Journal of Great Lakes Research Supplement 39 (2013) 137–150

Contents lists available at ScienceDirect

Journal of Great Lakes Research

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

Remote sensing reflectance in the Great Lakes: *In situ* measurements, closure analyses, and a forward model

David M. O'Donnell *, Steven W. Effler [1], Christopher M. Strait [2], Feng Peng [3], MaryGail Perkins [4]

Upstate Freshwater Institute, P.O. Box 506, Syracuse, NY 13214, USA

ARTICLE INFO

Article history:
Received 16 August 2012
Accepted 13 May 2013
Available online 25 July 2013

Communicated by George Leshkevich

Keywords:
Laurentian Great Lakes
Remote sensing reflectance
Optically active constituents
Underwater optics
Absorption
Backscattering

ABSTRACT

Observations of remote sensing reflectance (R_{rs}), the signal available to support remote sensing of optically active constituents (OACs) of water quality interest, are presented for multiple sites within each of the Laurentian Great Lakes based on *in situ* measurements made with a hyperspectral radiometer. $R_{rs}(\lambda)$ spectra are contrasted among these lakes and in time and space within selected systems. Qualitative analyses of spectra are provided that identify the inherent optical property (IOP) and coupled OAC conditions responsible for the differences in $R_{rs}(\lambda)$. The much higher R_{rs} peaks observed in the green wavelengths for the lower Great Lakes (Erie and Ontario) are attributed to elevated backscattering levels caused by higher concentrations of minerogenic particles. The credibility of the $R_{rs}(\lambda)$ spectra is established through successful closure analyses that demonstrate good matches with IOP-based predictions and consistency of coefficient values for radiative transfer expressions with related literature and theory. A mechanistic forward model of $R_{rs}(\lambda)$ is developed that accommodates the effects of three OACs, including metrics of phytoplankton biomass, minerogenic particles and colored dissolved organic material. This includes the development of the critical cross-section relationships that quantify the couplings between the OACs and IOPs, and in turn the IOPs and the $R_{rs}(\lambda)$ signal. The model is demonstrated to perform well in matching observations in Lake Erie, and to be sensitive to the representation of the spectral dependency of backscattering and likely variations in the dependence of phytoplankton absorption on chlorophyll. The modeled predicted responses of Lake Erie to different OAC levels are presented.

Introduction

Water color is quantified by measurements of remote sensing reflectance [$R_{rs}(\lambda)$, sr^{-1}; abbreviations and symbols listed in Table 1], an apparent optical property (AOP; *i.e.*, depends on the geometry of the light field). $R_{rs}(\lambda)$ is defined as the ratio of the water-leaving spectral radiance to downwelling spectral irradiance just above the surface. This signal provides rich quantitative information on the regulating optically active constituents (OACs) and mediating inherent optical properties (IOPs) of the absorption [$a(\lambda)$] and backscattering [$b_b(\lambda)$] coefficients that vary to different extents with wavelength (λ) in the visible domain (Lee et al., 2002; Lubac and Loisel, 2007). $R_{rs}(\lambda)$ is, in principle, proportional to the ratio $b_b(\lambda)$:$a(\lambda)$ in non-turbid water, and $b_b(\lambda)$:[$a(\lambda) + b_b(\lambda)$] in turbid systems (Gordon et al., 1988). It is the basis for development of remote sensing algorithms for retrieval of OAC concentrations as well as for satellite sensor calibration (Lee et al., 2010; Morel, 1980). Measurements of $R_{rs}(\lambda)$ have become spectrally robust and have been used to classify near-shore marine case 2 waters (non-phytoplankton OACs do not covary with, and may not be subordinate to, phytoplankton) according to various OAC cases (Lubac and Loisel, 2007).

There is an established successful history of development of strong empirical relationships between remotely sensed features of $R_{rs}(\lambda)$ and various OACs that have resulted in representative retrievals for case 1 waters (phytoplankton dominate, other OACs covary; Gordon et al., 1983; Lee et al., 1998; Morel and Prieur, 1977). System-specific empirical approaches and associated retrievals have also had some successes in case 2 waters (Doxaran et al., 2002, 2006), though dynamics, and particularly extreme events, may be problematic. Empirical remote sensing approaches, particularly retrieval of Chl, have been largely unsuccessful, or spatially and temporally limited (Gons et al., 2008), in the Great Lakes (Binding et al., 2012; Lesht et al., 2012; Mouw et al., 2013). A more mechanistic approach, using semi-analytical algorithms that incorporate a radiative transfer equation to describe the dependency of $R_{rs}(\lambda)$ on $a(\lambda)$ and $b_b(\lambda)$ and therefore the dependence of these IOPs on OACs, can support more robust remote sensing retrieval capabilities (Binding et al., 2012; Lee et al., 2002; Lubac and Loisel, 2007;

* Corresponding author. Tel.: +1 315 431 4962x119.
E-mail addresses: daveod@upstatefreshwater.org (D.M. O'Donnell), sweffler@upstatefreshwater.org (S.W. Effler), cstrait@upstatefreshwater.org (C.M. Strait), fpeng@upstatefreshwater.org (F. Peng), mgperkines@upstatefreshwater.org (M. Perkins).
[1] Tel.: +1 315 431 4962x102.
[2] Tel.: +1 315 431 4962x100.
[3] Tel.: +1 315 431 4962x105.
[4] Tel.: +1 315 431 4962x104.

0380-1330/$ – see front matter
http://dx.doi.org/10.1016/j.jglr.2013.06.016

Table 1
Abbreviations and symbols.

Abbreviations	
AOPs	Apparent optical properties
CDOM	Colored dissolved organic material
DOC	Dissolved organic carbon
IOP	Inherent optical property
NAP	Non-algal particles
OAC	Optically active constituent
OAC_{ax}	Optically active constituents for absorbing components
OAC_{bbx}	Optically active constituents for backscattering components
SAX	Scanning electron microscopy interfaced with automated image and X-ray analyses
Symbols	
$a(\lambda)$	Total spectral absorption coefficient (m^{-1}), at λ
$a_x(\lambda)$	Spectral absorption coefficient for component "x" (m^{-1}); "x" can be CDOM, NAP, particles (p), phytoplankton (φ), and water (w)
$a^*_{\varphi,Chl}(\lambda)$	Chl-specific a_φ at λ ($m^2 \cdot mg^{-1}$)
$b_b(\lambda)$	Backscattering coefficient at λ (m^{-1})
$b_{b,x}(\lambda)$	Backscattering coefficient for component x at λ (m^{-1}); x can be minerogenic particles (m), organic particles (o), and water (w)
$b_p(\lambda)$ and $b_{bp}(\lambda)$	Spectral particulate scattering and backscattering coefficient (m^{-1})
Chl	Chlorophyll *a* (μg L^{-1})
$E_d(\lambda)$	Downwelling irradiance ($\mu W \cdot cm^{-2} \cdot nm^{-1}$)
$E_s(\lambda)$	Irradiance above the surface ($\mu W \cdot cm^{-2} \cdot nm^{-1}$)
f	Coefficient in radiative transfer expression for $R_{rs}(\lambda)$
ISPM	Concentration of inorganic suspended particulate material (mg L^{-1})
$K_{L,u}(\lambda)$	Diffuse attenuation coefficient for upwelling irradiance (m^{-1})
$L_u(\lambda)$	Upwelling radiance ($\mu W \cdot cm^{-2} \cdot sr^{-1} \cdot nm^{-1}$)
$L_u(0^-, \lambda)$	Upwelling radiance just below the surface ($\mu W \cdot cm^{-2} \cdot sr^{-1} \cdot nm^{-1}$)
$L_u(0^+, \lambda)$	Water-leaving radiance ($\mu W \cdot cm^{-2} \cdot sr^{-1} \cdot nm^{-1}$)
$L_w(\lambda)$	Water-leaving radiance ($\mu W \cdot cm^{-2} \cdot sr^{-1} \cdot nm^{-1}$)
PAV_m	Projected area concentration of minerogenic particles (m^{-1})
Q	Coefficient in radiative transfer expression for $R_{rs}(\lambda)$ (sr)
$\langle Q_{bbm}(\lambda) \rangle$	Mean backscattering efficiency factor of minerogenic particle populations
R_{rs}	Remote sensing reflectance (sr^{-1})
S_{CDOM}	Slope of the $a_{CDOM}(\lambda)$ spectrum (nm^{-1})
S_{NAP}	Slope of the $a_{NAP}(\lambda)$ spectrum (nm^{-1})
λ	Wavelength of light (nm)

Mouw et al., 2013; Tzortziou et al., 2007). A widely used radiative transfer expression that describes the dependence of $R_{rs}(\lambda)$ on $a(\lambda)$ and $b_b(\lambda)$ is (Reynolds et al., 2001; Tzortziou et al., 2007) is

$$R_{rs}(\lambda) = 0.54(f/Q) \cdot [b_b(\lambda)/(a(\lambda) + b_b(\lambda))] \quad (1)$$

where the parameters f and Q are both variable, depending on solar zenith angle, the geometric structure of the radiance field, and the IOPs. However, f and Q tend to covary such that the f/Q ratio is subject to only modest variations with wavelength and for ambient conditions of interest (Morel and Gentili, 1993). Alternatively, f/Q has been represented as a single symbol(s) of uniform value(s) (Gordon et al., 1988).

Advancements in instrumentation have also enabled *in situ* spectral measurements of the IOPs including most recently the measurement of $b_b(\lambda)$ (Gallegos et al., 2008; Loisel et al., 2007; Snyder et al., 2008; Tzortziou et al., 2007) that have now been extended to the Great Lakes (Effler et al., 2013–in this issue; O'Donnell et al., 2010). Modern instrumentation for measurement of AOPs and IOPs represents a powerful basis to advance optical characterization and support the development and testing of mechanistic approaches in remote sensing, particularly when $b_b(\lambda)$ and $a(\lambda)$ are measured in concert with $R_{rs}(\lambda)$. This suite of IOP and AOP measurements enables an evaluation of their credibility through closure analyses that utilize the quantitative framework of an appropriate radiative transfer expression [*e.g.*, Eq. (1)]. Such closure analyses, that demonstrate good matches of measured $R_{rs}(\lambda)$ with predictions, based on paired observations of $a(\lambda)$ and $b_b(\lambda)$ and specification of f/Q, have been demonstrated for several case 2 systems (Gallegos et al., 2008; Tzortziou et al., 2006), but only for limited portions of the Great Lakes (Bergmann et al., 2004; O'Donnell et al., 2010, 2013–this issue). Another perspective, based on the availability of the same paired data sets and use of the same radiative transfer expression, is evaluation of the f/Q ratio with respect to λ dependency and variability (Reynolds et al., 2001; Tzortziou et al., 2007). This approach instead effectively transfers closure considerations to the values of f/Q relative to the accepted range based on the literature (Morel and Gentili, 1993; Reynolds et al., 2001).

Once closure of instrument measurements of $R_{rs}(\lambda)$ with $a(\lambda)$ and $b_b(\lambda)$ has been established, the testing of relationships between these IOPs and OACs through their effects on closure can be pursued. These relationships are the basis of the retrievals in mechanistic remote sensing approaches (Lee et al., 2002). These usually take the following general form, accepting the additive nature of contributing components to the IOPs (Babin et al., 2003; Wozniak and Stramski, 2004)

$$a(\lambda) = a_1^*(\lambda) \cdot OAC_{a1} + a_2^*(\lambda) \cdot OAC_{a2} \cdots a_n^*(\lambda) \cdot OAC_{an} \quad (2)$$

$$b_b(\lambda) = b_{b,1}^*(\lambda) \cdot OAC_{bb1} + b_{b,2}^*(\lambda) \cdot OAC_{bb2} \cdots b_{b,n}^*(\lambda) \cdot OAC_{bbn} \quad (3)$$

where $a_x^*(\lambda)$ and $b_{b,x}^*(\lambda)$ are cross-sections, or specific coefficients, for the optically active constituents for absorption, OAC_{ax}, and backscattering, OAC_{bbx}. The availability of cross-sections, together with paired observations of $R_{rs}(\lambda)$ and OAC_{ax} and OAC_{bbx}, supports a second form of closure analysis that represents a test of the appropriateness of the cross-sections. These can be described as forward tests of potential remote sensing algorithms, in contrast to the more complex inversion calculations that would be used to estimate OAC_{ax} and OAC_{bx} from the $R_{rs}(\lambda)$ signal. The cross-sections together with the radiative transfer expression for $R_{rs}(\lambda)$ constitute a forward model (Reynolds et al., 2001), that can be applied to project the effects of changes in OACs on the $R_{rs}(\lambda)$ signal, or test the sensitivity of $R_{rs}(\lambda)$ predictions to uncertainties in the coefficients embedded in the cross-sections. The effective partitioning of both $a(\lambda)$ and $b_b(\lambda)$ according to the contributions of multiple OACs, across a range of conditions in the Great Lakes, and the development of related cross-sections (Effler et al., 2013–in this issue; Perkins et al., 2013–in this issue), supports such a forward modeling initiative for this system.

This paper presents, analyzes and models $R_{rs}(\lambda)$ spectra from *in situ* measurements made throughout the Great Lakes. These were collected in concert with measurements of IOPs and OACs (Effler et al., 2013–in this issue; Perkins et al., 2013–in this issue) that support the analyses presented here. The goals of this paper are to: (1) advance characterization of the emergent light fields of the system and establish useful cases of $R_{rs}(\lambda)$ that correspond to certain IOP and OAC conditions, (2) demonstrate the credibility of the $R_{rs}(\lambda)$ measurements through closure analyses based on paired IOP data, in the contexts of both apparent f/Q values and predictions of $R_{rs}(\lambda)$, (3) extend the spectral representations of cross-sections, (4) develop and test a forward model for $R_{rs}(\lambda)$ for the west basin of Lake Erie, and (5) preliminarily apply the model to conduct sensitivity analyses for model coefficients and make example projections for OAC scenarios.

Methods

Study sites and supporting data

This paper provides a spatially extensive, though somewhat uneven, characterization of $R_{rs}(\lambda)$ in the Laurentian Great Lakes (Fig. 1). Measurements were made in the open waters (>10 km from shore) of each of the five lakes and along the primary axes of Keweenaw Bay (Lake Superior) and the inner portion of Green Bay (Lake Michigan). Paired measurements of IOPs, including $a(\lambda)$ and $b_b(\lambda)$, and OACs, were made, as described in parallel papers (Effler et al., 2013–in this