seawater \( P \) is expressed by a weighted sum of that of pure seawater \( P_w \) and suspended particles \( P_s \):

\[
P = (1 - W) P_w + WP_s. \tag{2}
\]
2.2.2 Non-backward-peaked phase function

The other characteristic shape of $P_\gamma$ predicted from Lorentz-Mie theory has a relatively flat shape in backward scattering angles (i.e. Non-backward-peaked phase function, Fig. 1c). Henyey-Greenstein phase function $P_{\text{HG}}$ represents such a shape:

$$P_{\text{HG}} = \frac{1}{4\pi} \frac{1-g^2}{[1+g^2-2g\mu]^{\frac{3}{2}}}$$  \hspace{1cm} (3)

where $g$ and $\mu$ represent the asymmetry factor and cosine of scattering angle. Fig. 2 shows that $P_{\text{HG}}$ (shown as $P_{60}$ for $W=1.0$) is similar to the non-backward-peaked $P_\gamma$ predicted by Lorenz-Mie theory shown in Fig. 1c. We use $P_{\text{HG}}$ here to represent the non-backward-peaked $P_\gamma$, rather than those determined by Lorentz-Mie theory, because $P_{\text{HG}}$ is expressed in an analytical form so that $P_\gamma$ can readily be assigned the same backscattering fraction $b_\gamma/b_\mu$, as that of PETZOLD $P_\gamma$. Resultant $g$ used here is 0.9185.

2.2.3 The phase functions of total water

Variations of $P$ calculated with $P_{\text{PET}}$ and $P_{\text{HG}}$ are shown in Fig. 2 for $W$ varying from 0.9 to 1.0. For $W=1.0$ (bold curves), $P$ is simply either $P_{\text{PET}}$ (solid) or $P_{\text{HG}}$ (dash-dot); see Eq. 2, too. It is seen that shape of backward $P$ calculated from $P_{\text{PET}}$ or $P_{\text{HG}}$ are different only when $W$ exceeds 0.9 due to the large contribution of $P_\gamma$ at $W<0.9$. $P_{60}$ has been used to represent $P$ for total (water + particle) seawater, and such approximation is not adequate for oceanic waters (HALTRIN, 2002). However, $P_{60}$ is used here for an approximation to $P_\gamma$, not to $P$. In addition, $P_{60}$ used as $P_\gamma$ still preserves a physical phenomenon that total $P$ obtained from $P_{\text{HG}}$ has the least variability at the scattering angle of 120 deg. (OISHI, 1990) (see inset of Fig. 2).
Thus, $P_{hc}$ would still be useful for oceanic application as long as it is used as one of the boundary shape of $P_r$.

### 2.3. Other input parameters

The radiative transfer simulations require not only $P$ but also the single scattering albedo $\omega = b_{tot} / (a_{tot} + b_{tot})$ as well as initial and boundary conditions. $\omega$ is calculated from $a_{tot}$ and $b_{tot}$ which are determined as follows. The absorption coefficient is decomposed into that by pure water ($a_w$) and by any other substances ($a_p$) so that $a_{tot} = a_w + a_p$. Subscript py means particle plus yellow substance. Due to lack of sufficient measurements to define natural variability of $a_p$ in the world oceans, $a_p$ is numerically varied from 0 to 1.59 m$^{-1}$; this range of values covers the maximal $a_p$ observed in coastal waters by Babin et al. (2003a). Effects of the upper limit chosen will be discussed in Section 3.2. Values of $a_w$ are taken from a measurement made by Pope and Fry (1997). The scattering coefficient may also be decomposed into $b_{tot} = b_w + b_p$ where subscript p means particles. Due to the same reason as $a_p$ above, $b_p$ is numerically varied from 0 to 7.37 m$^{-1}$; such a value of scattering corresponds to a sediment load of 7 to 15 g/m$^3$ (Babin et al., 2003b) and the maximum CHL considered here. Selection of the upper limit of $b_p$ will also be discussed in Section 3.2. Values of $b_w$ are taken from Morel (1974).

Table 1 summarizes values of $a_w$ and $b_w$ used in the present simulations. The initial condition to the ERT is determined from Harrison and Coombes (1988) and Gregg and Carder (1990) with variable solar zenith angle ($\theta_s$) from 0 to 75 deg. as shown in Table 1 (Results are shown only up to 58.3 deg. within the geometry for remote sensing, which does not affect a conclusion drawn in this paper). The boundary condition to the ERT is determined from Cox-Munk wave distribution with the wind speed of 7.2 m/s. The ocean is assumed to be optically deep. Actual simulations are performed for 15 discrete optical depths from $\tau = 0$ down to $\tau = 7$ with 0.5 interval, although we only focus on $\tau = \theta_s$ which is relevant remote sensing applications. Wavelength $\lambda$ is selected based on SeaWiFS bands (Table 1) but restricted to shorter wavelengths to minimise effects of inelastic scattering, including Raman scattering and fluorescence. The simulations are performed for all possible combinations of input parameters above (including any combination between $a_{tot}$ and $b_{tot}$). Radiance to derive $R_v$ is obtained from 0 to 49$^\circ$ of the viewing zenith angle and from 0 to 180$^\circ$ of the viewing azimuth angles (Table 1).

<table>
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<tr>
<th>$a_p$ [m$^2$]</th>
<th>$b_p$ [m$^2$]</th>
<th>Solar zenith angle [deg.]</th>
<th>Viewing zenith angle [deg.]</th>
<th>Viewing azimuth angle [deg.]</th>
<th>Wavelength [nm]</th>
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3. Results and discussions

The influence of \( P \) may be described by the ratio between \( R_s \), simulated with \( P_{\text{PET}} \) (denoted by \( R_{s,\text{PET}} \) hereafter) and \( R_s \) simulated with \( P_{\text{SIM}} \) (\( R_{s,\text{SIM}} \)): i.e. \( r_s = R_{s,\text{SIM}} / R_{s,\text{PET}} \). The influence of \( P_s \) is shown by the deviation of \( r_s \) from unity, and the largest influence can be evaluated by either of the maximum or minimum value of \( r_s \).

3.1 Estimation of the largest influence

Fig. 3a depicts \( r_s \) as a function of only \( \lambda \). All other variables, such as inherent optical properties (i.e. \( \alpha_{\text{tot}} \) and \( b_{\text{tot}} \), or \( \omega \)) and viewing and illumination angles, were varied. The maximum value of \( r_s \) (\( \approx 1.16 \)) is almost independent of \( \lambda \). The minimum values of \( r_s \) decreases from 0.70 to 0.65 as \( \lambda \) increases. Since deviation of the minimum \( r_s \) from unity is larger than deviation of maximum \( r_s \) from unity at all \( \lambda \), the maximum discrepancy between \( R_{s,\text{SIM}} \) and \( R_{s,\text{PET}} \) is represented by the minimum \( r_s \). The largest influence of \( P_s \) is found at \( \lambda = 555 \) nm.

Fig. 3b shows \( r_s \) as a function of only \( a_{\text{tot}} \) but wavelength is now fixed at 555 nm. All other variables except \( \lambda \) are allowed to vary. The maximum values of \( r_s \) are almost constant while the minimum values of \( r_s \) decrease with \( a_{\text{tot}} \). Since the greatest deviation of the minimum \( r_s \) from unity is larger than that of maximum \( r_s \), the largest influence of \( P_s \) is found by the minimum \( r_s \) at \( a_{\text{tot}} = 1.65 \) m\(^{-1}\).

Fig. 3c shows \( r_s \) as a function of only \( b_{\text{tot}} \) but now \( \lambda \) and \( a_{\text{tot}} \) are fixed at 555 nm and 1.65 m\(^{-1}\), respectively. Variation of the minimum \( r_s \) is not monotonic. It firstly decreases and then increases, as \( b_{\text{tot}} \) increases. Since the greatest deviation of the minimum \( r_s \) from unity is larger than that of maximum \( r_s \), the largest
influence of \( P_r \) occurs at \( b_{\text{cat}} = 1.01 \text{ m}^{-1} \).

\( r_r \) at \( \lambda = 555 \text{ nm}, \ a_{\text{cat}} = 1.65 \text{ m}^{-1} \) and \( b_{\text{cat}} = 1.01 \text{ m}^{-1} \) is shown in Fig. 3d as a function of solar zenith angle \( \theta_\odot \). The largest influence of \( P_r \) is found when \( \theta_\odot = 8.30 \text{ deg} \). Fig. 3e shows \( r_r \) at \( \lambda = 555 \text{ nm}, \ a_{\text{cat}} = 1.65 \text{ m}^{-1} \) and \( b_{\text{cat}} = 1.01 \text{ m}^{-1} \) and \( \theta_\odot = 8.30 \text{ deg} \). as a function of the viewing zenith angle \( \theta_\odot \), in which the largest influence is found at \( \theta_\odot = 7.00 \text{ deg} \). Finally \( \phi_\odot \), at which the largest influence of phase function is found is \( 0 \text{ deg} \), in which case \( r_r = 0.65 \). (Fig. 3f).

The largest influence of particle phase function is found at \( \lambda = 555 \text{ nm}, \ a_{\text{cat}} = 1.65 \text{ m}^{-1} \), \( b_{\text{cat}} = 1.01 \text{ m}^{-1}, \ \theta_\odot = 8.30 \text{ deg} \), \( \theta_\odot = 7.00 \text{ deg} \), and \( \phi_\odot = 0 \text{ deg} \), with \( r_r = 0.65 \), indicating that the influence of \( P_r \) can be significant to cause 35\%=100 (1\%-0.65) of maximum discrepancy in \( R_r \) according to the present simulations.

### 3.2 Effects of choice in upper limit of \( a_{\text{cat}} \) and \( b_{\text{cat}} \)

In the results shown above, the largest influence of \( P_r \) was found at \( a_{\text{cat}} = 1.65 \text{ m}^{-1} \) which is the upper limit of \( a_{\text{cat}} \) set in our simulations. Also the largest influence of phase function as a function of \( b_{\text{cat}} \) did not show a constant effect over \( b_{\text{cat}} \). These mean that our results obtained earlier depend on the choice of the upper limit of \( a_{\text{cat}} \) and \( b_{\text{cat}} \), or equivalently \( a_{\text{sym}} \) and \( b_\odot \) since \( a_{\text{cat}} \) and \( b_\odot \) are regarded as constants. for each wavelength In order to see effects of this choice, simulations are repeated by changing the upper limit of \( a_{\text{cat}} \) and \( b_{\text{cat}} \) (denoted hereafter by Max \( a_{\text{cat}} \) and Max \( b_{\text{cat}} \), respectively). Fig. 4 shows the largest influence of \( P_r \) in terms of \( r_r \), as functions of Max \( a_{\text{cat}} \) and Max \( b_{\text{cat}} \). If Max \( a_{\text{cat}} \) assumed in simulations is larger / smaller than “real” upper limit of \( a_{\text{cat}} \), the largest influence of phase function is over/under-estimated when Max \( b_{\text{cat}} \) is relatively large. When Max \( b_{\text{cat}} \) is relatively small however, the over/under estimation is less severe or even negligible, even if Max \( a_{\text{cat}} \) is incorrectly selected. This is consistent with Section 2.2.3 that the phase function
effects are remarkable only when $W>0.9$.

If Max $b_{tot}$ assumed is relatively larger/smaller than actual upper limit of $b_{tot}$, the largest influence of $P_r$ simulated is over/under-estimated, when the magnitude of actual $b_{tot}$ is small. When the magnitude of actual $b_{tot}$ itself is large however, the largest influence of $P_r$ simulated will be under/over-estimated if Max $b_{tot}$ assumed is relatively larger/smaller than actual upper limit of $b_{tot}$. The above results indicate that precise determination of the upper limit of $a_{tot}$ and $b_{tot}$ is required for quantitative prediction of the influence of $P_r$.

Morel and Maritorena (2001) proposed statistical relationships between $a_{tot}$ (or $b_{tot}$) and Chlorophyll a concentration (CHL) for oceanic water based on numerous in-situ observations, from which natural Max $a_{tot}$ and Max $b_{tot}$ may be determined in terms of an upper limit of CHL since the statistical relationship is non-linear but monotonic. Their data showed nearly 40 mg m$^{-3}$ of the maximum CHL in oceanic waters: see their Fig. 3 in Morel and Maritorena (2001). Thus, realistic Max $a_{tot}$ and Max $b_{tot}$ can be calculated for oceanic water by using CHL=40 mg m$^{-3}$. The largest influence of $P_r$ estimated using Max $a_{tot}$ and Max $b_{tot}$ derived in this way are shown in Fig. 4 as a star symbol. The largest influence of $P_r$ for CHL=0.03, 0.1, 1.0 and 10.0 mg m$^{-3}$ are also superimposed for comparison as well as for CHL=0.22 mg m$^{-3}$ which is a global annual average of CHL derived from SeaWiFS. When CHL is 0.22 mg m$^{-3}$, $r_s$ is 0.81 showing that 100 (1.00-0.81) = 19% of largest influence of $P_r$. The influence is relatively less for lower and higher CHL. The present result suggests that the influence of $P_r$ on $r_s$ (or equivalently $L_a$) can be significant for oceanic waters.

For coastal waters, a significant number of observations for $a_{tot}$ and $b_{tot}$ are required to define their maximum variability. Therefore quantitative prediction of the phase function effects cannot be made for coastal waters at the present stage. However, general tendency of the effects for coastal waters can be found at least qualitatively (Fig. 4). For absorbing waters (e.g. Baltic sea) where Max $a_{tot}$ is much larger than that for oceanic waters, the possible largest influence of $P_r$ on $r_s$ will be larger than that for oceanic waters, unless Max $b_{tot}$ (or $b_{tot}$) is also much larger than $b_{tot}$ for oceanic waters. For scattering waters (e.g. Black sea) where Max $b_{tot}$ is much larger, the largest influence of $P_r$ on $R_s$ will be reduced unless Max $a_{tot}$ is also much larger.

It is clear that a balance between the absorption and scattering play a significant role in the phase function effects, and the absorbing water or scattering waters may be defined based on $\omega$. However, it should be emphasized that absolute magnitude of $b_{tot}$ (or alternatively $b_0$) must also be considered together with $\omega$ when the phase function effects are estimated, since (1) we saw in Section 2.2.3 that significant difference in P is found only at $W>0.9$ and (2) a value of $\omega$ cannot specify a unique value of $W$.

Phase function effects for the absorbing waters implies that, even for oceanic waters, the effects can be significant at near-infrared wavelengths where the absorption by pure seawater itself is much larger than that at visible wavelengths. The near-infrared has a particular importance for atmospheric correction scheme of the ocean colour imagery, especially when the waters have a significant reflectance in the NIR; the bright pixel assumption (Moore et al., 1999). Thus, the present work implies that the phase function effects need to be considered in remote sensing application.

5. Conclusion

The largest influence of $P_r$ is estimated to be 19% for oceanic waters. For coastal waters, the influence can even be larger in absorbing waters, whereas it can be smaller in scattering waters. The influence of shape of phase function of suspended particles can be significant, especially when intensity of scattering of particle is large enough compared to that of pure seawater ($0.9<W$). The present results suggest that the shape of $P$ has to be taken into account in the ocean colour analysis, especially in highly absorbing waters.

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