Effects of bulk particle characteristics on backscattering and optical closure

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Abstract: Optical closure is essential for the determination of biogeochemical properties from ocean color remote sensing information. Mie scattering theory, a radiative transfer model, and a semi-analytical inversion algorithm were used to investigate the influence of particles and their properties on optical closure. Closure results were generally poor. Absorption coefficient (\(\alpha\)) inversions were more accurate for moderate particle size distribution slopes (3.50 ≤ \(\xi\) ≤ 3.75). The degree of success in the derivation of the backscattering coefficient (\(b_{bp}\)) was highest at moderate indices of refraction (1.15 ≤ \(n_p\) ≤ 1.20) and high values of \(\xi\) (> 3.75). Marked improvements in the estimates of \(b_{bp}\) were enabled by a priori knowledge of \(b_{bp}\) at one wavelength. At moderate values of \(n_p\), derivations of \(\alpha\) and \(b_{bp}\) were within 25% of Mie-modeled values when Gershun’s relationship was used in combination with the semi-analytical algorithm.

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References and links

4. C. J. Bohren and D. R. Huffman, Absorption and Scattering of Light by Small Particles (John Wiley, 1983).

1. Introduction

Optical closure involves solutions to the forward and inverse problems in ocean optics. Both problems are twofold: Forward – the determination of the inherent optical properties (IOPs) from characteristics of the particulate and dissolved material and the prediction of the apparent optical properties (AOPs) from the IOPs; Inverse – the derivation of the IOPs from the AOPs, and the determination of biogeochemical properties from the IOPs. The latter
component of the inverse problem is especially important for interpretation of ocean color remote sensing data to synoptically observe and monitor interdisciplinary processes such as biogeochemical cycling, particle transport, and ecosystem dynamics (e.g., see [1]). Other than the computation of the AOPs from the IOPs, i.e. component #2 of the forward problem [2], optical closure has proven problematic – particularly for global scale applications.

Optical theory suggests that the optical properties of particles depend on characteristics such as particle size, shape, composition, and index of refraction [3,4]. Mie scattering theory involves the estimation of the IOPs from characteristics for a single particle or a population of mono-dispersed or poly-dispersed particles. Briefly, Mie theory determines the scattering and extinction efficiency factors (and absorption by difference) for a homogeneous sphere at a given wavelength, index of refraction, and particle diameter. Ensembles of efficiency factors for spheres of different sizes can then be applied, using a specified particle size distribution (PSD) and number concentration to derive the respective IOPs, i.e. the absorption, scattering, and attenuation coefficients for a particle population.

The IOPs are in turn directly related to remote sensing reflectance through radiative transfer theory, which can be numerically modeled (e.g., [2]). A simpler approach to radiative transfer has been proposed, with remote sensing reflectance correlated to the absorption and backscattering coefficients and represented by:

\[
\text{r}_{rs}(\lambda) = \frac{f(\lambda)}{Q(\lambda)} \{ \frac{b_\text{bt}(\lambda)}{a_\text{t}(\lambda) + b_\text{bt}(\lambda)} \},
\]

where \(b_\text{bt}(\lambda)\) is total spectral backscattering, \(a_\text{t}(\lambda)\) is total spectral absorption, and the \(f/Q\) ratio (wavelength notation hereafter suppressed) is a parameter that depends on the shape of the upwelling light field and the volume scattering function (VSF) [5]. The parameter \(Q(\lambda)\) is a measurable quantity: the ratio of upwelling irradiance to upwelling radiance. However the value, \(f(\lambda)\), is often approximated for a single VSF [6] or using assumed scattering properties and sky conditions [7,8], which oftentimes leads to erroneous computations of \(r_{rs}(\lambda)\) from the IOPs and \textit{vice versa} when inverting this relationship (i.e. the inverse problem).

Empirical and semi-analytical algorithms have been developed to invert remote sensing reflectance signals to obtain the IOPs and biogeochemical constituents (e.g., chlorophyll concentration; [9]). Empirical algorithms have proven challenging for Case II waters, whose optical properties are not dominated by chlorophyll-containing particles but rather by inorganic particles, colored dissolved organic matter (CDOM), or both quantities. Semi-analytical algorithms based on Eq. (1) (e.g., see [10]) have been more successful when applied to widely varying optical water types, however, assumptions about the spectral and angular scattering properties and the upwelling light field can negatively impact inversion results.

The effects of particles and particle characteristics on the variability of remote sensing reflectance need to be understood in order to solve the forward and inverse problems in ocean optics and importantly, to better utilize ocean color data to obtain information about biogeochemistry and ecosystem dynamics. We present results from forward and backward approaches to optical closure with emphasis on the effects of particles and their characteristics on backscattering, the backscattering ratio, and ocean color. We build upon decades of theoretical, laboratory, and field results (e.g., see [3,4,11-20]).

2. Methods

Mie scattering theory and the radiative transfer model, Hydrolight, were used to compute the bulk IOPs and AOPs for a set of hypothetical water masses containing particle populations with variable bulk indices of refraction and PSDs. The influence of particles and their properties (e.g., bulk real index of refraction and PSD slope, \(n_p\) and \(\xi\), respectively) on the IOPs and AOPs and on inversion algorithms to derive the IOPs from AOPs was investigated using a semi-analytical remote sensing inversion algorithm.
2.1 Forward approach

Mie scattering theory was used to generate bulk IOPs for a series of hypothetical water masses. Mie model input values were determined based on four years of time series measurements of optical properties collected on a mooring at 4 m water depth in shallow coastal waters of the Santa Barbara Channel (Fig. 1). Optical water types in this region of the Santa Barbara Channel are highly biogeochemically complex and can vary rapidly from relatively clear waters dominated by biogenic particles to very turbid and comprised of mostly inorganic particles [21,22].

We used the Mie code provided by Bohren and Huffman [4] for scattering by homogeneous spheres (routines BHMIE and CALLBH), translated from Fortran language into Matlab by E. Boss (U Maine). This code computes the elements and efficiencies of the amplitude scattering matrix. The modeled PSDs were restricted to a size range of diameters, \( D \), ranging from 0.2 – 100 \( \mu \)m in 35 logarithmically spaced size bins. The PSDs followed a differential size distribution function where \( f(D) = N \times D^n \), where \( N \) is the particle concentration (held constant at 5 x 10^5 mL^-1), i.e. we assumed Junge-type PSDs. We used \( n_p \) values of 1.01, 1.05, 1.10, 1.15 and 1.20 and \( \xi \) values of 3.0, 3.25, 3.5, 3.75, 4.0 and 4.25 at nine wavelengths (\( \lambda = 412, 440, 488, 510, 532, 555, 650, 676, \) and 715 nm). The imaginary index of refraction of particles was held constant at \( n' = 0.01 \) for all Mie theory calculations. Flatter PSD slopes, i.e. lower values of \( \xi \), generally imply more large particles are present in a population, whereas steeper PSD slopes specify smaller particles. Lower values of \( n_p \) are indicative of biological particles (\( n_p^{phytoplankton} = 1.02 – 1.07; \) [23]) because of their high water content, and minerogenic particles are represented by higher values of \( n_p \) (\( n_p^{minerogenic} = 1.14 \) to 1.26; [24]). Two hundred and seventy sets of IOPs were determined from Mie modeling efforts. These Mie-computed IOPs were within the range of IOPs measured in the Santa Barbara Channel (Fig. 1).

![Fig. 1. Measured IOPs (Santa Barbara Channel). Thick black lines indicate the spectral mean and dashed black lines denote one standard deviation from the mean. The lower right-hand panel shows a data series of bulk \( n_p \) (red) and \( \xi \) (blue) computed using measured IOPs and methods presented by Boss et al. [25] and Twardowski et al. [12]. [The IOP property subscript 'p' denotes particulate material and 'g' represents dissolved matter.]](image)
Phase functions, together with Mie-computed scattering and attenuation (and absorption by difference) coefficients, were then inputted into the numerical radiative transfer model, Hydrolight, to compute the AOPs at the surface, just below the surface, and at 4 m geometric water depth in optically deep waters. Particle phase functions were generated from Mie-calculated VSFs using relevant phase function discretization operations in Hydrolight. Inelastic scattering processes were not included in computations and the following environmental conditions were assumed: wind speed = 5 m s\(^{-1}\), solar angle = 30°, and 0% cloud cover. Hydrolight calculations resulted in 270 arrays of AOPs representing five different bulk indices of refraction, six different PSD slopes, and nine different wavelengths.

2.2 Inverse approach

We employed a semi-analytical remote sensing inversion algorithm [10] in order to examine the influence of particles and their properties (\(n_p\) and \(\xi\)) on derivations of the IOPs from AOPs. This algorithm uses the relationship presented by Gordon et al. [26]:

\[
r_{rs}(\lambda) = g_0 u(\lambda) + g_1 [u(\lambda)]^2 \tag{2a}
\]

where

\[
u(\lambda) = b_{bt}(\lambda) / [a_t(\lambda) + b_{bt}(\lambda)] \tag{2b}
\]

and the g-constants are dependent on the particle phase function, oftentimes represented as \(g_0 = 0.084\) and \(g_1 = 0.17\) [10], which are the values we used in our computations. Due to the relatively large values of \(a_t(440) > 0.3\) m\(^{-1}\), \(a_t(650)\) was first parameterized as a function of Hydrolight-derived \(r_{rs}(\lambda)\), then \(b_{bt}(650)\) was derived from Eq. (2), as opposed to using the 555 nm wavelength method [10]. Next, \(b_{bt}(\lambda)\) was computed; it was assumed to monotonically decrease with increasing wavelength:

\[
b_{bt}(\lambda) = b_{bt}(\lambda_0) + b_{bp}(\lambda_0) \left(\lambda_0 / \lambda\right) \eta, \tag{3}\]

where \(\lambda_0 = 650\) nm and \(\eta\) is a function of \(r_{rs}(\lambda)\). Spectral \(a_t(\lambda)\) was calculated following Eq. (2). Details regarding empirical parameterizations of the IOPs and \(r_{rs}(\lambda)\) can be found in Lee et al. [10].

3. Results and discussion

To verify data and model integrity, we provide an independent parameterization of \(a_t(\lambda)\) derived from Gershun’s equation. The exact relationship (wavelength notation suppressed):

\[
a_t = K_d \mu_d \left[1 + R \left(\mu_d / \mu_u\right) \right]^{-1} \left[1 - R + (K_d)^{-1} dR/dZ\right], \tag{4}
\]

(where \(K_d\) is the diffuse attenuation coefficient for downwelling irradiance, \(\mu_d\) and \(\mu_u\) are the average cosines for downwelling and upwelling light, respectively, \(R\) is irradiance reflectance, and \(Z\) is depth) was applied to our Hydrolight-derived \(K_d\), \(\mu_d\), \(\mu_u\), and \(R\) at \(Z = 4\) m. Comparisons between Mie-modeled absorption coefficients, \(a_t^{Mie}(\lambda)\), and absorption coefficients inverted using Gershun’s equation, \(a_t^{Ger}(\lambda)\), at 4 m are shown in Fig. 2. The exact 1:1 correlation between \(a_t^{Mie}(\lambda)\) and \(a_t^{Ger}(\lambda)\) for all \(n_p\), \(\xi\), and \(\lambda\) indicates that no errors were made in Mie computed inputs to Hydrolight or Hydrolight modeling.
3.1 Forward approach - IOPs

The effects of variable $n_p$ and $\xi$ on spectral IOPs are shown in Fig. 3. The absorption, attenuation, scattering, and backscattering coefficients (minus water) all increased with increasing $n_p$ at all wavelengths. Harder particles (i.e. material with higher $n_p$-values) resulted in higher scattering and less transmission of light, which has been predicted from Mie theory (e.g., see [11,12]). The absorption coefficient was minimally affected by variations in $n_p$ and decreased with increasing $\xi$; spectral variability was more or less constant across all $n_p$ and $\xi$. PSD slope effects were similar between $c_p(\lambda)$ and $b_p(\lambda)$, i.e. attenuation was controlled more by scattering processes. In general, $c_p(\lambda)$ and $b_p(\lambda)$ decreased with increasing $\xi$ but at $n_p > 1.10$, $c_p(\lambda)$ and $b_p(\lambda)$ increased in the blue wavelengths as $\xi$ exceeded 4.0 (Fig. 3). Wozniak and Stramski [17] also showed higher blue-peaked spectra for mass-specific scattering coefficients at high values of $\xi$. Effects of $n_p$ variability were more pronounced at higher $\xi$ for $c_p(\lambda)$ and $b_p(\lambda)$. This implies that variability in $c_p(\lambda)$ and $b_p(\lambda)$ was more strongly affected by the presence of smaller, harder (i.e. minerogenic) particles.

![Fig. 2. Comparison between $a^\text{Mie}_p(\lambda)$ and $a^\text{Ger}_p(\lambda)$ [Eq. (4)] at nine wavelengths, five different values of $n_p$, and six different values of $\xi$.](image)

![Fig. 3. Spectral IOPs and IOP ratios as a function of $n_p$ (legend in top left panel; colors correspond to plot lines and not fill colors) and $\xi$ (x-axes).](image)
where biological particulates dominated. We also found that significant departures from a power-law function at lower \( n_p \), with the mean power-law exponent changing from \( \eta = -2.601 \) to \(-0.1056\), averaged over six different \( \xi \). The mean of \( \eta \) over the 270 Mie-computed \( b_{bp}(\lambda) \) spectra was calculated to be \(-0.8991\) with a standard deviation of 1.0844. In comparison, Snyder et al. [20] found that the mean and standard deviation of \( \eta \) for over 6000 field measurements of \( b_{bp}(\lambda) \) in coastal waters was \(-0.942 \pm 0.210\). They stated that, “…the spread in this value is not random and represents small, but real, spectral changes in the backscattering spectral properties of the water” [20]. Their results show that significant departures from the average power-law function occurred where biological particulates dominated. We also find that the spectral shape of \( b_{bp}(\lambda) \) deviated from a power-law function at lower \( n_p \) (at \( n_p < 1.10 \), \( b_{bp}(\lambda) \) exponentially decayed with increasing wavelength; not visible in Fig. 3), which is representative of particles with higher water content, i.e. biological particles. Spectral inflections in the particulate backscattering coefficient have been observed in modeling results that used input parameters based on measurements of phytoplankton cultures [27-30]. Direct measurements of the spectral backscattering properties of marine phytoplankton cultures have also shown spectral inflections [31]. Reduced backscattering in spectral regions of strong absorption (e.g. peaks in absorption by Chlorophyll-\(a\) around 440 and 670 nm) is caused by the change in the imaginary index of refraction at these wavelengths, an effect known as anomalous dispersion [3,32]. However, spectral inflections present in our results are somewhat surprising, given that we kept the real and imaginary portions of the index of refraction constant across wavelengths in our model runs.

Based on theoretical studies [11,12], the backscattering ratio, \( b_{bp}(\lambda)/b_p(\lambda) \), has traditionally been assumed to be spectrally flat. However, Ulloa et al. [11] assert that in the case of monodispersions or in waters dominated by minerogenic particles, \( b_{bp}(\lambda)/b_p(\lambda) \) can vary strongly with wavelength depending on the size of the particles and their refractive index. We found that Mie-modeled \( b_{bp}(\lambda)/b_p(\lambda) \) was spectrally flat only at \( \xi \leq 3.25 \) for all \( n_p \), i.e. larger particles. During all other conditions, \( b_{bp}(\lambda)/b_p(\lambda) \) varied spectrally with increasing \( n_p \) and \( \xi \). The spectral shape of \( b_{bp}(\lambda)/b_p(\lambda) \) exhibited increasing values with increasing wavelength, with the steepest spectral slopes observed at \( \xi = 4.25 \). The particulate backscattering ratios observed by Snyder et al. [20] also exhibited a wide range in wavelength dependence and were highly variable in space and time. However, others have found little spectral variation in \( b_{bp}(\lambda)/b_p(\lambda) \). Boss et al. [15] and Mobley et al. [33] reported that \( b_{bp}(\lambda)/b_p(\lambda) \) spectra varied by less than 10% and 24% for all values of backscattering measured in coastal New Jersey and modeled using Hydrolight, respectively. Whitmire et al. [19] found no significant spectral variability in a dataset of over 9000 observations that included data from diverse aquatic environments and particle populations, with rare exceptions in instances of monodispersions of large particles. Risović [13] found that Mie-modeled \( b_{bp}(\lambda)/b_p(\lambda) \) was only weakly dependent on wavelength but suggested additional research on the spectral behavior of \( b_{bp}(\lambda)/b_p(\lambda) \).

Risović [13] also suggested that \( b_{bp}(\lambda)/b_p(\lambda) \) can be overestimated with Mie theory when assuming a Junge-type particle distribution. However, our resultant \( b_{bp}(\lambda)/b_p(\lambda) \) values are quite similar to those measured in the Santa Barbara Channel (Figs. 1 and 3). The magnitude of \( b_{bp}(\lambda)/b_p(\lambda) \) generally increased with increasing \( n_p \) and \( \xi \), which has been shown by Mie theory (e.g., Fig. 5 in [11] and Fig. 1 in [12]). Theoretical studies have also indicated that \( b_{bp}(\lambda)/b_p(\lambda) \) is strongly affected by the presence of sub-micrometer particles and that its...
magnitude varies with the slope of the PSD [11]. Observed magnitudinal variability of \( b_p(\lambda)/b_\rho(\lambda) \) has been related to particle composition. Loisel et al. [34] indicated that, based on data collected in European waters, the amount of organic material has a strong influence on \( b_p(\lambda)/b_\rho(\lambda) \) and detrital particles resulted in higher values of \( b_p(\lambda)/b_\rho(\lambda) \). Boss et al. [15] also report that \( b_p(\lambda)/b_\rho(\lambda) \) is strongly related to the index of refraction particles. Snyder et al. [20], however, do not find any quantifiable evidence of particle type (organic vs. inorganic) with the magnitude of \( b_p(\lambda)/b_\rho(\lambda) \) and suggest that other factors need to be considered in quantifying the variability in \( b_p(\lambda)/b_\rho(\lambda) \).

The most striking results for the effects of particle characteristics on our set of hypothetical optical water types was the highly variable spectral shapes of the backscattering coefficient and the backscattering ratio. Contrary to assumptions made in the past, \( b_p(\lambda)/b_\rho(\lambda) \) was not always spectrally flat and spectral \( b_p(\lambda) \) did not always follow the widely used expression shown in Eq. (3). This suggests that spectral variability, in addition to magnitudinal variability in \( b_p(\lambda)/b_\rho(\lambda) \) and \( b_p(\lambda) \) could contain valuable information about the characteristics of particles. Importantly, variable spectral shapes (e.g., exponential versus power-law) at low \( n_p \) and spectral inflections at low \( \xi \)-values could have profound impacts on remote sensing and inversion algorithms for the derivation of the IOPs and biogeochemical properties.

3.2 Forward approach - AOPs

Hydrolight-computed AOP values were within the ranges of those reported in the literature (Fig. 4). For example, Morel et al. [35] reported field-measured and simulated values of \( Q(\lambda) \) between 0 and 8 sr and Loisel and Morel [36] found \( Q(\lambda) \) to vary between about 3 and 7 sr from numerical simulations of case II coastal waters with variable solar angles and scattering events. Loisel and Morel [36] also reported \( f/Q \) values between 0.06 and 0.20 sr\(^{-1} \) for the same simulations. \( K_d(\lambda) \) values and spectral shapes in Fig. 4 are typical of turbid coastal waters (e.g., Fig. 2 in [36]).

Spectral AOPs for variable \( n_p \) and \( \xi \)-values are shown in Fig. 4. \( K_d(\lambda) \) behaved similar to \( a_{pg}(\lambda) \), increasing with increasing \( n_p \) and decreasing with increasing \( \xi \) at all wavelengths.
Remote sensing reflectance and R(\(\lambda\)) (irradiance reflectance) spectral effects were as expected with increasing \(n_p\) and \(\xi\); spectral shapes shifted from blue-peaked (case I-like) at low \(n_p\) and \(\xi\) to green-peaked (case II-like) at high \(n\) and \(\xi\). The variability in the f/Q ratio was highly dependent on wavelength, \(n_p\), and \(\xi\). The f/Q ratio increased with increasing \(n_p\) at all wavelengths, however effects of variable \(\xi\) were spectrally and \(n_p\) dependent. This suggests that f/Q is strongly related to scattering processes and should not be treated as a constant (e.g., [37,38]) [note that the computation of f assumes that the relationship in Eq. (1) is true]. This has important implications for inversion algorithms to determine the IOPs and biogeochemical constituents from remotely sensed ocean color data as many radiative transfer-based inversion models employ empirically or numerically determined constants in the place of f/Q, e.g., Eqs. (1) and (2).

3.3 Inverse approach

Absorption and backscattering coefficients derived using a semi-analytical algorithm [10] were within 150% of “true” values, i.e. Mie-computed (Fig. 5). Lower values of \(a_\lambda(\lambda)\) were estimated more accurately than higher values, likely because the algorithm was formulated based on \(a_\lambda(\lambda)\) values of less than 0.3 m\(^{-1}\) whereas our Mie-computed \(a_\lambda(\lambda)\) values were much higher (mean of 0.5 m\(^{-1}\) at 412 nm; Fig. 1). The degree of success of derivation of \(a_\lambda(\lambda)\) was more influenced by \(\xi\) as compared to \(n_p\) or wavelength. For derivations of \(a_\lambda(\lambda)\), the inversion algorithm performed best at moderate \(\xi\)-values (3.50 \(\leq\) \(\xi\) \(\leq\) 3.75) for all values of \(n_p\) and at all wavelengths. Absorption was slightly overestimated for high values of \(\xi\) (i.e. smaller particles) and underestimated for low \(\xi\) (i.e. larger particles). On the other hand, successful derivations of \(b_{bp}(\lambda)\) were dependent on \(n_p\) and \(\xi\) but not necessarily on wavelength or the magnitude of \(b_{bp}(\lambda)\). We show that more accurate \(b_{bp}(\lambda)\) estimations were achievable at 1.15 \(\leq\) \(n_p\) \(\leq\) 1.20 and at higher values of \(\xi\) (i.e. smaller particles). Derivations were underestimated for lower \(\xi\).

Fig. 5. Derived \(a^{OAA}_\lambda(\lambda)\) and \(b^{OAA}_{bp}(\lambda)\) compared to \(a^{Mie}_\lambda(\lambda)\) and \(b^{Mie}_{bp}(\lambda)\). Wavelengths are represented by different colors from blue (400 nm range) to red (600 nm range). Open symbols in the first column denote the different \(\xi\)-values (triangles = 3.0, circles = 3.25, squares = 3.50, pluses = 3.75, stars = 4.0, and asterisks = 4.25) and closed symbols in the second column represent the different \(n_p\)-values (triangles = 1.01, circles = 1.05, squares = 1.10, crosses = 1.15, and stars = 1.20).
To investigate potential sources of error in the semi-analytical algorithm for these particular IOPs and AOPs, we assumed a priori knowledge of $b_{bp}(650)$ and then estimated $b_{bp}(\lambda)$ and $a_t(\lambda)$ using Eqs. (3) and (2). Results of this exercise are shown in Fig. 6a-d. Not surprisingly, derivations of spectral $b_{bp}(\lambda)$ are much more accurate with knowledge of $b_{bp}(\lambda)$ at one wavelength (Fig. 6c, d). Other than for $n_p = 1.01$, $b_{bp}(\lambda)$ was generally overestimated, more so at the blue wavelengths when $b_{bp}(650)$ is known. Thus, $a_t(\lambda)$ was also overestimated. The absorption coefficient was generally overestimated by up to 130%, even at $a_t(650)$ when $b_{bp}(650)$ is known, which suggests that $g_0$ and $g_1$ (Eq. 2) are not entirely accurate and should not be treated as constants, at least for this set of IOPs. This is evidenced by the highly variable f/Q ratio shown in Fig. 4 and discussed in the previous section.

The right two columns of Fig. 6 (e, f) show derivations of $a_t(\lambda)$ using a simplified version of Eq. (4), where $\mu_a = 0.40$, $\mu_d = 0.90$, and $dR/dZ$ is neglected [39]:

$$a_t(\lambda) = K_d(\lambda) 0.90 [1 + 2.25 R(\lambda)]^{-1} [1 - R(\lambda)]$$

and by assuming $R(\lambda) = 3.5 \times r_s(\lambda)$. Eq. (3) was then used to estimate $b_{bp}(\lambda)$ (Fig. 6g, h). The use of a simplified Gershun’s equation yielded more accurate derivations of $a_t(\lambda)$, mostly within 25% of Mie-computed values (Fig. 6e, f). The largest deviations in $a_t(\lambda)$ and $b_{bp}(\lambda)$ were found at higher $n_p$ values. Unsuccessful derivations of $b_{bp}(\lambda)$ at $n_p = 1.01$ in both cases are due to the fact that the spectral shape of $b_{bp}(\lambda)$ at the lowest $n_p$-value (Fig. 6d, h) is represented by an exponential, rather than a power-law function. This implies that for complex coastal waters, improvements need to be made to the empirical parameterization of the power-law exponent, $\eta$.

Wozniak and Stramski [17] also show that mineral particles in seawater can result in significant errors in the derivation of, in their case chlorophyll concentration from ocean color data. Marked improvements in the inversion algorithm are found by assuming a priori knowledge of $b_{bp}$ at one wavelength or by applying a simplified Gershun’s equation to first derive $a_t(\lambda)$. This shows that minimal in situ measurements can result in accurate assessments of the IOPs and hence biogeochemical properties from ocean color remote sensing data.
4. Summary and conclusions

Mie scattering theory and the radiative transfer model, Hydrolight, were used to compute the IOPs and AOPs for a set of hypothetical optical water types with variable bulk real indices of refraction and particle size distribution slopes. The influence of particles and their properties on inversion algorithms to derive the IOPs from modeled AOPs was investigated using a semi-analytical remote sensing inversion algorithm. Notable conclusions are highlighted here.

The spectral shape and magnitude of the absorption coefficient was minimally affected by variations in $n_p$, but its magnitude decreased significantly with increasing $\xi$. Variability in the attenuation and scattering coefficients was strongly influenced by the presence of smaller, harder particles. The spectral shape of the particulate backscattering coefficient was not always represented by a power-law function, and often exhibited spectral inflections. The particulate backscattering ratio was spectrally flat only in the presence of larger particles. During all other conditions, $b_{bp}(\lambda)/b_p(\lambda)$ varied spectrally with increasing $n_p$ and $\xi$. In evaluating the effect of particle properties on AOPs, we found that the f/Q ratio exhibited escalating spectral variability with increasing $n_p$ and $\xi$. In tests of the performance of a semi-analytical algorithm in predicting IOPs, the degree of success in the derivation of $a(\lambda)$ was more influenced by the magnitude of $a(\lambda)$ and $\xi$ as compared to $n_p$ or wavelength. Accurate derivations of $b_{bp}(\lambda)$ were dependent on $n_p$ and $\xi$ but not necessarily on wavelength or the magnitude of $b_{bp}(\lambda)$. Marked improvements in estimates of $b_{bp}(\lambda)$ were enabled by a priori knowledge of $b_{bp}$ at one wavelength. At $1.05 < n_p < 1.15$, derivations of $a(\lambda)$ and $b_{bp}(\lambda)$ were well within 25% of true values when Gershun’s equation was used in combination with the semi-analytical algorithm.

Our efforts here are focused on improving and quantifying understanding of the relationships between the bulk optical properties and the particle characteristics. The IOPs form the link between biogeochemical constituents and the vertical structure of the radiance field; therefore successful inversions of satellite-measured ocean color properties to derive biogeochemical products are dependent on efforts like these. We identify the need to better comprehend the effects of individual and bulk particle characteristics that are more detailed than $n_p$ and $\xi$ (e.g., individual particle composition and size) on the spectral shapes of the backscattering coefficient and backscattering ratio and on the variability of the f/Q ratio (or the g-constants) in order to properly parameterize inversion models. We also show that significant improvements to inversions can be achieved with minimal in situ measurements, i.e. ocean color remote sensing ground-truthing.

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