Re-examining the effect of particle phase functions on the remote-sensing reflectance

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Even though it is well known that both the magnitude and detailed angular shape of scattering (phase function, PF), particularly in the backward angles, affect the color of the ocean, the current remote-sensing reflectance \( R_{rs} \) models typically account for the effect of its magnitude only through the backscattering coefficient \( b_b \). Using 116 volume scattering function (VSF) measurements previously collected in three coastal waters around the U.S. and in the water of the North Atlantic Ocean, we re-examined the effect of particle PF on \( R_{rs} \) in four scenarios. In each scenario, the magnitude of particle backscattering (i.e., \( b_{bp} \)) is known, but the knowledge on the angular shape of particle backscattering is assumed to increase from knowing nothing about the shape of particle PFs to partially knowing the particle backscattering ratio \( B_p \), the exact backscattering shape as defined by \( \beta_p(\gamma \geq 90^\circ) \) (particle VSF normalized by the particle total scattering coefficient), and the exact backscattering shape as defined by the \( \chi_p \) factor (particle VSF normalized by the particle backscattering coefficient). At sun zenith angle \( \theta_s = 30^\circ \), the nadir-viewed \( R_{rs} \) would vary up to 65%, 35%, 20%, and 10%, respectively, as the constraints on the shape of particle backscattering become increasingly stringent from scenarios 1 to 4. In all four scenarios, the \( R_{rs} \) variations increase with both viewing and sun angles and are most prominent in the direction opposite the sun. Our results show a greater impact of the measured particle PFs on \( R_{rs} \) than previously found, mainly because our VSF data show a much greater variability in \( B_p \), \( \beta_p(\gamma \geq 90^\circ) \), and \( \chi_p \) than previously known. Among the uncertainties in \( R_{rs} \) due to the particle PFs, about 97% can be explained by \( \chi_p \), 90% by \( \beta_p(\gamma \geq 90^\circ) \), and 27% by \( B_p \). The results indicate that the uncertainty in ocean color remote sensing can be significantly constrained by accounting for \( \chi_p \) of the VSFs.

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1. INTRODUCTION

The study of ocean color is carried out by measuring the spectral irradiance \( (E_\lambda; \text{W m}^{-2} \text{sr}^{-1}) \) leaving the ocean and normalizing it by the incident irradiance \( (E_0; \text{W m}^{-2}) \) at the surface, forming the spectral remote-sensing reflectance \( (R_{rs}; \text{sr}^{-1}) \):

\[
R_{rs}(\lambda, \theta_v, \theta_s, \phi) = \frac{L_\lambda(\lambda, \theta_v, \theta_s, \phi)}{E_0(\lambda, \theta_s)},
\]

where \( \lambda \) is the wavelength; \( \theta_v \) and \( \theta_s \) are the sun zenith angle and the sensor viewing angle, respectively; and \( \phi \) is the azimuth angle of the sensor relative to the plane of sun. Through radiative transfer simulations, an approximate relationship was derived relating \( R_{rs} \) to two inherent optical properties (IOPs) of sea water, i.e., the absorption \( \alpha \) and backscattering \( b_b \) coefficients [1–5]:

\[
R_{rs} = \frac{f}{Q_a + b_b}.
\]

Here, the \( f/Q \) factor describes the bidirectional reflectance distribution function, which depends not only on the sun-sensor geometry but also on the IOPs [6,7]. Though not explicitly contained in Eq. (2), the volume scattering function (VSF or \( \beta \) \( \text{m}^{-1} \text{sr}^{-1} \)) plays a fundamental role in ocean color [8,9].

The VSFs influence the remote sensing reflectance [9,10] through both the backscattering coefficient and the bidirectional reflectance distribution function. \( b_b \) describes the overall magnitude of VSFs in the backward directions and is generally responsible for reflecting incident sunlight out of the water. Assuming azimuthal symmetry of scattering, \( b_b \) can be calculated as
\[ b_b = 2\pi \int_{\pi/2}^{\pi} \beta_b(\gamma) \sin \gamma d\gamma, \]

where \( \gamma \) is the scattering angle. The shape of VSFs influences the distribution of the underwater light field, which, in turn, impacts the \( R_a \). However, due to limited knowledge on the VSFs of natural particle assemblage, most of the current ocean color algorithms \([6,7,11]\) have ignored the shape effect. In ocean color \([4,8]\), the shape of a VSF in the backward angles is often described using two additional parameters, the backscattering probability (fraction or ratio),

\[ B = \frac{b_b}{b} = 2\pi \int_{\pi/2}^{\pi} \tilde{\beta}(\gamma) \sin \gamma d\gamma, \]

and the \( \chi(\gamma) \) factor \([18–21]\),

\[ \chi(\gamma \geq 90^\circ) = \frac{b_b}{2\pi \beta(90^\circ)} = \frac{B}{2\pi \bar{\beta}(\gamma)}. \]

While \( B \) can be considered as a measure of the general backward shape of a VSF, both the \( \chi \) factor and \( \bar{\beta}(\gamma \geq 90^\circ) \) describe its exact backward shape. From an ocean color perspective, the \( \chi \) factor is more relevant because it is normalized by the backscattering coefficient. Note that both \( B \) and the \( \chi \) factor can be derived directly from \( \bar{\beta} \).

The angular shape of \( \bar{\beta} \) is contributed by both molecules and particles. Since the scattering by pure seawater is relatively well known \([22,23]\), our focus in this study is on the effect of angular scattering by the particles, which represents the contribution by everything other than pure water and sea salt molecules and will be denoted by a subscript \( p \). While Gordon \([24]\) found that the PFs at angles \(<15^\circ\) have a \(<5\%\) impact on \( R_a \), other studies have shown that the VSF shapes at larger angles could have a significant impact.

Bulgarelli et al. \([12]\) found \( \sim40\% \) variation among simulated upwelling radiance using the Fournier–Forand (FF) \([25–27]\) PFs with \( B_p = 0.011 \) and 0.033 and the average Petzold PF, which was estimated using the measurements taken by Petzold \([28]\) in the San Diego harbor and has a \( B_p = 0.018 \).

Similarly, Tzortziou et al. \([17]\) found \( R_0 \) simulated using the average Petzold PF can differ by 50% from \( L_w \) measured in a water with considerably smaller \( B_p \) values, with an average of 0.0128 \( \pm \) 0.0032. Using FF and a few other theoretical PFs that have the same \( B_p \) value as the average Petzold PF, Mobley et al. \([25]\) found that simulated \( R_0 \) vary only by 10%. They further compared \( R_0 \) among measured, simulated with measured VSFs, and simulated with \( B_p \)-equal FF PF, and concluded that “...the exact shape of the phase function in backscatter directions does not greatly affect the light field, so long as ... the phase function have [sic] the correct backscatter fraction.” The conclusion has since been tested. Chami et al. \([29]\) found up to 20% differences in \( R_0 \) simulated using their measured PFs and the corresponding \( B_p \)-equal FF PFs. They also showed that an increase of the VSF between 10° and 100° could lead to increased reflectance due to multiple scattering. Tonizzo et al. \([16]\) also compared \( R_0 \) simulated using measured PFs and the corresponding \( B_p \)-equal FF PFs over a range of case I and II waters and found an average difference of 20%.

The phase functions used in these studies, some of which are based on simplified theoretical models, are limited in their representation of natural variability of the VSFs. In addition, these studies considered only the general backscattering fraction, not the full VSF shapes, while theoretical derivations \([8,9]\) indicates that the influence on \( R_a \) arises from both the magnitude and the exact shape of the VSF in the backward directions. For example, recent studies by Pitarch et al. \([15]\)

Fig. 1. (a) Comparison of particle PFs derived from: our measurements (gray lines); samples of historical Petzold’s measurements in clear water of the Tongue of the Ocean (black dotted line), in California offshore coastal water (black dashed line), and in very turbid water of San Diego harbor (black dotted-dashed line) \([32]\); the average particle PF of Petzold’s measurements in San Diego harbor \([33]\) (black solid line); the analytical Fournier–Forand (FF) formula having a \( B_p = 1.83\% \) \([25]\) (blue dashed line); and a series of particle PFs generated by linear mixing of \( B_p = 1\% \) FF PF and the average Petzold PF, as used in Lee et al. \([11]\) (green solid lines). The red line is one of the measured particle PFs referred to in Fig. 5. To highlight the variations, the x axes are in logarithmic scale for angles <30° and in linear scales for larger angles. (b) Corresponding \( \chi_p \) factors. (c) Histogram of \( B_p \) calculated from measured particle PFs.
and Lefering et al. [14] showed that accounting for the detailed shape of PFs is important in achieving optical closure in $R_n$.

We have measured VSFs over various coastal waters of the U.S. and in clear waters of the North Atlantic Ocean [30,31], with chlorophyll concentration ranging from 0.07 to 40 µg/L. The data show that the natural variability of particle VSFs is greater than what had been known or assumed previously in terms of both the backscattering probability and the detailed backward shape (Fig. 1). For example, $B_p$ values estimated from our measured VSFs vary over a factor of 30 from 0.0015 to 0.0543, which is much greater than the range of 0.0073–0.0194 estimated from Petzold’s measurements and the range of 0.002–0.020 measured in Tonizzo et al. [16], but comparable to the range of 0.0015–0.0454 reported in Mankovsky and Haltrin [34,35] over the oceans and lakes worldwide.

Therefore, we believe that the impact of angular scattering by oceanic particles on $R_n$ may have been underestimated. Using the latest measurements of the VSFs in a wide range of natural environments, we have re-examined the uncertainty that the particle PFs might have on the remote sensing of the color of the ocean. Our study differs from previous ones in two aspects. First, we are interested in the natural variability that the particle PFs might have on the remote sensing of the color of the ocean. Our study differs from previous studies in terms of both the backscattering probability and the detailed backward shape. $B_p$ is necessary for Eq. (8) to be physically valid [37]. There are 16 (out of 116) measured VSFs with $m > 2$. For these VSFs, we modified $B_p$ to ensure $m = 1.9$. The tests were performed with those VSFs with $m > 2$ by changing $m$ values between 1 to 1.9, and the results showed that the differences on HydroLight-simulated $R_n$ were <1.8%. These modified $B_p$ were used in generating the PF shapes in Fig. 1 and in the rest of this study.

B. HydroLight Simulation
We used HydroLight 5.2 to simulate $R_n$ following the methods described in the IOCCG report No. 5 [38]. Briefly, the absorption coefficients and backscattering coefficients of particles ($a_p$ and $b_{bp}$) were generated as a function of chlorophyll concentration in 20 discrete values between 0.03 and 30.0 µg/L, and at each value, 25 sets of spectral particle absorption and backscattering coefficients ($a_p$ and $b_{bp}$) at 532 nm were generated, providing a total of 500 sets of $a_p$ and $b_{bp}$. The values of $b_{bp}/(a + b_{bp})$ at 532 nm are between 0.03 and 0.34. For each generated synthetic data set of $a_p$ and $b_{bp}$, $R_n$ was simulated ingesting each of the 116 measured $B_p$. Also, the particle scattering coefficients ($b_p$) were estimated from $b_{bp}$ using $B_p$ associated with each $B_p$. Water is assumed homogeneous and infinitely deep, illuminated by a semi-empirical sky model (based on RADTRAN-X) with 0 cloud coverage and annual average climatology condition. The simulations were performed for $\theta_s$ ranging from 0° to 75° with an increment of $0.1°$.

\[ \beta_p(\gamma) = A \gamma^{-m}, \]  
(7)

where $A$ and $m$ are estimated using $\beta_p$ values at $\gamma_1 = 0.1°$ and $\gamma_2 = 0.2°$.

The particle scattering coefficient is then computed as

\[ b_p = \frac{2\pi}{2 - m} \beta_p(\gamma_1) \gamma_1^2 + 2\pi \int_{0.1}^{\pi} \beta_p(\gamma) \sin \gamma d\gamma. \]  
(8)

A precondition, $m < 2$, is necessary for Eq. (8) to be physically valid [37]. There are 16 out of 116 measured VSFs with $m > 2$. For these VSFs, we modified $\beta_p$ to ensure $m = 1.9$. The tests were performed with those VSFs with $m > 2$ by changing $m$ values between 1 to 1.9, and the results showed that the differences on HydroLight-simulated $R_n$ were <1.8%. These modified $\beta_p$ were used in generating the PF shapes in Fig. 1 and in the rest of this study.

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Fig. 2. $R_n(\theta_s = 30°, \theta_r = 0°)$ simulated with measured particle phase functions (color coded by the measurement locations) are shown as a function of $b_p/(a + b_p)$.
15°, θs ranging from 0° to 70° with an increment of 10°, and ϕ ranging from 0° to 180° with an increment of 15°. In total, we had 32,016,000 simulated \( R_{ns} \) over a range of optical and viewing conditions that we believe cover a sufficiently extensive variability that an ocean color sensor may encounter.

### 3. RESULTS

#### A. \( R_{ns} (\theta_s = 30°, \theta_v = 0°) \)

The \( R_{ns} \) simulated with different particle PFs at \( \theta_s = 30° \) and \( \theta_v = 0° \) are shown in Fig. 2. As expected, \( R_{ns} \) increases with \( b_b/(a + b_b) \). For a set of \( a \) and \( b_b \) values, the variability of \( R_{ns} \) also increases with \( b_b/(a + b_b) \). This confirms that the impact of the particle VSF shapes on \( R_{ns} \) increases with \( b_b \). In the following, we will examine the impact of the VSF shape in four scenarios with increasing constraint on the backscattering:

1. **No knowledge of \( \tilde{B}_p \)**
2. **Some knowledge of \( \tilde{B}_p \)**
3. **Some knowledge of exact backward shape of \( \tilde{B}_p \)**, i.e., \( \tilde{B}_p (\gamma \geq 90°) \)
4. **Some knowledge of both \( B_p \) and \( \tilde{B}_p (\gamma \geq 90°) \)

In all four scenarios, the particle backscattering coefficient \( \tilde{B}_p \) is assumed to be known. To quantify uncertainty for \( R_{ns} \) due to \( \tilde{B}_p \), we use pairwise percentage difference, \( dR_{ns} \), estimated as

\[
dR_{ns}(a, b_b, \theta_s, \theta_v, \phi) = \frac{|R_{ns}(i, a, b_b, \theta_s, \theta_v, \phi) - R_{ns}(j, a, b_b, \theta_s, \theta_v, \phi)|}{\frac{1}{2}[R_{ns}(i, a, b_b, \theta_s, \theta_v, \phi) + R_{ns}(j, a, b_b, \theta_s, \theta_v, \phi)]} \times 100%,
\]

where \( i, j \) denote two arbitrary phase functions. Given its definition in Eq. (9), \( dR_{ns} \) describes the variation arising entirely from the changes in particle PF for a given set of \( a \) and \( b_b \) in a given sun-viewing geometry.

#### 1. No Knowledge of \( \tilde{B}_p \)

For two waters with the same \( b_b \) (and \( a \)), the current ocean color models, e.g., Eq. (2), would predict the same \( R_{ns} \) for a given viewing geometry. Therefore, any variations shown in the simulated \( R_{ns} \) would represent the uncertainty caused by the difference in \( \tilde{B}_p \) shapes between the two waters [Fig. 3(a)].

With the natural variability exhibited by the \( \tilde{B}_p \) shown in Fig. 1, the median differences in \( R_{ns} \) are <15% but the maximum differences could reach >60%.

#### 2. Knowledge of \( B_p \)

Among the 116 measured \( \tilde{B}_p \), we found 44 pairs that have the same \( B_p \) values (within 0.5%). Since \( b_b \) and \( a \) are assumed to be the same, the same \( B_p \) effectively means the same \( b \) (and \( c \)).

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**Fig. 3.** Percentage difference between \( R_{ns} (\theta_s = 30°, \theta_v = 0°) \) simulated with two different particle phase functions. The whiskers boxes, showing the minimum, lower quartile, median, upper quartile, and maximum values, summarize the differences at the selected \( b_b/(a + b_b) \) values.

(a) Simulations performed with same \( b_b \) values. (b) Simulations performed with same \( b_b \) values and phase functions having the same \( B_p \) values. The dotted line at 10% represents the maximum difference found in Ref. [25], the dashed line at 20% represents the maximum difference found in Ref. [29], and the dotted-dashed line at 40% represents the maximum difference found in Ref. [16]. (c) Simulations performed with same \( b_b \) values and very similar \( \tilde{B}_p (\gamma \geq 90°) \) (logarithmic value within 1%). (d) Simulations performed with same \( b_b \) values and very similar \( \tilde{B}_p \) factor (within 1%).
With this additional constraint on the general backward shape, the median difference in $R_s$ decreased to <10%, and the maximum difference decreased to 35% [Fig. 3(b)]. Under the same set of constraints, Mobley et al. [13] found a difference of up to 10% [dotted line in Fig. 3(b)] using Petzold’s average $\bar{\beta}_p$ and a few other theoretical PFs with the same $B_p$ as the Petzold’s average $\bar{\beta}_p$. A difference of up to 20% [dashed line in Fig. 3(b)] was found by Chami et al. [29] using several measured PFs and the $B_p$-matched FF functions, while a similar study by Tonizzo et al. [16] found differences up to 40% [dot-dashed line in Fig. 3(b)]. Our results are consistent with these earlier studies, showing that the knowledge of $B_p$ is not sufficient to explain all the variations in $R_s$ caused by PF shapes.

3. Knowledge of $\bar{\beta}_p(\gamma \geq 90^\circ)$

Among the 116 measured $\bar{\beta}_p$, 66 pairs of measured particle PFs [Fig. 3(c)] have similar backward shape, with <1% difference between the logarithmic values of $\bar{\beta}_p(\gamma \geq 90^\circ)$. With this knowledge, the median difference in $R_s$ was lowered to <6% and the maximum difference to 20%.

4. Knowledge of Both $B_p$ and $\bar{\beta}_p(\gamma \geq 90^\circ)$

From Eq. (6), the same $B_p$ and $\bar{\beta}_p(\gamma \geq 90^\circ)$ are equivalent to the same $\chi_p$. Therefore, this scenario also represents the constraint of “knowledge of $\chi_p$.” Among the 116 measured $\bar{\beta}_p$, we found 25 pairs that have the $\chi_p$ factors similar to each other within 1% at all angles between 90° and 180°. The $R_s$ simulated with the same $b_{pp}$ and similar $\chi_p$ factors are very similar to each other, with a median difference <2% and a maximum difference of ~10% [Fig. 3(d)].

Common to all four scenarios is that $dR_s$ increases with $b_{pp}/(a + b_p)$, seemingly reaching a saturation at approximately $b_{pp}/(a + b_p) > 0.2$. As $b_{pp}/(a + b_p)$ increases, the backscattering will shift from water molecule-dominated to particle-dominated scattering, and therefore the shape of particle PFs will have an increasing impact on $R_s$. However, when $b_{pp}/(a + b_p)$ is high enough, the multiple scattering will be increased so much that the impact on $R_s$ due to the shape differences between particle PFs will not increase anymore [29].

B. $R_s(\theta_s, \phi_s)$

To examine how the impact of the particle PFs on $R_s$ varies with sun-viewing geometry, we plot the maximum percentage difference in $R_s$ in Fig. 4 as a function of sun zenith angles, viewing zenith, and azimuth angles. Without any knowledge on the shape of particle PF [corresponding to Fig. 3(a)], the maximum differences in $R_s$ vary between 52% and 107% [Fig. 4(a)]. With a knowledge of $B_p$ [corresponding to Fig. 3(b)], the simulated $R_s$ show a maximum difference varying between 26% and 54% [Fig. 4(b)]. If the backward shape of $\bar{\beta}_p$ is similar within 1% [corresponding to Fig. 3(c)], the maximum differences in $R_s$ vary between 17% and 30% [Fig. 4(c)]. A knowledge of both $B_p$ and $\bar{\beta}_p(\gamma \geq 90^\circ)$ [corresponding to Fig. 3(d)] will reduce the maximum variations in $R_s$ between 8% and 16% [Fig. 4(d)]. For all four cases, the difference in $R_s$ follows the same geometric pattern: increasing with both the sun and viewing zenith angles, and

![Fig. 4](image-url) Distribution of the maximum value of $dR_s$. In the polar plots, • indicates $\theta_s$, radial direction represents $\theta_s$, and polar direction represents $\phi$. Column (a) results with same $b_{pp}$; column (b) results with same $b_{pp}$ and $B_p$; column (c) results with same $b_{pp}$ and similar $\bar{\beta}_p(\gamma \geq 90^\circ)$ (logarithmic value within 1%); column (d) results with same $b_{pp}$ and similar $\chi_p$ factor (within 1%).
4. DISCUSSION AND CONCLUSIONS

Even though the commonly used $R_{ss}$ models do not explicitly account for the shape of the VSFs [e.g., Eq. (2)], its impact on the color of the ocean is well recognized [4,8,23,39,40]. In fact, Jerlov [40] pointed out that the observed variation of the reflectance with sun angles is a direct consequence of the shape of the VSF. In Eqs. (4)–(6), three commonly used parameters describing the backward shape of a VSF are introduced: $B$, $\tilde{\beta}(\gamma \geq 90^\circ)$ and the $\chi$ factor. So, a logical question to ask is which of these three shape factors is more important in affecting $R_{ss}$.

Under quasi-single-scattering approximation (QSS), Gordon [41] showed the remote sensing reflectance (the detailed derivation is given by Mobley et al. [42]):

$$R_{ss}(\theta, \phi, \theta_s) = \frac{1}{\cos \theta_s + \cos \theta a + b_b} \tilde{\beta}(\gamma),$$

where $\gamma$ represents the single scattering angle formed between the viewing and sun vectors. Since $\gamma$ is typically $>90^\circ$, it is clear from Eq. (10) that $R_{ss}$ is directly proportional to the backward VSF. Inserting the first equality of Eq. (6) into Eq. (10), we have

$$R_{ss}(\theta, \phi, \theta_s) = \frac{1}{2\pi \chi(\gamma)} \frac{1}{\cos \theta_s + \cos \theta a + b_b}. \tag{11}$$

It is clear from Eq. (11) that when $b_b$, and hence $b_{bb}$, is constrained, $R_{ss}$ is directly proportional to $1/\chi(\gamma)$, assuming $a$ is known in a fixed sun-viewing geometry. Since the $\chi$ factor for pure seawater is known [21], the uncertainty in $\chi_{pp}$ is directly reflected in $R_{ss}$. Our result showed that a complete lack of knowledge of particle backscattering shape would induce approximately 15% median and $>60$% maximum differences in nadir-viewed $R_{ss}$ [Fig. 3(a)]. On the other hand, Eq. (11) shows that if the $\chi_{pp}$ factor is constrained, $R_{ss}$ will be fixed. While this applies only to the QSS approximation, it does explain why the simulated $R_{ss}$ are very similar to each other, with median difference $<2$% and maximum difference $<10$%, when the $\chi_{pp}$ factor is constrained [Fig. 3(d)].

Inserting the second equality of Eq. (6) into Eq. (11), we have

$$R_{ss}(\theta, \phi, \theta_s) = \frac{\tilde{\beta}(\gamma)}{B} \frac{1}{\cos \theta_s + \cos \theta a + b_b}. \tag{12}$$

Apparently, when only one of $B$ and $\tilde{\beta}$ is constrained, there is still residual variance in $R_{ss}$ that arises from the other factor that is not constrained. For example, our results show that the median and maximum values of this residual variance due to unknown $\tilde{\beta}$ are approximately 10% and 35%, respectively [Fig. 3(b)], and are 5% and 20%, respectively, if $B_p$ is unknown [Fig. 3(c)].

As shown in Eq. (11), when either $\theta_s$ or $\theta$ increases, the value of $\frac{1}{\cos \theta_s + \cos \theta a}$ increases, and hence the impact of backward VSF increases. Therefore, the uncertainty due to the shape of VSF increases with both viewing and sun angles (Fig. 4).

For $B_p$, $\tilde{\beta}(\gamma \geq 90^\circ)$, or $\chi_p$, the field measurements indicate that the natural variability of the particle PFs is much greater than what has been assumed (Fig. 1). Consequently, the impact of the shape of the particle PFs on $R_{ss}$ may have been underestimated. For example, Fig. 5 compares the $R_{ss}$ predicted using the Lee's et al. [11] model, which was developed based on a limited range of phase functions (green lines in Fig. 1), with the $R_{ss}$ simulated using one particular phase function (red line in Fig. 1). Both Lee et al. [11] and our study followed the IOCCG Report No. 5 in generating the IOPs to drive the HydroLight. Since the final formula of the Lee et al. [11] model accounts for only a statistic average of the PFs used in their study, the scatter of the comparison shown in Fig. 5 is expected. However, the Lee et al. [11] model consistently over-predicted the $R_{ss}$ simulated for this particular PF by approximately 30%−50%. While the comparison shown in Fig. 5 represents an extreme case with the differences close to the maximum shown in Fig. 3(a), it does illustrate the potential impact of the VSF shape on the color of the ocean.

Our results have demonstrated the increasing importance of $B_p$, $\tilde{\beta}(\gamma \geq 90^\circ)$, and $\chi_p$, in regulating $R_{ss}$, and it will be of interest to quantify their respective importance in terms of fraction of total uncertainty in $R_{ss}$ due to the VSF shapes that they can explain. To do this, we started with $\tilde{\beta}_p$, which describes the general shape of a VSF, includes $\tilde{\beta}(\gamma \geq 90^\circ)$, and can be used to derive both $B_p$ and $\chi_p$ [Eqs. (5) and (6)]. Let $\sigma$, denote the total uncertainty in $R_{ss}$ explained by $\tilde{\beta}_p$. In the first test with no constraint on the shape, $R_{ss}$ were found to differ up to 65% for nadir-viewed geometries [Fig. 3(a)]. In other words, the maximum uncertainty due to VSF shapes is 65%, i.e., $\sigma = 0.65$. A constraint on $B_p$ was introduced in the second test, and, removing the uncertainty due to $B_p$, the maximum uncertainty due to VSF shapes was reduced to 35% [Fig. 3(b)], i.e., $\sigma = 0.35$, where $\sigma$ denotes the uncertainty in $R_{ss}$ explained by $B_p$. A constraint on $\chi_p$ was introduced in the third test, and, removing the uncertainty due to $\tilde{\beta}_p$, the maximum uncertainty due to VSF shapes was reduced to 20% [Fig. 3(c)], i.e., $\sigma = 0.20$, where $\sigma$ denotes the uncertainty in $R_{ss}$ explained by $\tilde{\beta}_p$.
to VSF shapes was reduced to 10% [Fig. 3(d)], i.e., \( \sigma^2_{\chi} - \sigma^2_{\gamma} = 0.10^2 \), where \( \sigma^2_{\chi} \) denotes the uncertainty in \( R_{\chi} \) explained by \( \chi^2 \). Eq. (13) summarizes the results of these four tests:

\[
\begin{align*}
\sigma^2_{\gamma} &= 0.65^2 \\
\sigma^2_{\gamma} - \sigma^2_{\beta_p} &= 0.35^2 \\
\sigma^2_{\gamma} - \sigma^2_{90} &= 0.20^2 \\
\sigma^2_{\gamma} - \sigma^2_{\chi} &= 0.10^2
\end{align*}
\] (13)

Solving Eq. (13), we have \( \sigma_{\beta_p} = 0.55 \), \( \sigma_{90} = 0.62 \), and \( \sigma_{\chi} = 0.64 \). Therefore, among the total uncertainties in \( R_{\chi} \) due to the shape of a VSF, about 71% (\( \approx \sigma^2_{\beta_p}/\sigma^2_{\gamma} \)) can be explained by \( B_{\rho} \) (about 90%) (\( \approx \sigma^2_{\gamma}/\sigma^2_{\beta_p} \)) by \( \tilde{b}_\chi(\gamma \geq 90^\circ) \), and 97% (\( \approx \sigma^2_{\chi}/\sigma^2_{\gamma} \)) by the \( \chi_p \) factor.

From the perspective of ocean color remote sensing, it is difficult to measure \( B_{\rho} \) or \( \tilde{b}_\chi(\gamma \geq 90^\circ) \), which requires b, which unfortunately cannot be retrieved from ocean color, at least for now. On the other hand, both the QSS approximation [Eq. (11)] and the exact \( R_{\chi} \) models, such as the one developed by Zaneveld [8,9], indicate that \( R_{\chi} \) is directly proportional to the \( \chi \) factor. Gordon [43] showed an example to retrieve the VSF shape, which was represented using an analytic equation first applied by Beardsley and Zaneveld [44]. Recently, Zhang et al. [45] found that the \( \chi_{\gamma} \) factor of a VSF can be represented by a linear mixing of two end members, the scattering by particles of sizes much smaller than the wavelength of light, and the scattering by particles of sizes much greater than the wavelength of light. The \( \chi_{\gamma} \) factors of both end members can be derived analytically. They also showed that the mixing ratio can be related to \( \tilde{b}_{\rho} \), which can be retrieved from ocean color observation. However, this relationship is still preliminary and needs further validation. Looking forward, it remains to be tested whether the uncertainty in \( R_{\chi} \) can be significantly constrained by directly accounting for the \( \chi_p \) factor of a VSF.

Our analysis was conducted at 532 nm, at which the VSFs are measured. Based on Eq. (11), how the particle PFs affect the spectral variation of \( R_{\chi} \) mainly depends on if and how the \( \chi_p \) factor varies spectrally. While some studies found no spectral dependence in \( \chi_p \) for oceanic particles [18] or phytoplankton cultures [46,47], Chang et al. [13] indicated that spectral differences could contribute to the up to 20% difference between simulated \( L_{\chi} \) and measured \( L_{\chi} \), and Chami et al. [19] found \( \chi_p \) varied spectrally by \( \pm 6\% \) in a non-blooming coastal water but up to \( \pm 20\% \) in algal cultures. How VSF shapes affect the spectral variation of \( R_{\chi} \), remains to be studied.

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**REFERENCES**


