SCALE CLOSURE IN UPPER OCEAN OPTICAL PROPERTIES: FROM SINGLE PARTICLES TO OCEAN COLOR

By

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ABSTRACT

Predictions of chlorophyll concentration from satellite ocean color are an indicator of phytoplankton primary productivity, with implications for foodweb structure, fisheries, and the global carbon cycle. Current models describing the relationship between optical properties and chlorophyll do not account for much of the optical variability observed in natural waters, because of the presence of seawater constituents that do not covary with phytoplankton pigment concentration. In an attempt to better understand variability in these models, the contributions of seawater constituents to ocean optical properties were investigated. A combination of Mie theory and flow cytometry was used to determine the diameter, complex refractive index (n+n′i), and optical cross-sections of individual particles, based on a method developed in the laboratory using phytoplankton cultures.

Individual particle measurements were used to interpret variability in concurrently measured bulk optical properties in New England continental shelf waters in two seasons. The summed contribution to scattering of individual particles in the size range of 0.1-50 μm accounted for approximately the entire scattering coefficient measured independently using bulk methods. In surface waters in both seasons, the large diameters and n′ of eukaryotic phytoplankton caused them to be the main particle contributors to both absorption and scattering. Minerals were the main contributor to backscattering, b_b, in the spring, whereas in the summer both minerals and detritus contributed to b_b. *Synechococcus* and heterotrophic bacteria were less important optically, contributing ≤11% each to attenuation in either season.

The role of seawater constituents in determining remote sensing reflectance, R_{rs}, was determined using radiative transfer theory. Seasonal differences in the spectral shape of R_{rs} were contributed to approximately equally by eukaryotic phytoplankton absorption, dissolved absorption, and non-phytoplankton b_b. A higher inverse wavelength dependence of non-phytoplankton b_b in the summer was caused by the contribution of small detritus, in contrast to larger minerals in the spring. Measurements of b_b and R_{rs} were compared to values from bio-optical models based on chlorophyll concentration. Differences in measured and modeled b_b and R_{rs} were caused by higher dissolved absorption and higher backscattering efficiencies and scattering by non-phytoplankton than were assumed by the model.

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CHAPTER 1:

INTRODUCTION

A primary motivation of this dissertation was to interpret, in a detailed manner, bulk optical properties in the ocean with the objective of improving model predictions of chlorophyll concentration from satellite ocean color. This motivation is in keeping with a longstanding goal in ocean optics of deriving ecologically important quantities, including chlorophyll concentration, phytoplankton absorption, and particulate carbon concentration, from measurements of bulk optical properties. Predictions of chlorophyll concentration from satellite ocean color are an indicator of phytoplankton primary productivity, with implications for foodweb structure, fisheries, and the global carbon cycle. Research began over 25 years ago on the development of bio-optical algorithms for the determination of chlorophyll concentration in the ocean from remotely sensed reflectance data (e.g. Clarke et al. 1970; Gordon et al. 1980), and this topic continues to be a major focus of current research (e.g. Morel and Maritorena 2001; Sathyendranath et al. 2001).

Bio-optical algorithms rely on the relationship between pigment concentration in the water and the bulk optical properties of the water. Bulk optical properties include both IOPs, which depend solely on the constituents of seawater (e.g. absorption, scattering, and backscattering), and AOPs which depend both on the constituents of seawater and the ambient light field (e.g. diffuse attenuation and reflectance). Unexplained variability exists in bio-optical algorithms in open ocean waters, and even more so in coastal waters, due to a lack of knowledge of seawater constituents besides phytoplankton. Recently, models have been developed for the inversion of reflectance spectra to determine IOPs, including absorption by phytoplankton, absorption by dissolved and detrital materials, and backscattering by particulates (Roesler and Perry 1995; Garver and Siegel 1997; Carder et al. 1999). Such models suggest that future research should focus on better understanding the ratio between absorption by phytoplankton and absorption by dissolved and detrital materials and on the types and optical properties of particles which contribute to backscattering. On the basis of recent measurements, it may also be possible to use satellite reflectance data in the estimation of particulate organic carbon in the ocean. Stramski et al. (1999) reported a relationship between measurements of particulate organic carbon and particulate backscattering in the Southern Ocean, suggesting that a similar relationship may exist for remote sensing reflectance.

The quantification of relationships between bulk optical properties and ecologically important quantities, such as chlorophyll and particulate organic carbon, depends on the ability to account for the seawater constituents that contribute to bulk optical properties. This dependence is an issue of "scale closure", defined as the use of measurements of single particles to account for changes in bulk properties (Mobley 1994). Model simulations have been performed to determine expected mean particle contributions to inherent optical properties in open ocean waters (Stramski and Kiefer 1991; Stramski and Mobley 1997; Stramski et al. 2001) and to apparent optical properties in both open ocean and coastal waters with two types of phytoplankton blooms (Mobley and Stramski 1997). These simulations show the power of summing over individual seawater consituents to explain modeled variability in optical properties and suggest that similar studies could describe important variability when applied to natural samples. Three studies have aimed at understanding scale closure in natural samples, all in Case 1 waters (DuRand and Olson 1996; Chung et al. 1998; Claustre et al. 1999). Variability in beam attenuation due to particles (c_p) at 660 nm was partially explained by accounting for changes in microbial particle types measured using flow cytometry. Based on these studies, eukaryotic phytoplankton of 0.2-20 μm in size accounted for 30-45% of total beam c_p, *Prochlorococcus* and heterotrophic bacteria accounted for ~10% each, *Synechococcus* contributed a negligible amount (≤5%), and non-plankton (not measured) were inferred to account for 40-50% of c_p. The results of Chung et al. (1998) for phytoplankton groups were not considered here because of seemingly erroneous findings (Binder and DuRand, 2002).

The application of flow cytometry in oceanography has allowed for the rapid determination of individual particle properties in mixed marine particle assemblages (Olson et al. 1993). The basis of modern flow cytometry, the sheath-flow principle, was first developed as a medical tool for the optical counting of red blood cells (Crosland-Taylor 1953). In the late 1970's and early 1980's, flow cytometry was applied to laboratory studies of phytoplankton in culture (Paau et al. 1978; Paau et al. 1979; Trask et al. 1982; Olson et al. 1983; Yentsch et al. 1983), and in 1985, flow cytometry was first used at sea for the study of marine phytoplankton distributions in natural samples (Olson et al. 1985). Since its initial application to the marine environment, methods have been developed for the identification of numerous particle types using flow cytometric forward and side angle scattering, fluorescence and labeling techniques. A comparison of forward scattering, red fluorescence, and/or orange fluorescence allows populations of *Prochlorococcus*, eukaryotic picophytoplankton, coccolithophorids, pennate diatoms, cryptophytes, *Synechococcus*, and non-phytoplankton particles to be enumerated and sized (Olson et al. 1993). Additionally, fluorescent staining techniques have allowed for the flow cytometric identification of heterotrophic bacteria (Marie et al. 1997), possibly viruses (Marie et al. 1999), and organic and inorganic particles (Moreira-Turcq and Martin 1998).

Mie theory provides the theoretical link between flow cytometric measurement of individual particles and the determination of their inherent optical properties. The absorption and scattering of light by a homogenous sphere, including the angular distribution of the scattered intensity, is solved using Mie theory (Mie 1908; Bohren and Hoffman 1983). The application of Mie theory to flow cytometry requires an understanding of how the optical properties of natural particles are related to those of homogenous spheres, as assumed by the theory. Measurements of angular scattering for phytoplankton cultures have shown deviations from angular scattering predicted by Mie theory (Quinby-Hunt et al. 1989; Volten et al. 1998), and modeling work has focused on better understanding the effects of non-sphericity and inhomogeneities on theoretical determinations of angular scattering (e.g. Quinby-Hunt et al. 1989; Kitchen and Zaneveld 1992; Herring and Boss 2000). With its assumptions in mind, Mie theory can provide a framework for calculating scattering at all angles from the forward and side angle scattering measurements of flow cytometry. Mie theory (or an approximation there of) has been applied to flow cytometric measurements of particles to determine particle diameter and real refractive index (n) (Ackleson and Spinrad 1988; Ackleson and Robins 1990) and the contribution of different phytoplankton species to beam attenuation (DuRand and Olson 1996; Claustre et al. 1999).

In addition to single particle measurements, the study of scale closure relies on the measurement of bulk optical properties. Remote sensing measurements of reflectance (ocean color) from space began with the launch of the Coastal Zone Color Scanner (CZCS) by NASA (National Aeronautics and Space Administration) in 1978 and have undoubtedly generated the widest interest in optical properties in the history of optical oceanography. As well, in situ methods exist for measuring AOPs using profiling radiometers, and measurement is generally made at wavelengths corresponding to those of current ocean color satellite sensors, such as the Sea Viewing Wide Field-of-View Sensor (SeaWiFS) (e.g. Morrow et al. 1994). In comparison to AOPs which depend on the ambient light field, instrumentation for measuring bulk IOPs is based on shining a characterized light source, such as a light emitting diode (LED), into or through a volume of water. Commercial, in situ instrumentation exists for measuring absorption, attenuation, backscattering, and the volume scattering function at selected angles (Zaneveld et al. 1990; Maffione and Dana 1997; Dana and Maffione 2000; Moore et al. 2001). In situ absorption is routinely measured on both filtered and unfiltered seawater to discriminate between