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Remote sensing of absorption and scattering coefficient using neural network model: Development, validation, and application

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ABSTRACT

The total absorption ($a(\lambda)$) and backscattering ($b_b(\lambda)$) coefficients of natural waters are the most significant factors affecting light propagation within water columns, and thus play indispensable roles in the estimation of aquatic biomass, primary production, and carbon pools. Despite its importance, no accurate retrieval model has been specifically developed for both oceanic and coastal waters, but significant efforts have been made in regard to oceanic inversion models. The objectives of the present study are to evaluate the applicability of the quasi-analytical algorithm (QAA) in deriving $a(\lambda)$ and $b_b(\lambda)$ from oceanic and coastal waters, and to improve it using a neural network-based semi-analytical algorithm (NNSAA). Based on a comparison of the $a(\lambda)$ and $b_b(\lambda)$ predicted by these models with field measurements taken from the national aeronautics and space administration bio-optical marine algorithm dataset (NOMAD), the Yellow Sea and China East Sea, it is shown that the NNSAA model ($R^2 > 0.82$ and mean relative error, $MRE = 20.6$–35.5%) provides a stronger performance than the QAA model ($R^2 < 0.73$ and $MRE = 32.2$–69.6%). The model was also applied to MODIS data after atmospheric correction using a near-infrared-based and shortwave infrared-based combined model. Through validation by field measurements, it was shown that the NNSAA model can predict $a(\lambda)$ and $b_b(\lambda)$ with high accuracy ($R^2 > 0.77$ and $MRE < 39.9\%$). Finally, the NNSAA model was used to map the global climatological seasonal mean $a(443)$ and $b_b(555)$ for the time range of July 2002 to September 2013. Except the coastal zones, it was shown that the $a(443)$ and $b_b(532)$ in some high-latitude areas are much higher than in the mid- and low-latitude regions, due to the effects of spurious signals from neighboring sea-ice. In the equatorial oceans, the $a(443)$ value in the surface water is considerably higher in the equatorial Pacific than in the equatorial Atlantic in the upwelling region, while the integrate $a(443)$ is much higher in the Atlantic than in the throughout the entire tropical gyre areas. The difference between $a(443)$ and $b_b(532)$ in the subsurface water is due to a pronounced deep biomass maximum existing in the equatorial Atlantic, which is associated with the higher nitrate in the lower euphotic zone.

1. Introduction

Absorption and backscattering coefficients are inherent optical properties (IOPs, see Table 1 for definitions of all symbols and acronyms used in this work). It has long been known that the visible radiation upwelling from a natural water body is partially dictated by the absorption and backscattering coefficients of the optically active constituents residing within that water body (Robert, Alexander, & Kirill, 1995), thus the total absorption and backscattering coefficients can be directly associated with a proper bio-optical treatment of the light regime of the ocean mixed layer and the related heat budget (Ohlmannn, Siegel, & Mobley, 2000). In general, an accurate estimation of the scattering and attenuation characteristics of the upper layer ocean may provide insight into the nature of the particles in suspension (Volpe, Silvestri, & Marani, 2011). Moreover, the total absorption and backscattering coefficients define the upwelling light field, and are also the most logical targets for the retrieval of the water-leaving reflectance spectrum determined from satellite observations (Mélin et al. 2005). At present, optical data, such as total absorption and backscattering coefficients, have been widely used for coastal and oceanic studies (Astoreca, Doxaran, Ruddick, Rousseau, & Lancelot, 2012; Garver & Siegel, 1997; IOCCG 2006), such as the optical classification of water bodies (Moore, Campbell, & Dowell, 2009).

Methods to accurately retrieve absorption and backscattering coefficients in oceanic waters have been under investigation for several decades, and models ranging from empirical to analytical have been proposed (Chen, Yao, & Quan, 2013; IOCCG 2006; Lee, Carder, & Arnone,

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Table 1
All symbols and definitions used in this work.

Symbol	Description	Unit
CDOM	Colored dissolved organic matter	
QAA	Quasi-analytical algorithm	
SAA	Semi-analytical algorithm	
MSAA	MODIS semi-analytical algorithm	
IOP	Inherent optical property	
AOP	Apparent optical property	
NNSAA	neural network-based semi-analytical algorithm	
NNS	Neural network model for $S(\lambda)$ retrieval	
NNB	Neural network model for $b_b(\lambda)$ retrieval	
NNA	Neural network model for $a(\lambda)$ retrieval	
NOMAD	NASA bio-optical marine algorithm dataset	
STDEV	Standard deviation	
NIR	Near-infrared	
SWIR	Shortwave-infrared	
ARE	Absolute relative error	%
MRE	Mean absolute relative error	%
$R_{rs}(\lambda)$	Remote sensing reflectance	sr^{-1}
R_{rg}	Band ratio of $R_{rs}(667)$ to $R_{rs}(488)$	
$a(\lambda)$	Total absorption coefficient	m^{-1}
$a_g(\lambda)$	Absorption coefficient for gelbstoff concentration	m^{-1}
$a_\varphi(\lambda)$	Absorption coefficient for phytoplankton pigment	m^{-1}
$a_w(\lambda)$	Absorption coefficient for water molecular	m^{-1}
$b_b(\lambda)$	Total backscattering coefficient	m^{-1}
$b_{bp}(\lambda)$	Backscattering coefficient for suspended particles	m^{-1}
$b_{bw}(\lambda)$	Backscattering coefficient for pure waters	m^{-1}
$S(\lambda)$	Ratio of $b_b(\lambda)$ to $a(\lambda)$	
λ	Wavelength	nm
g_i	Empirical coefficient ($i = 0, 1, 2,$ or 3)	
ξ	$a_g(\lambda_3)/a_g(\lambda_2) - \zeta a_g(\lambda_1)/a_g(\lambda_2)$	
ζ	$a_\varphi(\lambda_1)/a_\varphi(\lambda_3) + \xi a_\varphi(\lambda_2)/a_\varphi(\lambda_3)$	
$\varepsilon_{bb}(\lambda_1,\lambda_i)$	$b_b(\lambda_i)/b_b(\lambda_1)$ ($i = 2$ or 3)	
Y	Power value for spectral slope of backscatter of suspended particles	

2002; Lee, Werdell, & Arnone, 2009; Smyth, Moore, Hirata, & Aiken, 2006). Empirical models apply simple or multiple regressions to the desired optical property and the ratios of irradiance reflectance or remote sensing reflectance (Li et al., 2013). Such approaches do not require a full understanding of the relationship between the remote sensing reflectance and absorption and/or backscattering coefficients (Lee & Carder, 2004). Due to the statistical nature of regression, however, the accuracy of these models decreases when the bio-optical characteristics differentiate from the datasets used to empirically derive the covariance relationships, unless the waters are restricted to oceanic waters (Carder, Chen, Lee, Hawes, & Cannizzaro, 2003). The analytical model uses the radiative transfer theory to simulate the spectra at the top-of-atmosphere with different IOPs by satellite detector and atmosphere conditions (Gordon & Clark, 1981; Gordon et al., 1988). Using the water-leaving signals (e.g. remote sensing reflectance) detected by satellite, the IOPs can be accurately determined by a physical model (Mobley, 1994). However, this model requires the accurate profile information of the IOPs of the water and atmosphere for model initialization, which is not always available for the general application of remote sensing. The semi-analytical model is based on the relationship between the IOPs and AOPs, combined with several empirical relationships. This model works well for different water bodies and usually performs better than the empirical model (Chen, Zhang, Cui, & Wen, 2013; Li et al., 2013), thus it is a promising technique for IOP retrievals.

Despite the fact that there are several empirical and semi-analytical models available for computing IOPs (Chen, Yao, et al., 2013; Dupouy et al., 2010; Garver & Siegel, 1997; Hoge & Lyon, 2005; IOCCG 2006; Lee et al., 2009; Li et al., 2013; Mélin et al. 2005; Smyth et al., 2006; Tzortziou et al., 2007), at present there is a compelling need for an IOPs model for turbid coastal waters, as the existing models are essentially applicable only for clear oceanic waters or regional coastal zones. For example, the widely used QAA (Lee et al., 2009) models were originally developed for oceanic water, and thus may not be suitable for optically complex coastal waters due to the high concentrations of suspended sediment and CDOM (Chen, Cui, Tang & Song, 2014; D'Sa, MIller, & McKee, 2007; Li et al., 2013; Shanmugam, 2011). Such complexity is primarily manifested in the variation of the factors such as g_1 and g_2 which were proposed by Gordon et al. (1988) and lately modified by Lee et al. (2009) to describe the relationship between remote sensing reflectance and IOPs (Gordon et al. (1988) found that $g_1 \approx 0.0949$ and $g_2 \approx 0.0794$ for oceanic waters, while Lee et al. (2009) suggested that $g_1 \approx 0.089$ and $g_2 \approx 0.125$ are more suitable for higher scattering coastal waters). In fact, the relationship between remote sensing reflectance and IOPs may be very complicated, and is only vaguely understood. As a result, using constant g_1 and g_2 for different water types may be not appropriate (Aurin & Dierssen, 2012). In addition, in the QAA model the total absorption coefficient and backscattering at 555 nm are estimated by empirical models, and then extrapolated to the "unknown" shorter wave bands using a semi-analytical model. It is well known that empirical models are generally only suitable for application to waters with optical characteristics similar for application to waters with optical characteristics similar to those used in the development of the model. These reasons motivate us to build a more accurately model for deriving IOPs from remote sensing reflectance for both oceanic and coastal waters.

The performance of QAA model in the optical complex coastal waters may be improved by several recently developed semi-analytical and empirical models (Chen, Cui, Qiu & Lin, 2014; Garver & Siegel, 1997; IOCCG 2006; Li et al., 2013; Smyth et al., 2006). These models can be used to process satellite data efficiently, but some problems are encountered when they are applied to optically complex coastal waters such as the Yellow Sea and China East Seas. For example, when the IOP retrieval model developed by Garver and Siegel (1997) and Hoge and Lyon (2005) was used to process satellite data in the Yellow Sea and China East Seas, some negative backscattering values could be observed. Even though the model proposed by Li et al. (2013) may work better than QAA model in optically complex waters, due to the fact that this model is capable of accommodating the variation of g_1 and g_2 across