Remote Sensing of Environment 135 (2013) 150–166

Contents lists available at SciVerse ScienceDirect

Remote Sensing of Environment

journal homepage: www.elsevier.com/locate/rse

An inversion model for deriving inherent optical properties of inland waters: Establishment, validation and application

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ARTICLE INFO

Article history:
Received 24 December 2012
Received in revised form 28 March 2013
Accepted 30 March 2013
Available online 30 April 2013

Keywords:
IOPs estimation
Chlorophyll-*a*
Inherent optical properties
Inland waters
OCLI
AISA

ABSTRACT

The inherent optical properties (IOPs) of natural waters are the most significant factors affecting light propagation within water columns, and thus play indispensable roles on estimation of aquatic biomass, primary production, and carbon pools. Despite its importance, no IOPs retrieval model was specifically developed for inland water bodies, although significant efforts were made on oceanic inversion models. In addition, for inland waters, an IOPs-based model is often preferred for estimating chlorophyll-*a* (Chl-*a*) concentration, an application of IOPs, over empirical and some semi-empirical algorithms. Then developing a model for estimating both IOPs and Chl-*a* is of significance for understanding the bio-optical properties and occurrence of algal blooms in eutrophic reservoirs, lakes and estuaries. In this paper, an IOPs Inversion Model of Inland Waters (IIMIW) for deriving natural water IOPs and estimating Chl-*a* is proposed and validated. The results indicate that this model can be used to accurately retrieve absorption coefficients at 443 nm and 665 nm with $R^2 = 0.8347$ and $R^2 = 0.7550$ respectively for Indiana study sites, and to estimate Chl-*a* from the derived absorption coefficients at high accuracies ($R^2 = 0.9292$ and a mean relative error 21.65%) with samples collected from eight different study sites in the world and in different seasons. The model was also applied on Airborne Imaging Spectrometer for Application (AISA) images to map IOPs and Chl-*a*. Through validation by in situ measured Chl-*a*, results directly show that IIMIW can predict Chl-*a* with good accuracy even using the AISA bands, to as well indirectly prove that non-water absorption coefficients are retrieved accurately, at least within red and near-infrared region. Further biogeochemical information can be derived from these maps as well. These promising mapping results reveal possible remote routine surveillance of bio-optical states of inland waters.

1. Introduction

1.1. Deriving inherent optical properties (IOPs) for inland waters

Underwater light penetration is fundamentally important to aquatic ecosystems because the quantity and quality of underwater light drive the photosynthesis of algae dwelling in water bodies (Gallegos et al., 2005). The inherent optical properties (IOPs) of natural waters, including absorption ($a(\lambda)$, *referring to* Table 1 *for symbols and acronyms*) and backscattering ($b_b(\lambda)$) coefficients, are the most significant parameters governing the light propagation within the water column and thus indispensable to the estimation of aquatic biomass, primary production, heat flux, and carbon pools (Hirawake et al., 2011; Le et al., 2009a; Lee et al., 1996; Oliver et al., 2004; Wang et al., 2005; and references therein).

In recent years many efforts have been made to derive the IOPs from the apparent optical properties (AOPs), e.g. irradiance reflectance and remote sensing reflectance (e.g. Garver & Siegel, 1997; Hoge & Lyon, 1996, 2005; Le et al., 2009a; Lee et al., 1996; Wang et al., 2005). Among those existing algorithms, empirical algorithms use simple or multiple regressions to relate the IOPs to the ratio of the AOPs. They can be implemented rapidly, but their application is limited due to the variation of optical properties across different water bodies (Le et al., 2009a). Semi-empirical and analytical algorithms based on radiative transfer equations work better for different water bodies and usually perform better than the empirical algorithm. A derivation of IOPs from remote sensing reflectance is commonly based on the reflectance model shown in Eq. (1) (Gordon et al., 1988) that describes the relationship between remote sensing reflectance and IOPs.

$$r_{rs}(\lambda) = \frac{L_u(\lambda, 0-)}{E_d(\lambda, 0-)} = g_1\left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right) + g_2\left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^2 \quad (1)$$

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http://dx.doi.org/10.1016/j.rse.2013.03.031

Table 1
Symbols and acronyms.

Symbol/acronym	Description	Unit
$L_u(0-)$	Upwelling radiance below water surface	W m^{-2} sr^{-1}
L_x	Radiance. *x* could be *w*: water-leaving radiance; *sw*: total radiance of water surface; *sky*: Sky radiance; *p*: radiance of standard panel	W m^{-2} sr^{-1}
$E_u(0-)$	Upwelling irradiance below water surface	W m^{-2}
E_d	Downwelling irradiance. 0+: above water surface 0−: below water surface	W m^{-2}
$R_{rs}(\lambda)$	Remote sensing reflectance above water surface	sr^{-1}
$r_{rs}(\lambda)$	Remote sensing reflectance below water surface	sr^{-1}
f	Geometrical light factors	–
Q	Light distribution factor	sr
$a(\lambda)$	Total absorption coefficients of water column	m^{-1}
$a_x(\lambda)$	Absorption coefficients of *x*. *x* could be *w*: water; *ph*: in vivo phytoplankton; *sol*: in vitro phytoplankton; *t* − *w*: non-water constituents; *cdom*: colored dissolved organic matter; *cdm*: colored detritus matter	m^{-1}
$b_b(\lambda)$	Total backscattering coefficients of water column	m^{-1}
$b_{bx}(\lambda)$	Backscattering coefficients of *x*. *x* could be *w*: water; *p*: suspended particles	m^{-1}
IOPs	Inherent optical properties	m^{-1}
Chl-*a*	Chlorophyll-a (concentration)	mg m^{-3}
TSM	Total suspended matter (concentration)	g m^{-3}
CDOM	Colored dissolved organic matter	–
NAP	Non-algal particles (concentration)	g m^{-3}
CDM	Colored detritus matter, i.e. CDOM + NAP	–

where $r_{rs}(\lambda)$ is the remote sensing reflectance just beneath water surface, $L_u(\lambda, 0-)$ and $E_d(\lambda, 0-)$ are upwelling radiance and downwelling irradiance, respectively, and g_1 and g_2 are geometric factors. Hereafter the wavelength dependence of all model variables will be omitted for briefness unless it is necessary. Eq. (1) is simplified in many studies (e.g., Brando & Dekker, 2003; Giardino et al., 2007; Hakvoort et al., 2002; Hoogenboom et al., 1998; Jupp et al., 1994; Kutser, 2004; Kutser et al., 2006; Zhang et al., 2009) by omitting the quadratic term, resulting in Eqs. (2) and (3):

$$r_{rs} = \frac{f}{Q}\frac{b_b}{a+b_b} \tag{2}$$

$$R(0-) = \frac{E_u(0-)}{E_d(0-)} = f\frac{b_b}{a+b_b} \tag{3}$$

where f is a factor of light field, Q is the light distribution factor defined as $Q = E_u(0-) \,/\, L_u(0-)$; $R(0-)$, $E_u(0-)$ and $E_d(0-)$ are subsurface irradiance reflectance, upwelling and downwelling irradiance, respectively.

Built upon Eqs. (1)–(3), several semi-empirical and semi-analytical algorithms have been proposed for deriving the IOPs, including the Garver–Siegel–Maritorena (GSM) algorithm (Garver & Siegel, 1997; Maritorena & Siegel, 2005, 2006; Maritorena et al., 2002), the algorithm (referred to as HL) by Hoge and Lyon (1996, 1999, 2005) and the quasi-analytical algorithm (QAA) by Lee et al. (2002, 2009) and Lee and Carder (2004). The difference among them lies in that GSM and HL require pre-defined spectral shapes of phytoplankton absorption ($a_{ph}(\lambda)$) and colored detritus matter (CDM, colored dissolved organic matter (CDOM) + non-algal particles (NAP)) absorption ($a_{cdm}(\lambda)$) while QAA does not have such a requirement.

GSM, HL and QAA are all originally developed for ocean water and thus may not be suitable for optically complex inland waters due to high concentrations of suspended sediment (SS) and CDOM (Gons, 1999; Gons et al., 2000; Schalles, 2006; Schalles et al., 2001; Zhou et al., 2009). Such complexity is primarily manifested in the variation of the factors such as g_1, g_2, f and Q that are used in Eqs. (1), (2) and (3). However, previous studies assume g_1 and g_2 as constants (Garver & Siegel, 1997; Hoge & Lyon, 1996, 1999, 2005; Hoge et al., 1999a, 1999b; Lee & Carder, 2004; Lee et al., 1999, 2002, 2007, 2009; Maritorena & Siegel, 2005, 2006; Maritorena et al., 2002; Salama et al., 2009; Wang et al., 2005), f or $\frac{f}{Q}$ as a constant (Hakvoort et al., 2002; Hoogenboom et al., 1998), or f as a function of just light geometry (Brando & Dekker, 2003; Giardino et al., 2007; Jupp et al., 1994; Kutser, 2004; Kutser et al., 2006; Zhang et al., 2009). In fact, f, $\frac{f}{Q}$ [g_1 is equivalent to $\frac{f}{Q}$ (Maritorena et al., 2002)], and g_2 depend on ambient factors including bio-optical states, solar angles, and wind speed (Gould et al., 2001; Morel & Gentili, 1993, 1996; Zhang et al., 2009), and as a result may vary sample by sample or across different water bodies (Aurin & Dierssen, 2012; Gould et al., 2001). For example, the values assigned to g_1 and g_2 in QAA (Lee & Carder, 2004; Lee et al., 2002, 2009) differ from those used in GSM (Garver & Siegel, 1997; Maritorena & Siegel, 2005, 2006; Maritorena et al., 2002), and those used by Gordon et al. (1988), Lee et al. (1999), and Aurin and Dierssen (2012). The reported value for g_1 (or $\frac{f}{Q}$) could range from 0.08 to 0.15(Morel et al., 2002) even for spatially relatively homogeneous ocean waters. Aurin and Dierssen (2012) suggested that using constant g_1 and g_2 for different water types is not appropriate. In turbid inland water bodies, the variation of water properties at different sites is more complex (Zhang et al., 2009), leading to the dependence of g_1 and g_2 on study locations or sites. Therefore, g_1 and g_2 should be considered as variables when deriving the IOPs for optically complex inland waters is of interest. This motivates us to build an IOPs retrieval model that is capable of accommodating the variation of g_1 and g_2 across various inland water bodies and does not require recalibration when it is applied to different inland water bodies.

1.2. Application of IOPs for chlorophyll-a estimation

Chlorophyll-*a* (Chl-*a*) concentration is essential for monitoring algal blooms, especially toxic cyanobacterial blooms in reservoirs, lakes, and estuaries (Matthews et al., 2010; Randolph et al., 2008; Simis et al., 2005, 2007). Because of the optical complexity of inland waters, it is not easy to reliably retrieve Chl-*a* from remote sensing reflectance or water leaving radiance L_w using empirical algorithms such as band ratio (Dekker, 1993; Gitelson, 1992; Jupp et al., 1994; Kallio et al., 2001; Li et al., 2010), fluorescence line height (Gons et al., 2008; Gower & King, 2007; Hu et al., 2005), three-band tuning algorithms (Dall'Olmo & Gitelson, 2005; Duan et al., 2010; Gitelson et al., 2007, 2008, 2009), four-band algorithms (Le et al., 2009b, 2010), and other band combination methods (Budd & Warrington, 2004; O'Reilly et al., 1998). These algorithms are usually limited to the dataset on which they are calibrated (Giardino et al., 2007; Matthews et al., 2010). Particularly, when SS concentration is high, the scattering of SS usually masks the optical response of Chl-*a*, reducing the predictive power of the empirical algorithm (Bukata, 1995; Zhou et al., 2009). Therefore, IOCCG (2006) and Zhou et al. (2009) suggested to derive Chl-*a* from IOPs rather than directly from AOPs for highly turbid inland waters (e.g. Gilerson et al., 2010; Gons et al., 2002, 2008; Li et al., 2011; Simis et al., 2005, 2007). In this regard, several equations (e.g. Ritchie, 2008), can be used to quantify Chl-*a* from in vitro $a_{ph}(\lambda)$ in laboratory, and have potential