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Normalized difference chlorophyll index: A novel model for remote estimation of chlorophyll-*a* concentration in turbid productive waters

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ABSTRACT

We propose a normalized difference chlorophyll index (NDCI) to predict chlorophyll-a (chl-*a*) concentration from remote sensing data in estuarine and coastal turbid productive (case 2) waters. NDCI calibration and validation results derived from simulated and MEdium Resolution Imaging Spectrometer (MERIS) datasets show its potential application to widely varying water types and geographic regions. A quadratic function ($R^2 = 0.95$, $p < 0.0001$) accurately explained the variance in the simulated data for a chl-*a* range of 1–60 mg m^{-3}. Similarly a twofold calibration and validation of chl-*a* models using MERIS dataset, (chl-*a* range: 0.9–28.1 mg m^{-3}) yielded R^2 of 0.9, and RMSE of ~2 mg m^{-3} respectively. NDCI was applied on images over the Chesapeake Bay and Delaware Bay, the Mobile Bay, and the Mississippi River delta region in the northern Gulf of Mexico. The newly developed algorithm was successful in predicting chl-*a* concentration with approximately 12% overall bias for all above study regions. Findings from this research imply that NDCI can be successfully used on MERIS images to quantitatively monitor chl-*a* in inland coastal and estuarine waters. In case of remote coastal waters with no ground truth data, NDCI can be used to detect algal bloom and qualitatively infer chl-*a* concentration ranges very similar to NDVI's application in terrestrial vegetation studies.

1. Introduction

Accurate remote estimation of biophysical parameters such as chlorophyll-*a* (chl-*a*) and phytoplankton biomass in turbid productive waters is essential for large-scale and multi-temporal studies related to primary production, carbon cycle, biogeochemical cycles, and overall inland and coastal water quality. However, it is still a challenge because of the presence of non-covarying optically active constituents whose absorption features overlap with chl-*a*. Spectral channels in the blue-green part of the electromagnetic spectrum are heavily affected by the presence of constituents such as Colored Dissolved Organic Matter (CDOM), detritus, and tripton. Empirical algorithms (e.g., OC4v4) that use blue and green spectral channels often provide a relatively accurate estimate of chl-*a* in case 1 waters where the total non-water absorption is dominated by phytoplankton, however, do not provide reasonable estimates of chl-*a* in turbid productive waters (O'Reilly et al., 1998). In order to reduce the estimation error of chl-*a* in turbid productive waters, semi-analytical models have also been proposed (Gons et al., 2002; Maritorena et al., 2002). However, the success of these semi-analytical models depends on the accurate parameterization of the inherent optical properties of the medium that often poses a considerable challenge. Magnuson et al. (2004) re-parameterized the original semi-analytical model proposed by Maritorena et al. (2002) to make it suitable for the Chesapeake Bay and Mid-Atlantic Bight region. They reported that the re-parameterized model was successful in attributing CDOM absorption in the total absorption budget and offered accurate estimation when compared to OC4v4 model and the accuracy of chl-*a* estimation was within 30–50% of the in situ measured values. Even though the re-parameterized semi analytical model produced better accuracy than OC4v4, the uncertainty was still very high. Because of the difficulties in obtaining the information for re-parameterization, such as specific absorption coefficient of phytoplankton, $a_{ph}^*(\lambda)$, spectral slope of colored dissolved organic matter, S_{CDOM}, and spectral slope of detritus, $S_{detritus}$, alternative approaches have been encouraged to improve chl-*a* estimation in turbid productive waters. Over the past years numerous algorithms have been proposed to quantify chl-*a* in turbid productive waters using red-near infrared (NIR) bands and these algorithms can be classified into three primary groups such as 1) two-band empirical (Moses et al., 2009; Tzortziou et al., 2007), 2) three or four-band empirical (Dall'Olmo & Gitelson, 2005; Le et al., 2009), and 3) three-band semi-analytical (Gons, 1999; Gons et al., 2002) models. In this study, we have assessed the accuracy of red and NIR based empirical and semi-analytical algorithms in geographically diverse water bodies and propose a novel band difference algorithm for accurately mapping chl-*a* concentration in turbid productive waters.

We have selected four algorithms from the list above for further validation and examination of their performance and transferability to different water bodies. The selected algorithms discussed below are widely applied and unique in their band architecture.

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Moses et al. (2009) presented a two-band model (hereafter M09) using red and NIR bands to quantify chl-*a* in turbid productive waters. To match the band configuration of MERIS sensor, the conceptual model was designed as:

$$C_{chl-a} \propto R_{rs}^{-1}(665) \times R_{rs}(708) \tag{1}$$

They applied M09 on MERIS images over Azov Sea, Russia and reported the high accuracy potential of the model to estimate chl-*a* in turbid productive waters. Similarly, Tzortziou et al. (2007) collected an extensive bio-optical dataset to examine the relationship between inherent and apparent optical properties in the mid Chesapeake Bay, USA. They observed a better relationship ($R^2 = 0.54$) between remote sensing reflectance (R_{rs}) ratio at 677 and 554 nm, $R_{rs}(677)/R_{rs}(554)$, and chl-*a* concentration in the bay compared to blue-green spectral band ratios. In this study we have modified this ratio based on the MERIS band configuration, $R_{rs}(665)/R_{rs}(559)$ and named it T07 for further reference.

$$C_{chl-a} \propto R_{rs}^{-1}(559) \times R_{rs}(665) \tag{2}$$

Dall'Olmo and Gitelson (2005) (hereafter D05) presented a three-band model using red and NIR bands. The three-band model architecture was as follows:

$$C_{chl-a} \propto \left[R_{rs}^{-1}(665) - R_{rs}^{-1}(708)\right] \times R_{rs}(753) \tag{3}$$

The three band algorithm was based on several assumptions including, (i) the absorption by suspended solids and CDOM beyond 700 nm is approximately equal to that at 665–675 nm and the difference between them is very small and can be neglected, (ii) the total chl-*a*, CDOM, and total suspended sediment (TSS) absorption beyond 730 nm is nearly zero, and (iii) back-scattering coefficient of chl-*a* is spectrally invariant. They reported that D05 was successful to predict accurate estimate of chl-*a* in turbid productive water bodies with wide range of optical complexity. Moses et al.(2009) further validated D05 using MERIS data from the Azov Sea and documented that D05 was able to retrieve chl-*a* concentration with a RMSE of 5.02 mg m^{-3} (for a chl-*a* range: 18.37–47.86 mg m^{-3}).

Gons et al. (2008) presented a semi-analytical algorithm (hereafter G08) for chl-*a* retrieval using MERIS data which was a modification of the parent algorithm (Gons, 1999). G08 uses the relationship between inherent optical properties and the R_{rs} at three wavelengths, solves for chl-*a* absorption at 665 nm, and estimates chl-*a* by dividing a_{chl} (665) by the specific absorption coefficient of chl-*a*, $a_{chl-a}{}^{*}(665)$.

$$[Chl-a] = \left\{\left[\frac{R_{rs}(708.75)}{R_{rs}(665)}\right] * (0.70 + b_b) - 0.40 - b_b^{1.06}\right\}/0.016 \tag{4}$$

where b_b is the back-scattering coefficient and was expressed as:

$$b_b = \frac{1.61 * R_{rs}(775)}{0.082 - 0.6 * R_{rs}(775)}$$

Gons et al. (2008) reported that G08 successfully retrieved chl-*a* concentration in the Laurentian great lakes producing residuals less than 35% of the measured values. They also reported that G08 did not perform well in areas with chl-*a* less than 5 mg m^{-3} and even produced some negative values in oligotrophic waters.

Although, the three-band algorithms, D05 and G08, have excellent predictive ability, the biggest challenge of these models is that they require R_{rs} measurements at 753 and 775 nm. Based on existing atmospheric correction schemes for turbid productive waters, getting reliable estimates of R_{rs} at these wavelengths is a difficult task. In addition, another inherent difficulty of semi-analytical models such as G08 is the use of $a_{chl-a}{}^{*}(665)$. Any uncertainty associated with $a_{chl-a}{}^{*}(665)$ can contribute to inaccurate estimates of chl-*a*.

After carefully examining the strengths and weaknesses of the above models, our goal in this research was to develop an algorithm that can perform better than the existing algorithms. Two of the most important criteria for a successful spectral algorithm development include (1) applicability to satellite data, and (2) transferability to widely varying geographic regions without producing significant uncertainties. We have tested and analyzed both criteria in this study as part of the model validation. We propose a novel index, Normalized Difference Chlorophyll Index (NDCI), and demonstrate its sensitivity to chl-*a* concentration in turbid productive waters. We have calibrated and validated a chl-*a* model using NDCI by analyzing four datasets (one simulated and three field datasets) representing unique turbid productive water bodies and presented its potential use for chl-*a* estimation in optically complex waters. The purpose of using a simulated data was to test the model performance and sensitivity to a wide range of optical parameters in the water.

NDCI uses R_{rs} at 665 nm, $R_{rs}(665)$, and 708 nm, $R_{rs}(708)$, emulating the Medium Resolution Imaging Spectrometer (MERIS) channels. Similar to other turbid productive chl-*a* algorithms, this index uses the information from the reflectance peak centered at 700 nm which is maximally sensitive to the variations in chl-*a* concentration in water. Similarly, a wide spectral absorption peak between 665 nm and 675 nm is generally assigned to the absorption by chl-*a* pigments. We selected the two spectral features centered at 665 nm and 708 nm to develop NDCI and to avoid the confounding influence of CDOM and TSS on the water reflectance spectra at shorter wavelengths. Also, as both bands are closely located, we assume that the CDOM and TSS absorption is similar in magnitude. Based on the results from bio-optical modeling in this study, the combined range of CDOM and TSS absorptions at 665 nm (0.0193–0.1899 m^{-1}) and 708 nm (0.015–0.1603 m^{-1}) in the study regions are approximately equal and the difference between them can be assumed as negligible. Further, following the simplistic concept of normalized difference vegetation index (NDVI) applied in vegetation status monitoring; NDCI was developed by taking the spectral band difference at 708 nm and 665 nm and normalizing by the sum of their reflectance to eliminate any uncertainties in the estimation of R_{rs}, seasonal solar azimuth differences, and atmospheric contributions at those wavelengths. NDCI is formulated as:

$$C_{chl-a} \propto \frac{[R_{rs}(708) - R_{rs}(665)]}{[R_{rs}(708) + R_{rs}(665)]} \tag{5}$$

The overarching objective of this research was to improve the accuracy of chl-*a* retrieval in turbid productive waters using a simple, easy to implement, intuitive (such as NDVI for vegetation), and universal model. Throughout this paper, we have tested these criteria using several steps including, (1) developing a dataset simulating a wide range of bio-optical parameters to examine the conceptual model, (2) testing the model using an in situ dataset collected from a global bio-optical data archive and corresponding MERIS data, (3) evaluating the performance of several existing chl-*a* algorithms for turbid productive waters using the simulated and remotely sensed datasets, (4) applying the model in three unique study regions, such as Chesapeake-Delaware Bay, the Mississippi River Delta, and the Mobile Bay, and (5) finally and most importantly, developing a generalized but practical relationship between NDCI values and chl-*a* range in an attempt to make NDCI intuitive and applicable when/where ground truth data is not available.

2. Data and methods

2.1. Bio-optical modeling

The simulated R_{rs} spectra used for the model conception, calibration, and validation were approximated by the following method.