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An algorithm to retrieve absorption coefficient of chromophoric dissolved organic matter from ocean color

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ABSTRACT

We extended the quasi-analytical algorithm (QAA) architecture to analytically derive absorption coefficient of chromophoric dissolved organic matter (a_g). Specifically, we used an empirical formula based on total absorption and particle backscattering coefficients to estimate and then remove detritus absorption coefficient (a_d), and developed a scheme to use absorption coefficients at three wavelengths (412, 443, and 490 nm) for the separation of a_g and a_{ph} (absorption coefficient of phytoplankton). The algorithm was tested using an in situ data set collected in the South China Sea and the Taiwan Strait and a global in situ data set—the NASA Bio-Optical Marine Algorithm Data set (NOMAD). Our results indicated that this new analytical algorithm for retrieving a_g performed reasonably well with a mean absolute percentage error of approximately 45% for $a_g(412)$, while it also presented a satisfactory performance for a_{ph} and a_d in both coastal and oceanic waters. Furthermore, the applicability of this new algorithm for general oceanographic studies was briefly illustrated by applying it to MODIS measurements over the Taiwan Strait and the shelf region near the Mississippi River delta. Nevertheless, more independent tests with in situ and satellite data are needed to further validate and improve this innovative approach.

1. Introduction

Gelbstoff, or chromophoric dissolved organic matter (CDOM; frequently used abbreviations are summarized in Table 1), is an optically active component and plays an important role in carbon cycling (Coble, 2007). CDOM provides an effective sun shade, modulates the underwater light field and thus affects the growth of phytoplankton and other aquatic organisms (e.g., Jerlov, 1968; Karentz & Lutze, 1990). In addition, CDOM makes up part of the pool of dissolved organic carbon (e.g., Nelson et al., 1998; Vodacek et al., 1997). It is important therefore to study CDOM, including its abundance, source, composition, and final fate at local and global scales, in order to eventually model and forecast CDOM's variations as well as its contributions to global carbon budgets (e.g., Mannino et al., 2008).

Because field studies, although quite precise and extremely useful, provide limited information in space and time, CDOM property obtained through satellite remote sensing is the only feasible means to inform its distribution at global scales. In the past decades, semi-analytical algorithms to retrieve the absorption coefficients of the sum (a_{dg}; m^{-1}) of CDOM (a_g; m^{-1}) and detritus (a_d; m^{-1}), collectively named as CDM, have been developed (Carder et al., 1999; IOCCG, 2006), enabling the characterization of CDM on a global scale (e.g., Siegel et al., 2002). These algorithms, however, do not divide a_{dg} into a_g and a_d analytically, thus could not provide a precise evaluation for the spatial and temporal variations of a_g, a proxy for CDOM. Recently, Mannino et al. (2008) developed an empirical algorithm to retrieve a_g for coastal waters in the middle Atlantic Bight, but it is not clear if the empirical coefficients are applicable to other regions or oceanic waters. Separately, Zhu et al. (2011) used data measured in the Mississippi River plume to develop a semi-analytical algorithm for the separation of a_g from a_{dg} and achieved some successes for their data set. The derivation of a_d there followed the approach of Lee (1994), i.e., using derived particle backscattering coefficient (b_{bp}; m^{-1}) as an input to estimate a_d. Our latest in situ measurements suggest that this approach may be reasonable for turbid coastal waters where suspended particles are dominated by mineral particles (e.g., Mississippi River plume), but may have limitations for waters where particles are dominated by phytoplankton (e.g., oceanic waters). Therefore, for the evaluation of CDOM in both coastal and oceanic waters, there is still a lack of robust algorithm to estimate a_g from ocean color satellite measurements.

Here, we propose a new approach to derive CDOM absorption coefficient from ocean color based on the quasi-analytical algorithm (QAA; Lee et al., 2002). The performance of the approach is assessed using an in situ data set collected in the South China Sea and the Taiwan Strait (hereafter abbreviated as SCSD) and a global scale in

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Table 1
Symbols, abbreviations and definitions.

Symbol	Description	Unit
a_d	Absorption coefficient of detritus	m^{-1}
a_{dg}	Absorption coefficient of detritus and CDOM	m^{-1}
a_g	Absorption coefficient of CDOM	m^{-1}
a_p	Particulate absorption coefficient ($a_p = a_{ph} + a_d$)	m^{-1}
a_{ph}	Absorption coefficient of phytoplankton	m^{-1}
a_{phg}	Absorption coefficient of phytoplankton and CDOM	m^{-1}
a_{nw}	Total absorption coefficient without pure water contribution ($a_{nw} = a_{ph} + a_d + a_g$)	m^{-1}
b_{bp}	Backscattering coefficient of suspended particles	m^{-1}
CDOM	Chromophoric dissolved organic matter	
NOMAD	NASA Bio-Optical Marine Algorithm Data set	
QAA	Quasi-analytical algorithm (Lee et al., 2002)	
R_{rs}	Above-surface remote-sensing reflectance	sr^{-1}
S_{ag}	Spectral slope for CDOM absorption coefficient	nm^{-1}
S_{ad}	Spectral slope for detritus absorption coefficient	nm^{-1}
SCSD	In situ data set collected in the South China Sea and the Taiwan Strait	

situ data set—the NASA Bio-Optical Marine Algorithm Data set (NOMAD; Werdell & Bailey, 2005). As comparison, the performance of an earlier empirical-style algorithm (Mannino et al., 2008) and a semi-analytical algorithm (Zhu et al., 2011) was also assessed using the same data sets. The proposed algorithm is further applied to Moderate Resolution Imaging Spectroradiometer (MODIS) measurements over the Taiwan Strait and the shelf region near the Mississippi River delta to briefly illustrate its applicability for general oceanographic studies.

2. Data and methods

2.1. SCSD data set

The SCSD data were collected during 10 cruises over the years of 2003–2007. They included five parameters, which were remote-sensing reflectance (R_{rs}; sr^{-1}), total absorption coefficient without water (a_{nw}; m^{-1}), a_g, a_d, and absorption coefficient of phytoplankton (a_{ph}; m^{-1}).

The above-surface R_{rs} was derived from the measurements of (1) upwelling radiance (L_u; $W\ m^{-2}\ nm^{-1}\ sr^{-1}$), (2) downwelling sky radiance (L_{sky}; $W\ m^{-2}\ nm^{-1}\ sr^{-1}$), and (3) radiance from a standard Spectralon reflectance plaque (L_{plaque}; $W\ m^{-2}\ nm^{-1}\ sr^{-1}$). The instrument used was the GER1500 spectroradiometer (Spectra Vista Corporation, USA), which covers a spectral range of 350–1050 nm with a spectral resolution of 3 nm. From these three components, R_{rs} can be calculated as:

$$R_{rs} = \rho \times \frac{L_u - F \times L_{sky}}{\pi \times L_{plaque}} - \Delta \quad (1)$$

where ρ is the reflectance of the Spectralon plaque with Lambertian characteristics, and F is the surface Fresnel reflectance (around 0.023 for the viewing geometry). $\Delta(sr^{-1})$ accounts for the residual surface contribution (glint, etc.), which was determined either by assuming $R_{rs}(750) = 0$ (clear oceanic waters) or through iterative derivation according to optical models for coastal turbid waters, as described in Lee et al. (2010).

Measurements of a_g were performed according to the Ocean Optics Protocols Version 2.0 (Mitchell et al., 2000), and were detailed in Hong et al. (2005) and Du et al. (2010). Briefly, seawater was filtered with a thoroughly cleaned 0.2-μm Millipore filter, and the absorbance of the filtered water was measured in a 10-cm quartz cell between 250 and 800 nm with 1 nm increment using a Varian Cary100 dual-beam spectrophotometer. The reference was 0.2-μm filtered MilliQ water. After converting the absorbance to absorption coefficient, a nonlinear least square regression (Eq. 2 with $\lambda_0 = 443$ nm) was employed to obtain the spectral slope (S_{ag}; nm^{-1}) over a wavelength range from 300 to 500 nm (Bricaud et al., 1981).

$$a_g(\lambda) = a_g(\lambda_0) \times \exp\left(-S_{ag}(\lambda - \lambda_0)\right) \quad (2)$$

The particulate absorption coefficient (a_p; m^{-1}) was measured by the filter-pad technique (Kiefer & Soohoo, 1982) with a dual-beam PE Lambda 950 spectrophotometer equipped with an integrating sphere (150 mm in diameter), in accordance with a modified Transmittance-Reflectance (T-R) method (Dong et al., 2008; Tassan & Ferrari, 1995). This approach was selected instead of the T method recommended in the NASA protocol (Mitchell et al., 2000), because some of the samples were rich in highly scattering non-pigmented particles; as a result, the standard T method overestimated the sample absorption (Dong et al., 2009; Tassan & Ferrari, 1995). Coefficient a_d was obtained by repeating the measurement on samples after pigment extraction by methanol (Kishino et al., 1985), and then a_{ph} was calculated by subtracting a_d from a_p. Eq. (3) with $\lambda_0 = 443$ was fitted by a nonlinear least square regression to obtain the spectral slope (S_{ad}; nm^{-1}) over a wavelength range from 400 to 600 nm.

$$a_d(\lambda) = a_d(\lambda_0) \times \exp(-S_{ad}(\lambda - \lambda_0)) \quad (3)$$

In total, there were 104 sets of in situ data, of which 86% was from the Taiwan Strait and the other 14% was from the South China Sea (see their locations in Fig. 1). The Taiwan Strait, a shallow channel connecting the South China Sea with the East China Sea, has complex hydrographic conditions determined by influences of several currents under the forcing of monsoonal winds (e.g., Jan et al., 2002). Several medium-sized rivers and numerous bays are located on the west coast (on mainland China) of the strait. Algae blooms often occur during spring in these bays (e.g., Wang et al., 2009). Also along this coast, upwelling develops in summer, driven by the prevailing southwest monsoon, which runs parallel to the coast due to Ekman transport (e.g., Hong et al., 2009). The Taiwan Strait portion of the SCSD mainly consisted of summer upwelling samples, intensive algae bloom samples in two bays (Xiamen Bay and Huangqi Bay), and samples in the vicinity of river mouths.

The South China Sea is one of the largest marginal seas in the world. Its basin is deep (~5000 m) and oligotrophic, with surface chlorophyll concentration lower than 0.1 mg/m^3 except in winter (e.g., Liu et al., 2002; Shang et al., 2012). Two large rivers, the Pearl River and the Meikong River, discharge into the South China Sea. Plume-induced blooms are often observed (e.g., Dai et al., 2008). Meso-scale eddies and upwelling events are also prominent, resulting in significant biological enhancements (e.g., Chen et al., 2007; Gan et al., 2009).

In summary, this in situ data set used for algorithm assessment covered a variety of coastal and oceanic water regimes, and thus a wide range of absorption properties, with $a_{nw}(443)$ ranging from 0.021 to 2.16 m^{-1}, and the ratios of $a_{ph}(443)/a_{nw}(443)$, $a_g(443)/a_{nw}(443)$, and $a_d(443)/a_{nw}(443)$ varying in a range of 8.9%–78.9%, 5.4%–54.8%, and 6.9%–85.7%, respectively.

2.2. NOMAD data set

The NOMAD data set was downloaded from the website: http://seabass.gsfc.nasa.gov/. This is a publicly available, global, in situ bio-optical data set for use in ocean color algorithm development and satellite data product validation activities (Werdell & Bailey, 2005). In this data set, 89 sets contain concurrent R_{rs}, a_{nw}, b_{bp} and a_d, which were used to derive empirical functions (see Eqs. 7–8 in