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An optical water type framework for selecting and blending retrievals from bio-optical algorithms in lakes and coastal waters

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ABSTRACT

Bio-optical models are based on relationships between the spectral remote sensing reflectance and optical properties of in-water constituents. The wavelength range where this information can be exploited changes depending on the water characteristics. In low chlorophyll-*a* waters, the blue/green region of the spectrum is more sensitive to changes in chlorophyll-*a* concentration, whereas the red/NIR region becomes more important in turbid and/or eutrophic waters. In this work we present an approach to manage the shift from blue/green ratios to red/NIR-based chlorophyll-*a* algorithms for optically complex waters. Based on a combined *in situ* data set of coastal and inland waters, measures of overall algorithm uncertainty were roughly equal for two chlorophyll-*a* algorithms—the standard NASA OC4 algorithm based on blue/green bands and a MERIS 3-band algorithm based on red/NIR bands—with RMS error of 0.416 and 0.437 for each in log chlorophyll-*a* units, respectively. However, it is clear that each algorithm performs better at different chlorophyll-*a* ranges. When a blending approach is used based on an optical water type classification, the overall RMS error was reduced to 0.320. Bias and relative error were also reduced when evaluating the blended chlorophyll-*a* product compared to either of the single algorithm products. As a demonstration for ocean color applications, the algorithm blending approach was applied to MERIS imagery over Lake Erie. We also examined the use of this approach in several coastal marine environments, and examined the long-term frequency of the OWTs to MODIS-Aqua imagery over Lake Erie.

1. Introduction

Water quality properties are used as primary indicators for assessing lake and coastal water environmental viability by agencies to guide resource management and public safety decisions. These water quality properties include chlorophyll-*a* concentration, total suspended matter, Secchi depth, and nutrient concentrations, as well as the plant and animal species that inhabit these environments. Of these, chlorophyll-*a* concentration is arguably the most comprehensive environmental descriptor as it a measure of algal biomass and indicator of water clarity. *In situ* sampling remains the most accurate way of determining chlorophyll-*a* concentration, yet the use of satellite remote sensing for routine and synoptic chlorophyll-*a* monitoring has been increasing in the last decade in these types of environments (e.g., Binding, Jerome, Bukata, & Booty, 2010; Hunter, Tyler, Carvalho, Codd, & Maberly, 2010; Kloiber, Brezonik, Olmanson, & Bauer, 2002; Kutser, 2004; Olmanson, Brezonik, & Bauer, 2013; Yacobi et al., 2011).

Historically, the main applications of ocean color satellites and bio-optical algorithms have been directed towards open-ocean conditions. The optical properties of these environments are largely dictated by the concentration of phytoplankton and covarying material in the water, and have been referred to as 'case 1' waters (Morel & Prieur, 1977). Optical models designed to retrieve geophysical properties (e.g., chlorophyll-*a* concentration) in case 1 water have been modeled using the spectral light field in the blue-green part of the spectrum (e.g., Maritorena, Siegel, & Peterson, 2002; O'Reilly et al., 1998). These models begin to break down in environments where the optical properties are governed by materials other than phytoplankton—the so-called 'case 2' waters. Coastal regions and inland waters are highly susceptible to case 2 conditions from land effects (e.g., runoff of sediments, nutrients and organic matter) and re-suspension of sediments from shallow bottoms. In addition, the concentrations of particles including phytoplankton can be much higher compared to open ocean environments. As a consequence, bio-optical algorithms developed for the open ocean are less effective in more optically-complex waters found in coastal and inland waters (Melin et al., 2011; Moore, Campbell, & Dowell, 2009).

The development of bio-optical algorithms for eutrophic conditions more common to lakes and coastal regions has focused on wavelengths in the red and near-infrared (NIR) region of the light spectrum (Gitelson, Gurlin, Moses, & Yacobi, 2011; Gower, King, Borstad, & Brown, 2005; Hu et al., 2010; Matthews, Bernard, & Robertson, 2012;

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Yacobi et al., 2011). These algorithms achieve higher performance in highly eutrophic conditions compared to the open ocean case 1 algorithms (Gilerson et al., 2010), but often times it is not known which algorithm is best suited for a particular place or time in ocean color image scenes that contain both types of optical cases. The iconic case 1/case 2 system view that has predominated the view of aquatic optical classification for the last several decades is actually not an objective classification system, but a way to think about where and when algorithms are appropriate. If, as the evidence suggests, bio-optical algorithms perform better under certain situations and worse at times under different conditions, then a classification scheme is needed that can differentiate the environment and choose the more appropriate algorithm for the given environmental conditions.

Previous studies focused on optical classification of coastal and inland waters for bio-optical algorithm development/selection have been tested in a variety of environments. Melin et al. (2011) utilized a classification scheme that could select and blend type-specific bio-optical algorithms between two water types in the Adriatic Sea. Based on cluster analysis of remote sensing reflectance data, Vantrepotte, Loisel, Dessailly, and Meriaux (2012) showed that optical classes developed from coastal *in situ* data could identify the types in ocean color imagery. In addition, these optical classes could sufficiently represent other coastal areas not included in their data set. Le et al. (2011) developed a bio-optical classification scheme based on data from several lakes in China which could all be considered case 2 waters. Their results showed that optical classes were successful in selecting the best-performing algorithm for given optical case 2 conditions. Lubac and Loisel (2007) and Feng, Campbell, Dowell, and Moore (2005) developed optical classes for case 2 waters in the English Channel and Tokyo Bay, respectively. These studies support the emerging view that optical classes and algorithms vary within coastal and lake environments for waters that could collectively be termed as case 2, and not just between case 1 and case 2 waters.

Observed reflectance spectra from different case 2 waters share common features, as their optics are governed by similar factors including eutrophic/hypereutrophic trophic conditions, high loads of suspended sediments and colored dissolved organic matter (CDOM). Thus, coastal and lake environments may benefit from a common classification scheme using aggregate data that avoids specific regions or separation of fresh and marine waters. We have previously proposed a classification and blending scheme based on *optical water types* (OWTs) for oceanic regional and global scales (Moore, Campbell, & Feng, 2001; Moore et al., 2009). This global OWT system was based on open ocean and coastal waters with low to moderate levels of chlorophyll-*a*, and is not designed for lakes with moderate to extreme values of chlorophyll-*a*. Therefore, we are interested in adapting the application of the OWT method to inland lakes formed from a new data set representative of these types of waters. However, our interest is also to generalize complex optical water types across both coastal and inland water bodies to provide continuity from freshwaters to marine environments.

Our main objective is to 1) describe optical water types for coastal and lake environments which share similar levels of optical complexities, and to provide transition along the continuum of optical conditions between optical environments. Furthermore, we aim 2) to assess the feasibility of an optical classification system for blending the retrievals from multiple bio-optical algorithms for these optically-complex waters. The goal was not to advocate or promote any single algorithm, but to use two existing algorithms as case studies for the proposed classification framework.

2. Methods

To achieve the main goal, we sought to implement a classification system through defining *optical water types* from *in situ* remote sensing reflectance (R_{rs}) measurements covering a wide range of optical conditions in coastal and inland lake waters. This involves identifying the water types, sorting the data into respective subsets, and developing membership functions for the water types. The membership functions are the heart of the classification method, and the class memberships produced are used as the basis of weighting factors for blending algorithm retrievals into a single product when applied to satellite imagery. This process will be detailed in the following Sections.

2.1. Data sets

We assembled an aggregate data set from multiple sources with two requirements: 1) the reflectance measurements must have hyperspectral resolution collected from an above-water or near-surface radiometer, and 2) have co-measured chlorophyll-*a* measurements. These requirements were needed for two reasons: first, we are focused on capturing spectral features throughout the visible spectrum and into the NIR, and therefore need hyperspectral resolution. This also provides flexibility in adapting the derived OWT spectral reflectance characteristics to any satellite-specific band configuration and accommodates the use of existing and planned algorithms. Secondly, the need for reflectances in the red/NIR limits the use of profiling sensors that may not be sensitive enough to resolve the light field when descending through the water column. Additionally, our main interest was in evaluating chlorophyll-*a* products, although the conceptual approach applies to other bio-optical products from other types of algorithms (e.g., semi-analytical).

Several data sets from numerous freshwater lakes and coastal marine sites were combined. They comprise three main sources: a data set collected by the University of New Hampshire (UNH) in various northeastern US lakes as well as the Great Salt Lake in Utah (Bradt, 2012); a data set from Spain covering many lakes and trophic conditions (Ruiz-Verdu, Simis, de Hoyos, Gons, & Pena-Martinez, 2008); and a data set obtained from NASA's SeaBASS archive primarily from U.S. coastal marine sites (Werdell et al., 2003). All reflectance data were collected with hyperspectral instruments, which were binned at 3 nm intervals from 400 to 800 nm. The reflectance data were visually examined individually, and obvious erroneous spectra were not included in the final data set. The total number of reflectance data that passed our inspection with co-measured chlorophyll-*a* data was 488 points (Table 1).

In all cases, we are basing our analysis on the remote sensing reflectance denoted as the vector R_{rs}, which is defined as the ratio of the upwelling spectral light field to the downwelling spectral irradiance. All of our *in situ* data are in the above-water form $R_{rs}(0+)$; that is, it is the remote sensing reflectance just above the air–water interface. In our analyses with optical water types, we have converted the above-water form to below-water form, $R_{rs}(0-)$; that is, the remote sensing reflectance just below the air–sea interface. These two quantities are directly related, and we use the standard NASA conversion from above-water to below-water:

$$R_{rs}(0-) = \frac{R_{rs}(0+)}{0.52 + 1.7 * R_{rs}(0+)} \tag{1}$$

For clarity, the $R_{rs}(0+)$ form is used for all chlorophyll algorithm input.

Table 1
In situ data set summary.

Data set	N	Location	Source
UNH	140	NH lakes, Great Salt Lake	UNH
Spain	179	Assorted Spanish lakes	CEDEX
NASA	169	Coastal marine, U.S.	SeaBASS, NASA