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An optical model for the remote sensing of coloured dissolved organic matter in coastal/ocean waters

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A B S T R A C T

An optical model is developed for the remote sensing of coloured dissolved organic matter (CDOM) in a wide range of waters within coastal and open ocean environments. The absorption of CDOM (denoted as a_g) is generally considered as an exponential form model, which has two important parameters – the slope S and absorption of CDOM at a reference wavelength $a_g(\lambda_0)$. The empirical relationships for deriving these two parameters are established using in-situ bio-optical datasets. These relationships use the spectral remote sensing reflectance (R_{rs}) ratio at two wavelengths $R_{rs}(670)/R_{rs}(490)$, which avoids the known atmospheric correction problems and is sensitive to CDOM absorption and chlorophyll in coastal/ocean waters. This ratio has tight relationships with $a_g(412)$ and $a_g(443)$ yielding correlation coefficients between 0.77 and 0.78. The new model, with the above parameterization applied to independent datasets (NOMAD SeaWiFS match-ups and Carder datasets), shows good retrievals of the $a_g(\lambda)$ with regression slopes close to unity, little bias and low mean relative and root mean square errors. These statistical estimates improve significantly over other inversion models (e.g., Linear Matrix-LM and Garver-Siegel-Maritorena-GSM semi-analytical models) when applied to the same datasets. These results demonstrate a good performance of the proposed model in both coastal and open ocean waters, which has the potential to improve our knowledge of the biogeochemical cycles and processes in these domains.

1. Introduction

Coloured dissolved organic matter (CDOM), defined as materials passing through a 0.2 μm filter and often described as yellow substance or gelbstoff, plays a critical role in a broad range of marine aquatic ecosystems. It primarily absorbs ultraviolet and blue light radiation in 350–500 nm range and plays an important role in determining the underwater light fields. In addition, CDOM represents a significant component of ocean optical signals for satellite-based measurements of ocean colour and can interfere in global and regional estimates of primary production. The optically active fraction of CDOM affects the ocean colour, underwater light fields and aquatic chemistry through a suite of sunlight-initiated photochemical processes. CDOM is a highly complex macromolecular material containing humic and fulvic [check fulvic at proof] substances. In the open ocean, where coastal runoff and riverine input are negligible on annual time scales and Chlorophyll-a concentrations (Chl-a) are typically less than 0.5 mg m^{-3}, CDOM exhibits a featureless absorption spectrum that decreases exponentially with increasing wavelength from ultraviolet (UV) into visible wavelength and influences the spectral distribution and light availability in the water column. The CDOM spectral slope (S) indicates the rate at which the CDOM absorption decreases with increasing wavelength. Changes in the shape of CDOM absorption spectrum or S have been attributed to solar photo-bleaching or photo-oxidation (increase in S) or to the differing nature of CDOM sources (Blough and Del Vecchio, 2002; Twardowski and Donaghay, 2002), thus providing additional insights into the nature of CDOM. Moreover, absorption of sunlight by CDOM has important implications to carbon cycling in the marine environment. For example, the process of photo-oxidation can result in photoproducts and a variety of organic compounds with low molecular weights (Gao and Zepp, 1998). Absorption by CDOM can mitigate the damaging effect of solar UV radiation in the aquatic system, while its loss due to photo-oxidation can decrease absorption in the UV and visible spectral regions. In the visible range of the electromagnetic spectrum, CDOM absorption can reduce the amount of photosynthetically active radiation (PAR) available to the phytoplankton and thus can affect primary productivity or can interfere with satellite determinations of seawater constituents such as phytoplankton pigments (Blough and Del Vecchio, 2002).

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The spectral variations of absorption and scattering of clear and turbid waters have been studied over the wavelength range from 400 to 700 nm. The behaviour of S in natural waters is highly sensitive with respect to the wavelength range over which it is estimated. In CDOM studies, variability in S is associated with changes in the composition of the CDOM pool (Carder et al., 1989), and in the open ocean it is usually associated with degradation (solar and bacterial) and mixing of different CDOM pools (Brown, 1977; Gao and Zepp, 1998). However, the source of CDOM (in concert with the blue colour reflected by ocean water) can be tracked effectively. For instance, the largest source of CDOM is end members (riverine and marine) that are determined from the conservative mixing model (Kowalczuk et al., 2006). Stedmon and Markager (2001) established an algorithm to distinguish CDOM of terrestrial or marine origin based on the relationship between CDOM absorption and the spectral slope.

Modelling the spectral shape of the absorption coefficient spectra $a_g(\lambda)$ (m^{-1}) in the optical region has been reported by various researchers (Bricaud et al., 1981; Roesler et al., 1989; Kowalczuk et al., 2006), who have shown that it should follow the exponential decay function. Therefore, the spectral information with respect to $a_g(\lambda)$ can only be obtained by measuring a_g at a specific wavelength (e.g., 412 nm) and with known mean slope of exponential decay constant. The S coefficients change with wavelength and season, and co-vary with CDOM concentration.

For developing remote sensing algorithms, a complete characterization of the water is required. For instance, understanding the variability of inherent and apparent optical properties and water constituents is essential for correct retrievals of the CDOM, suspended sediment (SS) and Chl concentrations. Remote sensing algorithms have been developed for many optical properties of seawater, including spectral absorption and spectral backscattering, and are frequently evaluated in a number of regional field studies. Spectral band ratios are widely used to interpret the remote sensing data. In coastal waters where the spatial distribution of optically active constituents is variable, these ratios seem to have local and regional characteristics (Kahru and Mitchell, 1998; Kutser et al., 2001). However, various empirical and semi-analytical algorithms have been additionally proposed for the retrieval of CDOM absorption coefficient (a_g) from remote sensing data at the specific wavelengths (Kahru and Mitchell, 1998; Kutser et al., 2001; Maritorena et al., 2002; Boss and Roesler, 2006). These algorithms/models fail to provide the spectral dependence of a_g, which may vary from region to region according to the specific biogeochemical constituents of CDOM.

The objectives of this paper are (1) to develop a robust optical model for the remote sensing of CDOM in coastal and open ocean waters, and (2) to validate the proposed model using in-situ bio-optical datasets as well as satellite match-ups datasets.

2. Data and methods

2.1. Data sets

An updated NASA bio-Optical Marine Algorithm Dataset (hereafter referred to as NOMAD) was obtained from the NASA Ocean Biology Processing Group. It consists of two types of datasets – in-situ bio-optical dataset and satellite corresponding data with concurrent SeaWiFS observations of remote sensing reflectance (R_{rs}) and in-situ a_g at key wavelengths. The in-situ datasets are high quality data acquired over 4459 stations and stored in the system for use in algorithm development and validation (O'Reilly et al., 1998, 2000). Fig. 1 shows the frequency distribution of the in-situ $R_{rs}(443)$ and $a_g(490)$ collected in coastal and ocean waters ($N = 223$). The lower end of the histograms represents clear waters while the higher end represents the coastal waters. These data were used to develop the empirical relationships for the new model. Another suite of NOMAD dataset (composing NOMAD in-situ data) includes SeaWiFS-remote sensing reflectances and coincidently measured in-situ $a_g(\lambda)$ data from the coastal and open ocean regions (NOMAD-2). These satellite corresponding data together with the Carder bio-optical dataset ($N = 618$) obtained during cruises in the west coast of Florida in different seasons and years from 1999 to 2006 were used to validate the performance of the proposed model.

2.2. Performance assessment

To assess the performance of the model, two basic statistical measures were used: the root mean square error (RMSE, random error) and mean normalized bias (MNB, systematic error). In addition, the slope (S), intercept (I) and correlation coefficient (R^2) were also obtained from regression analysis for further assessment. Because the in-situ and model data are independent and are both subject to errors, systematic and random errors were calculated as follows:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(M_i - I_i)^2} \quad (1)$$

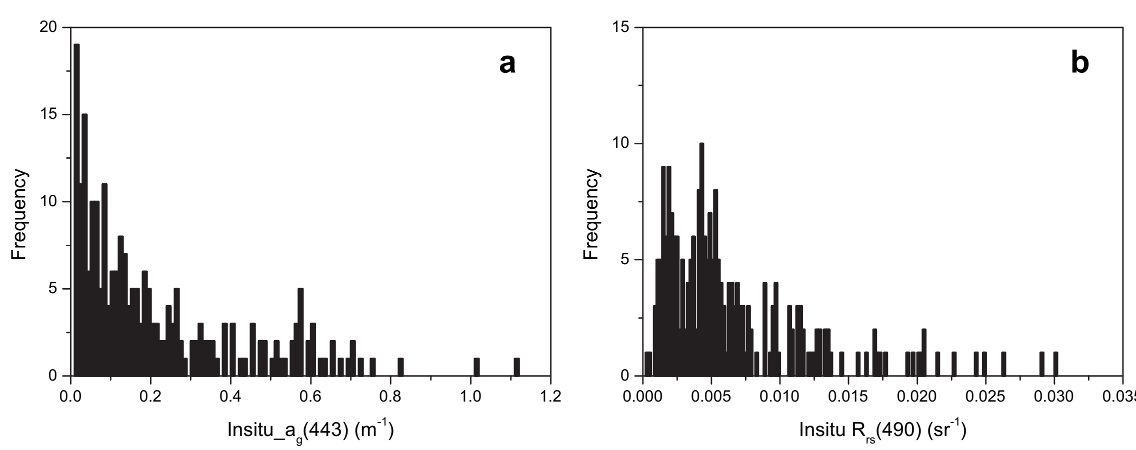

Fig. 1. Histograms of the (a) $a_g(443)$ (m^{-1}) and (b) $R_{rs}(490)$ (sr^{-1}) from NOMAD in-situ datasets ($N = 233$).