Interpretation of scattering by oceanic particles around 120 degrees and its implication in ocean color studies

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Abstract: Field observations and theoretical studies have found that the volume scattering functions (VSFs) of oceanic particles exhibit minimum variability at angles near 120°. However, its physical interpretation is still unknown. We find this minimum variability angle represents the intersection of two backscattering-normalized VSFs, one representing particles of sizes smaller than the wavelength of light and the other larger than the wavelength of light. This also suggests that the VSFs of oceanic particles at angles between 90° and 180°, which play a critical role in ocean color study, can be modeled by linear mixing of these two end members. We further validate this mixing model using measured VSFs in coastal and oceanic waters around the US and develop a two-component model predicting the backward shapes of the VSFs.

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References and links

1. Introduction

The volume scattering function (VSF, m⁻¹ sr⁻¹; \( \beta(\theta) \)) in the backward direction (i.e., \( 90 \leq \theta \leq 180^\circ \)) largely dictates the magnitude and shape of reflected solar radiation from the ocean [1] that is amenable to above-water observation. As the VSFs by pure water and seawater are known relatively well [2–4], understanding the backward scattering by oceanic particles is critical for properly interpreting ocean color observations [5].

The backscattering coefficient (\( b_{\text{bb}}, \text{m}^2 \)) is often used to describe the overall magnitude of backward scattering,

\[
b_{\text{bb}} = 2\pi \int_{\theta_{\text{bb}}}^{\pi} \beta(\theta) \sin \theta \, d\theta.
\]
Normalizing $\beta(\theta)$ with $b_b$ describes the overall shape ($\chi$) of the VSFs in the backward angles,

$$
\alpha(\theta) = \frac{1}{\chi(\theta)} = \frac{2\pi\beta(\theta)}{b_b} = \frac{\beta(\theta)}{\int_{\pi/2}^{\pi} \beta(\theta) \sin \theta d\theta}.
$$

For simplicity in notation, we will use $\alpha$ to represent $1/\chi$ hereafter, understanding that both $\alpha$ and $\chi$ are equivalent in representing the shapes of the VSFs from $90^\circ$ to $180^\circ$. From first principles, $\chi$ is very sensitive to the shape [6], composition [7], and size distributions of particles and is expected to vary significantly for different aquatic environments with differing particle assemblages [5]. However, field measurements of the VSFs collected over a wide range of global waters show an intriguing feature of $\chi$, which exhibits minimum variability at angles around $120^\circ$ [8–11]. Denoting this minimum variability angle as $\theta^*$, Oishi [8] found $\theta^* = 120^\circ$ and $\chi(\theta^*) = 1.14 \pm 5\%$; Boss and Pegau [9] found $\theta^* = 118^\circ$ and $\chi(\theta^*) = 1.10 \pm 2\%$; Sullivan and Twardowski [10] found $\theta^* = 113 – 116^\circ$ and $\chi(\theta^*) = 1.0 \pm 2.0\%$; Zhang et al. [11] found $\theta^* = 122^\circ$ and $\chi(\theta^*) = 1.10 \pm 1.45\%$. This behavior was also spotted in mono-specific phytoplankton cultures [12] and confirmed by Mie simulations which show $\theta^* = 112 - 120^\circ$ [8, 9, 13, 14] for spherical particles following the power-law size distributions.

In a further investigation, Zhang et al. [11] found $\theta^*$ to be very close to the angles representing the classic mean values for differentiation of the VSFs, i.e.,

$$
\beta'(\theta^*) = \frac{2}{\pi} (\beta(\pi) - \beta(\pi/2)),
$$

where the symbol $'$ denotes differentiation. The low variability is due to the fact that this classic mean value for the VSFs varies little with the composition and sizes of particles [11]. However, Zhang et al. [11] could not find the physical root for this intriguing behavior of $\chi$ and concluded with an open statement: “It remains to be investigated as to what physical connotation the classic mean value of $\beta(\theta)$ in the backward angles carries that leads to such a constrained variability.” Attempting to answer this question leads to the objectives of this study: (i) to offer a physical interpretation on why backward scattering exhibits constrained variability at angles around $120^\circ$; and (ii) to explore its application for better interpreting ocean color observations.

2. Theoretical interpretation

In nature, particles form a continuum in sizes, ranging from molecules to particulates millimeters or larger. Those that are optically significant have sizes between approximately $0.01 – 1000 \mu m$ [15]. Within this size range, we first examine two end members: particles of sizes less than the wavelength of light ($\lambda$), i.e., size $< \lambda/m_0$, where $m_0$ is the refractive index of water ($\approx 1.33$) and particles of sizes greater than the wavelength of light, i.e., size $> 20\lambda/m_0$ [16]. For visible light ($\lambda = 400 – 700$ nm), particles smaller than the wavelength of light are roughly $< -0.1 \mu m$ (denoted as $P_S$) and those larger than the wavelength of light are $> -10 \mu m$ (denoted as $P_L$). For oceanic $P_S$, the VSF can be approximated as [16],

$$
\beta(\theta) \approx 1 + \frac{1 - \delta}{1 + \delta} \cos^2 \theta,
$$

where $\delta$ represents the depolarization ratio. The corresponding $\alpha_S$ is,

$$
\alpha_S(\theta) = \frac{3}{2} \frac{1 + \delta + (1 - \delta) \cos^2 \theta}{2 + \delta}.
$$

Operationally, $P_S$ is in the dissolved portion of the particle continuum and consists of small colloidal particles [17] and large polymeric molecules, such as dissolved organic matter [18]. While the depolarization ratio for oceanic $P_S$ has been seldom measured, we think that
its range of values is well constrained for the following two reasons: First, the depolarization ratio typically decreases with increasing molecular weight [19]. For example, the laboratory experiments estimated $\delta$ of 0.02 – 0.03 for proteins having a molecular weight of 10,000 – 70,000 g mol$^{-1}$ [19]. In comparison, the current best estimate of $\delta$ for water is 0.039 [20]. Second, for long-chain type molecules, which, if assumed to be rigid, would exhibit strong anisotropic scattering, the random orientation and coiling of molecules would dramatically reduce its effect. For example, if an ~0.2 µm long rod-type particle is rigid, $\delta$ is estimated to be 0.19 – 0.59; however, if it is flexible (consisting of multiple elements, each of which can orient independently of the next), $\delta$ values would be reduced to 0.01 – 0.04 [19]. In this study, we assumed the depolarization ratio for oceanic $P_S$ has values < 0.05, with smaller values being more likely. $\alpha_S$ computed for $P_S$ using $\delta = 0.01$, 0.03, and 0.05 are shown in Fig. 1. Clearly, within this range of possible $\delta$ values, $\alpha_S$ is not very sensitive to the actual value of $\delta$.

For oceanic particles larger than the wavelength ($P_L$), the scattering in the backward angles is predominantly due to reflected light [21] and “the scattering pattern caused by reflection on very large convex particles with random orientation is identical with the scattering pattern by reflection on a very large sphere of the same material and surface condition” [16]. Following Fournier [22], the VSF due to reflection can be approximated as

$$\beta(\theta) \propto |r_m|^2 + |r_l|^2 + |r_m|^2 (1 - |r_m|^2)^2 + |r_l|^2 (1 - |r_l|^2)^2,$$ (5)

where $r_m = \frac{\cos \theta - m \cos \theta_i}{\cos \theta + m \cos \theta_i}$, $r_l = \frac{m \cos \theta - \cos \theta_i}{m \cos \theta + \cos \theta_i}$, $\sin \theta_i = m \sin \theta$, $\theta = \pi - 2\theta_i$, and $m$ is the refractive index of particles relative to water. The backscattering coefficient for $P_L$ is [23]

$$b_h \propto b_{h_0} + b_{h_L}$$

$$b_{h_L} = \frac{3m^4 - 16m^3 + 12m^2 - 1 + 2(2m^2 - 1)^{3/2}}{6(m^2 - 1)^2}$$

$$b_{h_0} = \left[3 - \ln 16\right] + \frac{37(m - 1)}{40(m + 1)} b_{h_L}.$$ (6)

Inserting Eqs. (5) and (6) into Eq. (2), we estimated $\alpha_L$ for $P_L$ (Fig. 1) for $m = 1.02 – 1.20$, the typical range of refractive index values for oceanic particles [24]. $\alpha_L$ shows similar shapes for different refractive indexes with an average difference < 20%.

![Fig. 1. $\alpha(\theta)$ computed between 90 and 180° for very small ($P_S$) particles with different depolarization ratio ($\delta$) and for very large ($P_L$) particles with different refractive indexes ($m$).](image)

While both $\alpha_S$ and $\alpha_L$ vary within a similar range of values between 90° and 180°, their trends of variation are completely different. From 90° to 180°, $\alpha_S$ increases from 0.75 to 1.45 – 1.50, whereas $\alpha_L$ decreases from 1.32 – 1.58 to 0.82 – 0.90. It is also interesting to note that
two groups of $\alpha$’s intersect at angles around 120°, where minimum variability of scattering was found for natural particles [e.g., 11]. Mathematically, this also means that affine combinations of various $\alpha_S$ and $\alpha_L$.

$$\alpha(\theta) = \sum_{i=1}^{n} f_{Si} \alpha_S(\theta) + \sum_{j=1}^{m} f_{Lj} \alpha_L(\theta),$$

where $f_{Si}$ and $f_{Lj}$ are coefficients, satisfying

$$\sum_{i=1}^{n} f_{Si} + \sum_{j=1}^{m} f_{Lj} = 1,$$

would also intersect at angles around 120°. In other words, if $\alpha_S$ and $\alpha_L$ can serve as end members, then their linear mixings would produce $\alpha$’s that exhibit minimum variability at 120°. Now the question is if natural VSFs in the backward angles can be represented by mixings of $P_S$ and $P_L$. To assess this question, first we estimated $\alpha(\theta)$ from measured VSFs, from which the scattering by pure seawater, estimated following [4], was subtracted. Then we tested if the affine combination of the theoretical $\alpha_S(\theta)$ and $\alpha_L(\theta)$ could reproduce the measured $\alpha(\theta)$. A total of 116 VSF measurements have been collected using a prototype instrument, Multispectral Volume Scattering Meter (MVSM) [25], in three coastal waters of the US (Chesapeake Bay, Mobile Bay, and Monterey Bay) and in North Atlantic Ocean. The details of these data sets and their applications have been reported in several studies [11, 25–28]. Basically, the MVSM measures VSFs from 0.5° to 179° with an angular step of 0.25°, which gives 357 measurements at backward angles. Comparison of VSF measurements at a few backward angles by the MVSM and two commercial instruments (HS-6 by HOBI Labs Inc., Bellevue, Washington; and ECO-VSF by WET Labs Inc., Philomath, Oregon) shows an inter-instrument agreement with differences <10% [28].

With each $\alpha(\theta)$ derived from measured VSFs, we used the three $\alpha_S(\theta)$ and five $\alpha_L(\theta)$ shown in Fig. 1 as potential end members and applied a constrained Least-squared regression to solve Eq. (7) for coefficients $f$’s. To ensure physical soundness of the solution, the coefficients to be solved are constrained to be non-negative. If $f_i = 0$, then the corresponding $\alpha_S(\theta)$ or $\alpha_L(\theta)$ is not an end member. The criteria of success are: (i) the sum of coefficients satisfies Eq. (8); and (ii) a significant portion of variability in the VSFs can be explained by these end members. Figure 2(a) (blue bars) shows the distribution of the sums of $f$’s, which has a mean value of 1.01 ± 0.01. Since Eq. (8) is not a required constraint for the inversion, its automatic fulfillment by the solutions indicates that the $\alpha_S(\theta)$ and $\alpha_L(\theta)$ shown in Fig. 1 can indeed serve as the end members. The reproduced backward scattering by linear combination of these end members agree with the measured values within 5 – 10% at angles from 90° to ~170° and within 30% at angles >170° (blue curve in Fig. 2(b)). Results shown in Figs. 2(a) and 2(b) confirm that natural VSFs in the backward angles can be represented by a mixing of $P_S$ and $P_L$ at least for angles from 90° to 170°. Since the points of intersection of these end members are around 120°, the affine combination of them also intersect at approximately the same angle, which explains why the backward shapes of VSFs by natural particles exhibit minimal variability at ~120°.
Fig. 2. Fitting Eq. (7) with $\alpha_S$ and $\alpha_L$ shown in Fig. 1 to measured $\alpha(\theta)$. (a) the sum of derived coefficients $f$, which has a mean value $= 1.011 \pm 0.009$ with 8 end members (EM) and $1.006 \pm 0.014$ with 2 end members; (b) percentage root mean square differences between measured and fitted $\alpha(\theta)$ with 8 and 2 end members, respectively; (c) the total numbers of $\alpha_S$ and $\alpha_L$ that have non-zero coefficients; (d) the distribution of end members that have non-zero coefficients. For the x-axis in (d), the first three values (0.01, 0.03 and 0.05) are for $\delta$ needed to compute $\alpha_S(\theta)$ using Eq. (4) and the rest of the values (1.02, 1.06, 1.10, 1.14 and 1.18) are for $m$ needed to compute $\alpha_L(\theta)$ using Eqs. (5) and (6).

3. A Two-component model for backscattering

Nearly 90% of results (101 out of 116) have only two end members (Fig. 2(c)); one from $P_S$ and the other from $P_L$. For $P_S$, the dominant end member is $\alpha_S$ with a depolarization ratio $\delta = 0.01$; for $P_L$, the dominant end member is $\alpha_L$ with a refractive index $m = 1.02$ (Fig. 2(d)). Since the difference among $\alpha$’s within either $P_S$ or $P_L$ group is relatively small, exactly which end member becomes dominant within each group really depends on the initial condition. For example, the results shown in Fig. 2 are obtained using the $\alpha$’s shown in Fig. 1 as end members. If we drop the $\alpha_L(m = 1.02)$ from the $P_L$ group, then the $\alpha_L(m = 1.04)$ would become the dominant end member in this group with negligible penalty in regression performance (results not shown). This led us to believe that probably using just two end members are sufficient in reproducing the shape of backward scattering.

We repeated the test using $\alpha_S(\delta = 0.01)$ and $\alpha_L(m = 1.02)$ as the two end members and the results (red bars in Fig. 2(a) and red line in Fig. 2(b)) are very similar to those with eight end members. Four examples are shown in Fig. 3, one from each experiment site. Most of the variability in the shape of backward scattering by particles can be explained by the linear mixing of just two end members, representing very small and very large particles, respectively.

Mathematically, the two-component model can be summarized as:
\[ \alpha(\theta) = f_s \alpha_s(\theta) + f_L \alpha_L(\theta), \quad (9) \]

where \( f_s + f_L = 1 \). Optically, for a particle population consisting of one \( P_s \) and one \( P_L \), whose VSFs are \( \beta_s(\theta) \) and \( \beta_L(\theta) \), and backscattering coefficients are \( b_{bS} \) and \( b_{bL} \), respectively, the total VSF \( \beta(\theta) = \beta_s(\theta) + \beta_L(\theta) \) and total backscattering coefficient \( b_b = b_{bS} + b_{bL} \). Also, it can be easily derived from Eq. (2) that

\[ \alpha(\theta) = \frac{b_{bS}}{b_b} \alpha_s(\theta) + \frac{b_{bL}}{b_b} \alpha_L(\theta). \quad (10) \]

Let \( f_s = b_{bS}/b_b \) and \( f_L = b_{bL}/b_b \), then \( f_s + f_L = 1 \) and Eq. (10) becomes identical to Eq. (9). This suggests that the backward VSF of a particle population can be reproduced by a hypothetical mixing of two particle populations of \( P_S \) and \( P_L \). The coefficients \( f_s \) and \( f_L \) in Eq. (9) simply represent the fractional backscattering contributions by \( P_S \) and \( P_L \), respectively.

Comparison of possible angular variations of \( \alpha(\theta) \) produced by the two end members (Fig. 4(a)) with the measured \( \alpha(\theta) \) (Fig. 4(b)) demonstrates the potential of using the two-component model (Eq. (9)) to reproduce the shape of backward scattering of natural particle populations. Note that for better display and for highlighting overall angular variation, the measured \( \alpha(\theta) \) shown in Fig. 4(b) were smoothed to removed high frequency variability, such as those shown in Fig. 3 (gray lines), that are frequently seen in the measurements. The values of \( f_S \) or the backscattering fraction by \( P_S \) seem to co-vary with the total particle backscattering coefficient, with a best-fit regression of

\[ f_s = 0.45(\pm0.05)(\log b_b)^2 + 1.90(\pm0.21)\log b_b + 2.29(\pm0.21). \quad (11) \]

![Fig. 4.](image)

4. Discussion and conclusions

Most of the variability in the shape of backward scattering \( \alpha(\theta) \) by particles can be explained by the linear mixing of just two groups of end members, one representing backscattering by very small particles and the other large particles. Because the backward angular scattering within each group are very similar to each other, we further showed that applying linear mixing by using just one end member from each group can adequately reproduce the measured \( \alpha(\theta) \) with an uncertainty < 10% for angles from 90 – ~170° (Figs. 3 and 4). Since the point of intersection of these end members is at angles around 120°, the affine combination of these end members also intersect at the approximately the same angle, which
explains why the backward shapes of VSFs by natural particles exhibit minimal variability at ~120°.

Tan et al. [29] showed recently that the ratio of scattering at 170° and 120° is a good indicator of the shape differences of the VSFs measured for natural particles as well as for cultures of phytoplankton. This finding can be easily derived from Fig. 4(a), which shows that $\beta(170)/\beta(120)$ correlates well with the mixing ratio of $a_S$ and $a_L$, and hence the general shape of the VSFs in the backward angular range.

As shown in Fig. 2(b), uncertainty is relatively high (up to 30%) in reproducing the scattering at angles > 170°. Technically, it is extremely challenging to measure scattering at the immediate backward angles because both the light source and detector have finite physical sizes. On the other hand, natural particles, such as clouds [16, 30] or bubbles [31], do generate glory, an enhancement of scattering at angles $\approx 180°$. Therefore, we are not certain what could be the cause for the relatively greater uncertainty at angles > 170°; but at least a part of it could be due to instrumental difficulty. However, this uncertainty has little impact on our results because (i) in estimating the backscattering coefficient $b_b$ (Eq. (1)), $\beta(\theta)$ is weighted by $\sin(\theta)$, which goes to zero as $\theta$ approaches 180°; and (ii) part of the uncertainty would be cancelled out in forming $a(\theta)$, which represents the ratio of $\beta(\theta)$ to $b_b$ (Eq. (2)).

While particle sizes are an important factor determining the shape of the angular scattering as shown in Fig. 1, other particle characteristics also play a role. For example, if particles have roughened surfaces, such as coccoliths, Fournier and Neukermans [23] have shown that their backward scattering can be approximated by diffuse scattering [16], which is very close in shape to the scattering by $P_S$. Therefore, caution should be used in interpreting relative contributions by $P_S$ and $P_L$ to the angular backscattering, because in this study they represent more a type of angular shape in scattering than a particular particle size class.

Kopelevich [32] proposed a two-component particle phase function model, including a small fraction representing mineral particles less than 1.3 µm in radius and having a relative refraction index of 1.15 and a large fraction representing biological particles larger than 1.3 µm in radius and having a relative refraction index of 1.03. Haltrin [33] provided a regression formula for each of the components and used their linear mixing to represent the VSFs of particles in the ocean. While the model might be able to reproduce the overall shape of particle scattering over the entire angular range of 0 – 180°, we found that it does not represent the backscattering very well. For example, $\alpha$’s corresponding to the small and large fractions in the Kopelevich’s model have approximately similar shapes and intersect at two angles: ~110° and ~168°. On the other hand, the two-component we proposed in this study is focused on the backscattering and can explain approximately 90% of variability in the shape of backward angular scattering.

Our model also has significant implication to the study of ocean color. From the radiative transfer equation, Zaneveld [1, 34] showed that the color of the ocean, or the remote sensing reflectance $r_s(\lambda)$ is directly proportional to the VSFs, i.e., $r_s = \beta(\theta_m)$, where $\theta_m$ represents mean scattering angle of reflecting the downwelling radiance field back to a sensor. Since $\theta_m$ is predominantly in the range of 90 – 180°, knowledge of the backward VSFs plays a critical role in interpreting the ocean color measurements. While the magnitude of backward VSFs, i.e., the backscattering coefficient $b_b$ can be derived from the measurement of $r_s$ [35–37], the effect of the shape of the backward VSFs, i.e., $a(\theta)$ or $\chi(\theta)$ has been largely unknown and typically lumped into the BRDF (or the $f/Q$) factor [38, 39]. The two-component model (Eqs. (10) and 11) we proposed in this study offers a possibility of including the shape as well as the magnitude of backward scattering in studying the color of the ocean. We are currently developing a model to derive both $a(\theta)$ and $b_b$ from the ocean color measurements. While its technical details will be reported separately, the model conceptually involves the iterative estimates of (i) $b_b$ using the conventional ocean color algorithms [e.g., 40], (ii) $a(\theta)$ from $b_b$.
using Eq. (11), (iii) BRDF effect from $\alpha(\theta)$ following [e.g., 1], and (iv) improved $b_h$ using estimated BRDF.

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