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An algorithm to retrieve chlorophyll, dissolved organic carbon, and suspended minerals from Great Lakes satellite data

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ABSTRACT

An algorithm that utilizes individual lake hydro-optical (HO) models has been developed for the Great Lakes that uses SeaWiFS, MODIS, or MERIS satellite data to estimate concentrations of chlorophyll, dissolved organic carbon, and suspended minerals. The Color Producing Agent Algorithm (CPA-A) uses a specific HO model for each lake. The HO models provide absorption functions for the Color Producing Agents (CPAs) (chlorophyll (chl), colored dissolved organic matter (as dissolved organic carbon, doc), and suspended minerals (sm)) as well as backscatter for the chlorophyll, and suspended mineral parameters. These models were generated using simultaneous optical data collected with in situ measurements of CPAs collected during research cruises in the Great Lakes using regression analysis as well as using specific absorption and backscatter coefficients at specific chl, doc, and sm concentrations. A single average HO model for the Great Lakes was found to generate insufficiently accurate concentrations for Lakes Michigan, Erie, Superior and Huron. These new individual lake retrievals were evaluated with respect to EPA in situ field observations, as well as compared to the widely used OC3 MODIS retrieval. The new algorithm retrievals provided slightly more accurate chl values for Lakes Michigan, Superior, Huron, and Ontario than those obtained using the OC3 approach as well as providing additional concentration information on doc and sm. The CPA-A chl retrieval for Lake Erie is quite robust, producing reliable chl values in the reported EPA concentration ranges. Atmospheric correction approaches were also evaluated in this study.

Introduction

Satellite remote sensing of the Great Lakes has become increasingly important over the past two decades. The Great Lakes account for approximately 20% of the Earth's surface fresh water and supplies drinking water for forty million United States and Canadian people (Van der Leeden et al., 1991). Lakes Michigan and Huron in particular have undergone major changes in lower food web production as witnessed by decreases in average chlorophyll, primary productivity, *Diporeia*, and fish populations (Fahnenstiel et al., 2010a,b; Nalepa et al., 2009). Lake Erie and to a lesser extent Lake Ontario continue to exhibit multiple Harmful Algal Blooms (HABs) each summer (Boyer, 2008; Rinta-Kanto et al., 2005). Remote sensing observations from satellites allow for the synoptic long term monitoring of all the Laurentian Great Lakes to document changes in water quality parameters and primary productivity as a result of the climate, anthropogenic, and invasive species forcing functions.

Only visible radiation penetrates into a water column to any great extent (Jerlov, 1976). As light travels through the water column it interacts with both molecules and particles that comprise the chlorophyll (chl), colored dissolved organic matter (cdom) and inorganic suspended minerals (sm) resulting in alterations of the upwelling radiative flux (Pozdnyakov and Grassel, 2003). Thus the backscattered flux emerging from beneath the water surface contains information about the optical properties of the water column which when observed over time provides insight into the dynamic processes of the Great Lakes (Shuchman et al., 2006).

For the open ocean case, the satellite retrieval of the chlorophyll and other related water quality parameters is straight forward. For example the OC3, OC4 and other algorithms currently used by NASA for the open ocean (Ackleson, 2001; O'Reilly et al., 1998, 2000a) are empirical, visible (blue/green) band ratio techniques. These algorithms are effective due

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to the optical simplicity of the ocean water which is dominated by indigenous phytoplankton and are referred to as Case I waters by Morel and Prieur (1977).

Some waters in the Great Lakes and coastal ocean areas, known as the Morel and Prieur Case II waters, have optical properties that are influenced not only by phytoplankton, but also by inorganic terrigenous particulate matter in suspension (sm) and the colored portion of dissolved organic carbon (doc). In some areas of the Great Lakes and in particular the near shore, bays, river mouths, and areas of concern (AOCs) the content of sm and doc in the water column is abundant enough to compete with the phytoplankton in influencing the resultant composite optical properties, thus creating optically complex water (Bukata et al., 1985; Mortimer, 1988). It is this complexity that impacts the performance of ocean based ratio techniques.

Recent attempts to generate optical algorithms to retrieve chlorophyll concentrations in complex Great Lakes waters are also producing promising results. Binding et al. (2012) have constructed a model that uses both red and near-infrared wavelengths to retrieve both concentrations of chlorophyll and suspended sediments in Lake Erie. This model is unaffected by the presence of cdom which is not only detected in the blue wavelengths but is also sensitive to suspended sediment reflectance in the red wavelengths. Lesht et al. (2013) have modified the blue–green band ratio technique created for use in the open ocean by generating sensor specific coefficients from near simultaneous satellite and field data sets that produce good chlorophyll estimates in the offshore “open” portions of the Great Lakes. While these algorithms show great potential in certain portions of the Great Lakes, a full spectrum algorithm, like the CPA-A, with robust water optical characterization can be implemented for all types of Great Lakes water.

When observing Case II waters from space over the full visible electromagnetic spectrum, it is impractical to retrieve the concentration of a single component like chl without also inferring the content of the other major water constituents determining the overall color, the so called color producing agents (CPAs) (Pozdnyakov et al., 2005). Bukata et al. (1995) determined through simultaneous optical and in situ measurements on Lake Ontario that in the Great Lakes the other two CPAs in addition to chl are cdom and sm. A principal component analysis reported by Shuchman et al. (2006) further confirmed Bukata supposition that chl, cdom, and sm generate the color of the Great lakes observed from space.

Thus, in summary, water color in inland and coastal water results mainly from three different parameters, referred to as CPAs. They include: 1) chlorophyll, chromophoric dissolved organic matter and suspended minerals. Chlorophyll (chl) is the green pigment found in plant cells that are suspended in the water and produce a green-yellow color. Chl not only absorbs light but also contributes to the overall water light scattering through complex interactions as well (Bukata et al., 1995). Dissolved organic carbon is a product micro-organism metabolism and can be produced in situ in the lake or transported from decaying vegetation via rivers and streams. The cdom portion of the doc both absorbs and scatters light, however due to a small number of doc molecules per unit volume compared to the number of water molecules in this unit volume, the cdom contribution to molecular scattering is believed to be negligible (no backscatter component). Suspended minerals (sm) constitute inorganic particles that can both scatter and absorb light.

The Color Producing Agent Algorithm (CPA-A) presented here uses a Levenberg–Marquardt (L–M) multivariate optimization procedure (Levenberg, 1944; Marquardt, 1963) to estimate chl, cdom, and sm based on hydro-optical (HO) models. These HO models were generated using simultaneous near surface optical data collected with in situ water chemistry measurements of the three primary components collected during research cruises in all the Great lakes using multiple regression analysis as well as using specific absorption and backscatter coefficients at specific chl, doc, and sm concentrations. The algorithm is non-satellite specific and the number of spectral bands used is variable depending on application. The algorithm identifies and discards pixels with poor atmospheric correction and/or water optical properties incompatible with the applied HO models. Pixels in optically shallow water (reflected light from the lake bottom) are also discarded during the retrieval process. Unlike the original algorithm used in the previous Lake Michigan Study (Shuchman et al., 2006) the CPA-A algorithm does not use neural net techniques for generation of the initial starting point of the retrieval process.

The cdom reflectance signature recorded from satellite observations is inverted to a doc concentration estimate via the HO model to provide a more meaningful water quality parameter to the user and also to be consistent with the chl and sm concentrations, rather than retrieved band specific cdom absorption. The methodology to derive doc from cdom is discussed in the Hydro-optical model generation and algorithm description section of the paper. Hence throughout this paper doc is presented as one of the three outputs of the CPA-A, but it should be noted that cdom is the constituent actually contributing to the satellite measured water reflectance signature.

Atmospheric correction of satellite data is a very important factor in determining the accuracy of the CPA-A estimates (Land and Haigh, 1997; Ruddick et al., 2000). The challenge over Case II waters is obtaining a highly precise assessment of the path radiance originating from photon interactions with atmospheric aerosols, particularly in the lower troposphere. In Case I waters, typically offshore, the atmospheric aerosols are generally homogeneous throughout the optical path length, dominated by scattering from the aerosols and can be adequately corrected to within 5% (Pozdnyakov et al., 2000a). Because they are generally located near shore or in waters closely bounded by land, the aerosols found over Case II waters are more likely to be influenced by varied continental sources and are no longer uniformly distributed and include both scattering and absorption components. The aerosols come from a number of point and distributed sources often anthropogenic in nature. Atmospheric aerosol correction models that rely on the Near Infrared (NIR) black pixel assumption (Gordon and Clark, 1981) also can fail in some Case II waters where sufficient quantities of CPAs can reflect enough NIR light to violate this assumption. Case II atmospheric correction error, with respect to corrected satellite observed reflectance compared to in situ spectra, can be as high as 15% which can adversely affect the performance of the retrieval algorithms (Pozdnyakov et al., 2000b). Thus, an aspect of this study was to evaluate the recommended suite of atmospheric corrections available to MODIS data users on three Great Lakes data sets where coincident ship based radiometer data was available.

A number of investigators (Budd and Warrington, 2004; Kerfoot et al., 2008; Lesht et al., 2012; Stumpf, 2001) have used OC3 retrievals of chl for Great Lakes investigations with success. These studies which included some limited comparisons with field campaigns show in general that chl retrieval in the open/offshore portions (optically deep) of Lakes Michigan, Huron, Superior and portions of Ontario where the color component observed is dominated by chl can be used to generate meaningful time series. However, Bergmann et al. found that in Lake Michigan there were statistically significant deviations between in situ measured and OC3 modeled chlorophyll concentrations when cryptophytes make up a large percentage (>40%) of the total chlorophyll (Bergmann et al., 2004) indicating potential limitations of ratio based methods to produce accurate chlorophyll retrievals in dynamic phytoplankton regimes. In areas of the Great lakes such as the near shore and bays where the observed color is a result of chl, cdom and sm the OC3 retrieval values are overestimated, a consequence of the band ratio approach assuming a single CPA component, namely phytoplankton (Lohrenz et al., 2008). The high shallow water chl concentrations provided by the OC3 blue–green band ratio technique in the near shore are also exacerbated by reflection off the lake bottom in optically shallow water (D'Sa et al., 2002; Lee et al., 2001). Comparison of standard OC3 retrievals in Lakes Erie and the western basin of Ontario does not consistently compare well with in situ observations (Witter et al., 2009) again due to the fact that all