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Modeling the contributions of phytoplankton and non-algal particles to spectral scattering properties in near-shore and lagoon waters

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ABSTRACT

Particular attention was focused on modeling the spectral scattering properties of phytoplankton ($b_{ph}(\lambda)$) and non-algal particles (detrital organic and inorganic sediments $b_{NAP}(\lambda)$) from absorption and attenuation measurements in near-shore and lagoon waters. The absorption line height ($a_{LH}(676)$) measured above a linear background between 648 nm and 714 nm in particulate and dissolved organic matter absorption spectra ($a_p(\lambda)$) is a spectral feature that is primarily associated with the chlorophyll with significantly less pigment package effect compared to the blue peak, and hence it is solely attributed to the phytoplankton absorption (a_{ph}). The correlation of $a_{ph}(\lambda)$ with $b_{ph}(\lambda)$ in terms of the spectral shape and the relation of $a_{LH}(676)$ with chlorophyll concentration hold the key to derive $b_{ph}(648)$ from the $a_{LH}(676)$ measurements. $b_{NAP}(648)$ values are then determined by subtracting the $b_{ph}(648)$ from $b_p(648)$, allowing the power-law model to derive the $b_{NAP}(\lambda)$. In-situ determination of b_{ph} (λ) is subsequently achieved by subtracting the featureless $b_{NAP}(\lambda)$ from $b_p(\lambda)$ provided by the *ac-s* sensor. These data form the basis for the development of models for independent estimates of $b_{ph}(\lambda)$ and $b_{NAP}(\lambda)$ based on the measurements of a_{LH} and suspended sediment concentration or turbidity. The validity of this method was demonstrated in a wide variety of samples from coastal and inland environments. Comparison of the modeled and measured spectral variations of $b_{ph}(\lambda)$ showed the mean relative percent difference between these two data to be within 20%. $b_{NAP}(\lambda)$ predictions also had an error a few percent and the correlation coefficient close to unity. When comparing the modeled $b_{ph}(\lambda)$ with laboratory culture data, the results were exceptionally good although discrepancies in size and refractive index of cells of monospecific lab culture samples and natural assemblages due to the simultaneous presence of different species. The proposed approach and models are highly instrumental in investigating the scattering properties of phytoplankton and non-living constituents, and will provide new tools for improving our current understanding of particle dynamics, advancing biogeochemical and ecosystem modeling, and assessing phytoplankton blooms and sediment plumes within inland and coastal environments.

1. Introduction

Knowledge of light absorption and scattering properties and their variability is essential for addressing many scientific and practical problems linked to coastal and near-shore environments largely dominated by land-ocean interaction processes. Absorption, attenuation and scattering are inherent optical properties (IOPs) that are solely dependent on the contents of the medium and have been recognized as powerful tools for particle dynamics and biogeochemical studies (Yentsch, 1962; Roesler and Perry, 1995; Boss et al., 2001; Xu et al., 2005; Snyder et al., 2008; Woźniak et al., 2010; Astoreca et al., 2012; Maier et al., 2012; Shi et al., 2014; Kiefer et al., 2015; Pérez et al., 2010; Baffico, 2013; Raeder et al., 2010). Among the IOPs, scattering is generally considered one of the most fundamental optical properties that can be used to optically detect and characterize major algal blooms including harmful algal blooms (because each phytoplankton species has a characteristic scattering spectra (Ahn et al., 1992; Whitmire et al., 2010)) and sediment plumes within coastal and inland environments. Scattering is the part of the incident visible radiation scattered out of the beam in every direction and is obtained by subtracting the absorption coefficient from the attenuation coefficient. The absorption and attenuation properties can be directly measured in-situ with existing commercial instruments (*e.g.,* WET Labs *ac-s*, *ac-9*) that have become widely adopted instruments within the hydraulic optics and ocean color remote sensing community (Boss et al., 2001; Boss and Pegau, 2001; Huot et al., 2008; McKee et al., 2013). The total scattering coefficient is the sum of the scattering coefficients of seawater and particles. Eliminating the scattering coefficient of pure seawater from

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total scattering gives the particulate scattering coefficient which is directly related to aquatic particles and depends on the refractive index, size distribution and concentration of those particles (Morel and Maritorena, 2001; Twardowski et al., 2001; Biber et al., 2008; Woźniak et al., 2010; McPherson et al., 2011; Sahu and Shanmugam, 2015). Scattering properties are strongly wavelength dependent and have characteristic spectral shapes for different water constituents (such as phytoplankton and non-algal particles), thus it is essential to derive their specific scattering properties and understand their spectral dependency behavior and variability. Furthermore, a prior knowledge of their specific scattering properties is necessary to improve parameterizations and bio-optical models for retrieving the biogeochemical variables and detecting algal blooms from remote sensing measurements.

Experimental and observational studies found that total suspended particulate matter (TSM) directly influences particulate scattering through relationships that vary depending on the TSM composition (Stramski et al., 2007; Lund-Hansen et al., 2010; Shi et al., 2014). The relationship of particulate scattering coefficient and TSM concentration considerably varies with respect to the refractive index and particle size distribution (Babin et al., 2003; Stramski et al., 2007). They found that the mass-specific scattering coefficient in coastal waters with a high inorganic content was smaller than in open-ocean waters with a low inorganic content. Furthermore, it was speculated that the algal absorption would decrease the mass-specific scattering coefficient in productive waters with a high chlorophyll concentration. Morel (1988) theoretically showed the inverse power-law spectra of scattering for non-absorbing particulate matters. This power-law function has been previously used for deriving the particulate scattering coefficients (Morel et al., 2006; Sun et al., 2009). Though few studies reported to have departures from the power-law spectra in bands known to have strong absorption features (Stramski et al., 2001; Babin et al., 2003), the power-law model fits well in waters with low phytoplankton pigment content and high sediment concentration (Sun et al., 2009).

Theoretical models based on homogenous, spherical particles have been used to describe the variations of scattering and backscattering properties of phytoplankton. The anomalous diffraction approach of Van de Hulst forms the basis of this approach (Bricaud and Morel, 1986; Bernard et al., 2001). Many ocean optical studies have relied on this approach to study the influence and variation of phytoplankton scattering in different environmental conditions (Stramski et al., 1993, 2001, 2004). Nevertheless, the assumption of homogeneous sphere significantly deviates from reality because algal cells have diverse, complex inner structure and shapes. Similar studies have indicated departures from the homogeneous sphere simulated models of scattering spectra (Volten et al., 1998; Witkowski et al., 1998). Zhou et al. (2012) studied the variations of scattering spectra for 14 phytoplankton species based on laboratory experiments and found that the highly featured scattering and backscattering spectra of phytoplankton cannot be modeled satisfactorily based on Mie theory for homogeneous spheres. The scattering and backscattering spectra of phytoplankton are highly featured and differ significantly (departure) with the power-law behavior in waters with high phytoplankton concentration (Bricaud et al., 1983; Ahn et al., 1992; Whitmire et al., 2010), although their variability for different species of phytoplankton is yet to be well understood (Zhou et al., 2012).

Scattering by phytoplankton highly depends on size, shape and refractive index of all components of the phytoplankton cell (Volten et al., 1998; Jonasz and Fournier, 2011) and significantly contributes to the total particulate scattering because of their internal structure and membranes, complex morphology, and composition (Quirantes and Bernard, 2004). Modeling the scattering properties of phytoplankton through anomalous diffraction approximation and Mie theory calculations is difficult (Gordon and Du, 2001) because of the inappropriate assumption of spherical homogeneity and non-absorbing particles used to simplify these theoretical calculations. In reality, phytoplankton possess heterogeneous intracellular refractive indices, associated with a variety of complex internal structures (e.g., silicate, cellulose or calcite cellular coatings or plates, absorbing chloroplasts, and other membrane bound organelles, gas vacuoles and starch granules, in addition to their taxonomic diversity with a wide range of cellular shapes) (Quirantes and Bernard, 2004). Taking into account many of these components in theoretical approximations of phytoplankton scattering for a variety of algal species with cellular heterogeneity is thus extremely difficult (Volten et al., 1998; Quirantes and Bernard, 2004). Accurate calculations require the use of the full non-spherical theory. Models using two and layered spheres with the chloroplast as the central layer have found that cellular heterogeneity resulted in both spectral changes and an increase in magnitude of scattering by several times (Zaneveld and Kitchen, 1995; Quirantes and Bernard, 2004). On the other hand, the thickness and real refractive index of the phytoplankton cells (larger cells occurs in turbid productive/eutrophic waters) seem to have a significant effect on the magnitude of scattering (Quinby-Hunt et al., 1989; Kitchen and Zaneveld, 1992). Shape is also considered as a minor contributor to scattering, which depends mainly on particle size and composition (i.e., refractive index for a heterogeneous scatterer). Despite these complications and constraints for theoretical studies, many of the above investigators noted that phytoplankton scattering properties are of significant importance to the coastal oceanographic and environmental studies.

Characterization of the spectral scattering properties of different particulate matters is particularly important for improving the bio-optical models to retrieve water quality parameters and biogeochemical variables in aquatic environments (Stramski et al., 2001, 2004; Platt et al., 2008). Moreover, these scattering properties have implications in underwater imaging (e.g., mitigating the effect of scattering induced distortion) which is extensively used in various underwater environmental and engineering applications (Mortazavi et al., 2013), biological studies (Sun et al., 2008), underwater target detection (Rao et al., 2009), and underwater structure investigations (Kondo and Ura, 2004). The information on bulk scattering and backscattering of phytoplankton can greatly help in remote sensing detection of dominant species of phytoplankton during algal bloom events (Roesler and McLeroy-Etheridge, 1998; Cannizzaro et al., 2008) and act as a synoptic tool to understand the phytoplankton variations in world oceans (Kostadinov et al., 2009). Recent studies (e.g., Sun et al. (2010)) have reported that phytoplankton have a weaker contribution in particulate scattering coefficient for inland lake waters. The weak contribution by phytoplankton makes it difficult to infer the phytoplankton scattering from the particulate scattering. Stavn and Richter (2008) proposed another method to partition the scattering coefficient into suspended sediments (SS) and organic particulate components utilizing mass-specific scattering cross sections for northern Gulf of Mexico waters. In the present study, a novel method is proposed for deriving the scattering properties of phytoplankton and non-algal particles from in-situ measurements in marine and inland waters. Independent models are developed based on these data to predict their spectral scattering properties from measurements of the absorption line height and suspended sediment concentrations. The validity of this method is demonstrated using biogeochemical and optical measurement data from several cruises and field campaigns. In addition, the results are compared with lab culture data and those predicted by the existing models.

2. Data and methods

2.1. Sampling site

Field measurements were carried out in three contrasting coastal environments: clear-moderately turbid waters around Chennai, highly turbid waters around Point Calimere and productive eutrophic lagoon waters (Muttukadu) on the southeast coast of India. Three cruises were