On the non-closure of particle backscattering coefficient in oligotrophic oceans

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Abstract: Many studies have consistently found that the particle backscattering coefficient ($b_{bp}$) in oligotrophic oceans estimated from remote-sensing reflectance ($R_{rs}$) using semi-analytical algorithms is higher than that from in situ measurements. This overestimation can be as high as ~300% for some oligotrophic ocean regions. Various sources potentially responsible for this discrepancy are examined. Further, after applying an empirical algorithm to correct the impact from Raman scattering, it is found that $b_{bp}$ from analytical inversion of $R_{rs}$ is in good agreement with that from in situ measurements, and that a closure is achieved.

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OCIS codes: (010.4450) Oceanic optics; (280.0280) Remote sensing.

References and links


1. Introduction

The spectrum and amplitude of the light leaving the ocean depends on the constituents therein and therefore can be used to obtain information about these constituents. For remote sensing application, the water-leaving radiance \( L_w \) (W m\(^{-2}\) sr\(^{-1}\)) is used to describe this light, and because \( L_w \) is proportional to the incoming light on the ocean, described by the downwelling irradiance \( E_d \) (W m\(^{-2}\)), \( E_d \) is used to normalize \( L_w \) and remove the dependence of variable incident irradiance. The ratio \( L_w/E_d \) termed the remote sensing reflectance \( (R_{rs}, \text{sr}^{-1}) \) [1], depends on the concentration of optically active constituents in the water and the geometry of observation (angular distribution of the light field and observation direction of the sensor).

The impact of the optically active constituents on \( R_{rs} \) can be described by inherent optical properties (IOPs) [2]. The IOPs depend only on the type and concentration of constituents and not on the ambient light field [3]. These IOPs are the absorption coefficient \( (\alpha, \text{m}^{-1}) \) which describes the loss of photon by absorption, and the volume scattering function (V SF, m\(^{-1}\) sr\(^{-1}\)) which represents the angular distribution of scattered photons. Because photons leaving the
The particulate backscattering coefficient ($b_{bp}$, m$^{-1}$), the fraction of the total backscattering coefficient that is not due to water molecules, is an important IOP. Not only does it describes how light is returned to the ocean surface and thus forms the signal collected by satellite sensors, but it’s value, when interpreted in terms of particle population, has also been proposed to infer concentrations of organic and inorganic constituents in the oceans [12–15]. Because of this importance, both remote sensing [13,16] and in situ methods [17] have been developed to obtain measurements of $b_{bp}$ in surface waters in the global oceans.

Remote sensing methods to retrieve $b_{bp}$ are based on its relationship to $R_{rs}$. For empirical algorithms [13], functional relationships are described based on concurrent measurements of $b_{bp}$ and $R_{rs}$. For such empirical algorithms, there is no involvement of the radiative transfer equation (RTE), where all the information required for the algorithms is provided by the measurements and consequently any measurement bias are directly reflected in the output. Empirical algorithms will also include all relevant trans-spectral effects as they covary with the input $R_{rs}$ and do not require knowledge of the optical properties of waters. Semi-analytical methods [16,18], on the other hand, obtain $b_{bp}$ based on approximations of relationships found through the radiative transfer theory between $R_{rs}$ and the IOPs and employ a few optical and bio-optical properties and/or relationships. Thus, $b_{bp}$ derived semi-analytically from $R_{rs}$ is independent of measured $b_{bp}$ in situ but depends on using an accurate approximation of the relationship between $R_{rs}$, IOPs and trans-spectral processes.

If every step necessary for both determinations is well controlled and understood, $b_{bp}$ from both methods should agree with each other, i.e. there should be a closure [19–21], as demonstrated in Gordon et al. [22]. But the study 22 covered just two cases, and the inversion scheme uses vertical profiles of upwelling radiance and downwelling irradiance as inputs, which is very different from remote sensing inversion. Empirical approaches also indicated good matches [13,15], but such results do not indicate a closure between two independent determinations. Various studies, in particular those using $R_{rs}$ as the input to analytically retrieve $b_{bp}$ [23–25], however, have found that $b_{bp}$ values derived from semi-analytical algorithms are generally higher than those estimated from in situ measurements, i.e. there is no closure on $b_{bp}$. For instance, it was found that $b_{bp}$ derived from MODIS-Aqua $R_{rs}$ is systematically higher than $b_{bp}$ inferred from chlorophyll-a concentration ([Chl], mg/m$^3$) by a factor of 2-3 (see Fig. A1 in Huot et al. [23] and Fig. 11 in Brown et al. [15]), where the relationship between $b_{bp}$ and [Chl] was developed based on concurrent measurements of [Chl] obtained by HPLC and $b_{bp}$ obtained by a BB3 sensor (Wetlabs, Inc.) [26]. Beyond the study by Huot et al. [23], the $R_{rs}$-derived $b_{bp}$ in oligotrophic waters via spectral optimization
algorithms is also found much higher (up to a factor of 2) than that measured in situ in recent evaluations of algorithm performances [25,27].

In principle, the uncertainty in the $b_{bp}$ derived analytically from $R_s$, are small at least for oligotrophic waters [28] where the absorption coefficients in the longer wavelengths (550 nm and longer) are nearly constant (see more detailed discussions below). This is well demonstrated when the semi-analytical algorithms [25,29] were applied to a data set [16] obtained from radiative transfer simulations with the Hydrolight software when trans-spectral effects were not included. Comparison showed that the retrieved $b_{bp}$ generally contains errors ~20% or less for oligotrophic conditions [16,25]. Errors in measured $R_s$ will certainly contribute to analytically derived $b_{bp}$, but the errors in measured $R_s$ are not systematic [31,32], therefore we should not expect systematically and significantly higher $b_{bp}$ from errors in $R_s$. It is necessary to address such large systematic overestimations of $b_{bp}$, and more importantly, it is necessary to demonstrate if a closure can be achieved after these sources of error are taken into consideration. Here, we focus on a semi-analytical algorithm, the quasi-analytical algorithm (QAA) developed by Lee et al. [29], to examine these discrepancies. After rapidly reviewing the algorithm, we further address the sources that could contribute to the non-closure in $b_{bp}$, and then followed with evaluations of ocean color $b_{bp}$ products after the sources of uncertainties/errors are considered.

### 2. Brief description of the QAA

For the retrieval of inherent optical properties (IOPs) from spectral $R_s$, a quasi-analytical algorithm (QAA) was developed by Lee et al. [29]. QAA uses the relationship between IOPs and $R_s$ derived from the RTE, and makes very few assumptions in the process of algebraically solving for $b_{bp}$ from $R_s$. The uncertainty in QAA-derived $b_{bp}$, at least for oligotrophic waters, is small and well understood.

From the RTE, a simplified relationship between IOPs and reflectance derived from radiative transfer computations, where the trans-spectral effects are omitted, is

$$r_s(\lambda) = \left( g_0 + g_1 \frac{b_w(\lambda)}{a(\lambda) + b_w(\lambda)} \right) \frac{b_s(\lambda)}{a(\lambda) + b_s(\lambda)}. \quad (1)$$

Here $r_s$ is the subsurface remote-sensing reflectance, which can be derived from $R_s$ with an uncertainty ~10% [6,33]. The coefficients $g_0$ and $g_1$ are wavelength-independent model parameters, which depend on sun-sensor angular geometry as well as the shape of particle phase functions [7,34]. $b_w$ can be expressed as

$$b_s(\lambda) = b_{sw}(\lambda) + b_{bw}(\lambda), \quad (2)$$

with $b_{bw}$ representing the backscattering contribution from water molecules, and is taken as a constant for the global oceans [35,36], although $b_{bw}$ varies slightly with temperature and salinity [36]. Therefore, when $b_w$ is known, it is straightforward to derive $b_{bp}$ using Eq. (2).

As Eq. (1) indicates, once $g_0$ and $g_1$ are known, that there are just two unknowns for any given $r_s$: $a$ and $b_{bw}$, so $b_s$ can be easily derived when $a$ is known. In the QAA scheme, $a$ at a reference wavelength ($\lambda_0$) is estimated with

$$a(\lambda_0) = a_w(\lambda_0) + \Delta a(\lambda_0), \quad (3)$$

with $a_w(\lambda_0)$ the contribution of water molecules, and $\Delta a(\lambda_0)$ estimated empirically from the $R_s$ spectrum. For the oceanic waters, $\lambda_0$ is set as 550 nm for MODIS and 555 nm for SeaWiFS, where $R_s$ at these wavelengths are available, respectively.

The first step of the algorithm consists in estimating $a(\lambda_0)$ using an empirical algorithm based on $R_s$ band ratios to estimate $\Delta a(\lambda_0)$. As described in Lee et al. [29], for oligotrophic waters $a(\lambda_0)$ is dominated (~95%) by $a_w(\lambda_0)$, thus $a(\lambda_0)$ can be accurately estimated; errors in
estimating $\Delta a(\lambda_o)$ have negligible impact on $a(\lambda_o)$ for such waters. This is particularly true for the oceanic gyres, where the amount of optically active constituents other than water (such as phytoplankton and gelbstoff) are scarce [37,38]. Therefore, as long as $R_{rs}(550)$ (or $R_{rs}(555)$) is measured accurately and Eq. (1) is valid, $b_{bbp}(550)$ (or $b_{bbp}(555)$) can be estimated accurately. If $b_{bw}$ is accurately known, or at the very least is the same value as that used when processing the in situ validation measurements, $b_{bbp}(550)$ (or $b_{bbp}(555)$) estimated from $R_{rs}$ should match that from in situ measurements.

3. Impact of errors in the QAA components on the $b_{bbp}$ retrieval

As mentioned above, the QAA algorithm when applied to data simulated by the radiative transfer equation retrieves $b_{bbp}$ with very low errors [16], as is expected in waters where the optical properties are consistent with those of oligotrophic waters. Because QAA is essentially based on such simulations, this highlights that the algorithm structure and approximations allow accurate retrieval of $b_{bbp}$ for such conditions. The discrepancy found when compared with in situ measurements must thus originate from one of three sources. The first is that the radiative transfer simulations are not representing accurately the relationships between $R_{rs}$ and IOPs in situ as expressed in Eq. (1) (and those that allow going from $R_{rs}$ to $R_{rs}$). The second is that the optical properties of pure saltwater, used in Eqs. (2) and (3), are incorrect. The third is that there are errors or biases present in measured $b_{bbp}$. We now examine these different potential sources of variability.

3.1 $R_{rs}$-IOP relationship

The relationship between $R_{rs}$ and $b_{bbp}/(a + b_{bb})$ as described by Eq. (1) is not exact and other mathematical models were also developed in the past decades [39–42]. Instead, it is an approximate solution of the RTE with no trans-spectral effects present. For an hypothetical ocean without trans-spectral effects, this simplification results in errors up to ~12% compared with the simulations [6]. Depending on inputs used in data simulations (e.g., phase function of particle scattering, range of IOPs, etc.), slightly different $g_0$ and $g_1$ values are obtained. By changing the values of $g_0$ and $g_1$ using two sets of published values (i.e. from 0.0949 and 0.0794 [6] to 0.089 and 0.125 [29]), it is found that the retrieved $b_{bbp}$ values with the latter coefficients are higher than that with the former, and this difference is higher for smaller $b_{bbp}$ (see Fig. 1), with the maximum difference around 12% (for $b_{bbp}(555)$ ~0.0005 m$^{-1}$). This analysis shows that the selection of values to represent $g_0$ and $g_1$ cannot be the reason leading to ~200-300% difference between $R_{rs}$-retrieved $b_{bbp}$ and in situ measured $b_{bbp}$. This is further supported by the fact that in more eutrophic waters the retrieved and measured $b_{bbp}$ are much closer; therefore, for errors in $g_0$ and $g_1$ to be the source of the significant differences in $b_{bbp}$ observed it would require substantial changes in $g_0$ and $g_1$ with trophic status. The values of $g_0$ and $g_1$ vary mostly due to the geometry of observation (including angular distribution of the incident light field) and angular shape of the particle phase function in the backward domain [5,34]. While the former does not change with trophic status, observations [23,43,44] suggest that the latter also does not change strongly across trophic states.

A major caveat of Eq. (1) in modeling $R_{rs}$ is the omission of contributions from in-elastic processes, which include those from chlorophyll $a$ and CDOM fluorescence and Raman scattering [1]. Chlorophyll $a$ fluorescence is centered around 685 nm (with a roughly Gaussian shape at a half-height width around 25 nm), so its influence in the QAA-retrieved $b_{bbp}$ is nil as QAA uses measurements around 550 nm to retrieve $b_{bbp}$. For oceanic waters, the contribution from the CDOM fluorescence is small, so the impact of this effect is also negligible [11,45]. However, the contribution from the Raman scattering to $R_{rs}$ can be as high as 20% in the longer wavelengths for oceanic waters [8,9,46], thus the impact of Raman scattering on the retrieval of $b_{bbp}$ could be significant for clear oceanic waters [47,46,48]. Indeed for simulated waters with Raman contribution so extreme that $b_{bbp} = 0$ and an absorption consistent with a chlorophyll concentration of 0.01 mg/m$^3$, the QAA scheme
returns a $b_{bp}(550)$ value of $\sim 0.00025 \text{ m}^{-1}$ as it interprets the light from Raman scattering to particulate backscattering; this value is approximately half of the lowest values of $b_{bp}(550)$ measured in the NOMAD data set [49].

To effectively process ocean color satellite imageries, an empirical algorithm has been developed to correct this contribution in $R_{rs}$ inversion [50], and Fig. 2 presents $b_{bp}$ retrievals before and after the correction of Raman contribution for measurements made in the South Pacific gyre. For these “clearest” water of the global oceans [37,51], the ratio of $R_{rs}$ -derived $b_{bp}$ to in situ $b_{bp}$ decreased from $\sim 300\%$ to $\sim 200\%$ (for lowest $b_{bp}(555)$), removing on average $0.00022 \text{ m}^{-1}$ of retrieved $b_{bp}(555)$ from $R_{rs}$, clearly echoing the importance of removing Raman effect in the analytical retrieval of $b_{bp}$ from $R_{rs}$ [22,46–48]. As presented, however, $b_{bp}$ from $R_{rs}$ is still generally higher than that from in situ measurement, and this difference is $\sim 0.00025 \text{ m}^{-1}$ for all samples.

The scheme to empirically correct the Raman effect has a maximum error of about 15% in estimating the Raman contribution to $R_{rs}$ [50]. The impact of a 15% adjustment in the Raman correction, however, results in just $\sim 3\%$ uncertainty in the $R_{rs}$ derived $b_{bp}$. This indicates that the empirical scheme is sufficient for the correction of Raman scattering contribution in oceanic waters and that the origin of the remaining differences cannot originate from incorrect Raman correction.
3.2 Pure-water absorption coefficient

Another source of error in the QAA-derived $b_{bp}$ is the uncertainty in the absorption coefficient of pure water at the reference wavelength (550 or 555 nm), since this value is used in the estimation of $a(\lambda_0)$ before the analytical derivation of $b_{bp}(\lambda_0)$. Based on Eq. (1), higher $a(555)$ will result in higher $b_{bp}(555)$ and consequently higher $bbp$(555). Modern laboratory and field measurements (see a list of $aw$ values in Mobley 1) of $aw(555)$ span approximately 0.0596 m$^{-1}$ [52] to 0.0673 m$^{-1}$ (spectrally interpolated from Smith and Baker [53]). QAA uses the lowest published $aw$ values [52], leading to the lowest values of $b_{bp}(555)$. Pope and Fry [52] also provide the standard deviation of the error on their measurement at 555 nm as 0.0012 m$^{-1}$, this translates in QAA in an error of ~4% on the determination of $b_{bp}(555)$ for the data shown in Fig. 2. Obtaining optically pure water is very challenging and the value published may still suffer from minor contamination by absorbing components (as was the case with previous determinations). However, above ~450 nm [37], the $aw(555)$ values of Pope and Fry [52] are consistent with values obtained from the diffuse attenuation coefficient of the clearest water which imposes a strong upper limit on the $aw$ value and strongly support the assertion that these are nearly devoid contribution from colored substance at 555 nm.

4. Uncertainties in $b_{bp}$ measured in situ

The non-closure of $b_{bp}$ does not have to originate only from errors or uncertainties in $R_{rs}$ inversion; it also includes errors from in situ measurements [56]. While significant efforts were deployed to obtain accurate values in the clearest Pacific waters, these measurements are extremely challenging and push the sensitivity and resolution of the instruments to their limit.

Since the advent of commercial instruments, measurements of $b_{bp}$ in situ are generally made with active instruments (e.g., Hydroscat, HOBI Lab, Inc.; BB3, WET Labs, Inc.). In these sensors, light from a pulsed LED is emitted into the water and the backscattered light (usually with a scattering angle of ~120° to 140°) from this source is recorded, and this...
energy is converted to $b_{bp}$ after subtracting the contribution of pure saltwater. Calibration of this system is usually carried out in the lab with well-characterized materials (reflecting surface or beads) [51]. Apart from possible calibration errors, there are two main sources of errors that can arise from these measurements. The first is caused by an estimation of $b_{bp}$ from a measurement of the volume scattering function at 120$\theta$ or 140$\theta$, while the other may arise from the undersampling of the backscattering from larger and less abundant particles due to the limited observation volumes.

The error caused by the estimation of $b_{bp}$ from a measurement of the VSF between 120$\theta$ to 140$\theta$ (a constant factor $\chi$ is used for this conversion) has been studied by different authors [57–59]. All authors report that errors caused by this approximation should be less than ~10%. This conclusion arises in all cases from measured VSF in coastal waters as well as simulated VSF from Mie scattering. Although a thorough study of the conversion factor hasn’t been carried out in oligotrophic ocean waters it appears unlikely that the error could increase by a factor of 10 and could explain the discrepancies observed. Therefore, the measurement strategy at a single angle does not seem to be a plausible source of error to explain the differences observed.

The passive measurement systems have a sampling volume in the range of 10s to 1,000s m$^3$, while the instruments measuring $b_{bp}$ in situ have a sampling volume around $10^{-6}$ m$^3$, i.e. there is a many orders of magnitude difference in the sampling volume between the active backscatter sensors and the passive remote systems. In oceanic waters, larger particles are generally scarcer, thus the sampling volume of an active sensor will likely miss some of the larger particles during individual observations. This is demonstrated in Briggs et al. [60] where the observed spikes in $b_\theta$ time series are indicators of large particles, although larger particles generally have a smaller backscattering efficiency [61]. The difference in sampling volume may help to explain the slightly (~0.0003 m$^{-1}$) higher $b_{bp}$ by Hydroscat than that by BB3 in the clearest waters, although both sensors were carefully calibrated for the field measurements (see Stramski et al. [54,51] for details). This is because Hydroscat has larger sampling volume than BB3 (or BB9) due to measurement geometry, thus more particles might be “counted” for by a Hydroscat sensor, although Hydroscat will not be able to cover all particles in the bulk water during a measurement scan. Indeed, if Hydroscat underestimated $b_{bp}(555)$ by 0.0002 m$^{-1}$ (a very small number) [54], much better closure of $b_{bp}$ is achieved between $R_{rs}$ inversion and in situ measurements for waters in the South Pacific gyre (see Fig. 3), with the ratio of $R_{rs}$-derived $b_{bp}(555)$ to the adjusted (adding 0.0002 m$^{-1}$ to the Hydroscat measured value) $b_{bp}(555)$ in a range of ~0.8-1.2 (which was ~1.1 - 2.2, see Fig. 2). The ± 20% difference (transfers to ~0.0001 m$^{-1}$ absolute difference) is beyond the precision of either remote sensing measurements or in situ determinations. Indeed, even the value of 0.0002 m$^{-1}$ that we added is within the instrument offset uncertainty (specified as between 5x10$^{-5}$ to 5 x $10^{-4}$ m$^{-1}$, http://www.hobilabs.com/). These results suggest that it is necessary to take appropriate average over a long time or wide spatial range of in situ $b_\theta$ measurements to have a “ground truth” to match the large volume observed by remote sensing systems. In particular, if the objective is to compare products of backscattering sensors with that from passive sensors, whether remotely or in situ, the removal of “spikes” must be carried out only if the spikes are caused by instrument malfunction and not by rare large particles (see user manual of the backscattering sensors).
In-situ \(bbp(555)\) \([m^{-1}]\)

\[
Rrs \rightarrow \frac{bbp(555)}{in-situ bbp(555)}
\]

0.0000 0.0005 0.0010 0.0015 0.0020

0.8 1.0 1.2

Fig. 3. Ratio of Rrs-derived \(bbp(555)\) to \(in situ\) measured \(bbp(555)\) for waters in the South Pacific Gyre, with Rrs-derived \(bbp(555)\) after correcting the Raman contributions in the \(Rrs\) inversion process, and Hydroscat-measured \(bbp(555)\) was increased by 0.0002 m\(^{-1}\) from the original measurements.

In an attempts to examine the impact of Raman scattering on the remote sensing retrieval globally, we carried out an analysis similar as Huot et al. [23], where we compared the MODIS derived \(bbp\) using QAA with \(in situ\) statistical relationships that have been derived (Fig. 4). As opposed to Huot et al. [23] the comparison is done at 555 nm instead of 443 nm to avoid spectral errors when extrapolating the value from 555 nm to 443 nm; furthermore, care was taken to use the same value of the backscattering coefficient of pure saltwater (though at constant salinity) for the remote sensing estimates as was used for the processing of the Hydroscat data underlying the Huot et al. [23] relationships. Before the Raman corrections there is clearly an overestimation of \(bbp(555)\) (Fig. 4(a), blue line vs pink line); this overestimation disappears after the correction, and the running median of the remote sensing data follows very closely the Hydroscat parameterization of the backscattering and is just below the global statistical relationship derived by Brewin et al. [24]. These results confirm that the Raman effect is a big contributor to the non-closure of \(bbp\) in previous studies and that the empirical scheme to correct this effect is plausible [23].

5. Conclusions

The results of this study highlighted the two major sources that contributed to the non-closure of \(bbp\) in oligotrophic oceans shown in previous studies. One is the Raman scattering, which resulted in an increased \(bbp\) when it is analytically derived from \(Rrs\) when the Raman effect was not considered; another is associated with the uncertainty in \(in situ\) measured \(bbp\) (see Table 1 for summary). In particular, it is extremely difficult to get the “ground truth” of \(bbp\) of such clear waters, as the values of \(bbp\) are generally smaller than 0.001 m\(^{-1}\). A closure in \(bbp\) for oligotrophic water is achieved after correcting the Raman contribution in the inversion process and using the adjusted \(bbp\) values (adding 0.0002 m\(^{-1}\) to that measured by Hydroscat, a value well within the measurement uncertainty). This closure in \(bbp\) demonstrated the effectiveness of the empirical scheme in correcting the Raman scattering contribution, and provided a confidence in satellite ocean-color \(bbp\) products, as long as all relevant processes are considered in its analytical inversion.
Fig. 4. Comparison of $b_{bp}(555)$ from QAA before (panel A) and after (panel B) Raman correction. The colored points represent the number of $b_{bp}(555)$ observations obtained from the QAA algorithm (see color bar) when applied on a global Level 3 (SMI) data set from the MODIS sensor for March 2007 (all daily level 3 values are temporally averaged). The Magenta lines (see legend in Panel A) are for three fits (i.e., with different values of the “Beta parameter”, see Huot et al. [23]) to three $b_{bp}$ data sets obtained during the BIOSOPE cruise: “adopted” stands for the Hydroscat and BB3 data set, “Hydroscat Beta” stands for the Hydroscat data only and “BB3 Beta” stands for the BB3 data set only. C) Same as B but after Raman correction. The black line corresponds to Eq. (6) in Brewin et al. [24] as parameterized on their Data set “A”. The blue line is a 1001 points running median on the MODIS data set.

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Acknowledgments

Financial support from the NASA Ocean Biology and Biogeochemistry and Water and Energy Cycle Programs and the JPSS VIIRS Ocean Color Cal/Val Project is greatly appreciated. We are grateful for the comments, and discussions, about $b_{bp}$ measurements from Drs. Jim Sullivan, Robert Brewin, and Giorgio Dall'Olmo. The acquisition of BIOSOPE data where funded through CNRS[1]-INSU[2] grants; we thank Marlon Lewis for sharing the Rrs data and Dariusz Stramski for sharing the Hydroscat data. Comments and suggestions from two anonymous reviewers significantly improved this article and are greatly appreciated.