Bio-optical water quality dynamics observed from MERIS in Pensacola Bay, Florida

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Abstract: Observed bio-optical water quality data collected from 2009 to 2011 in Pensacola Bay, Florida were used to develop empirical remote sensing retrieval algorithms for chlorophyll a (Chla), colored dissolved organic matter (CDOM), and suspended particulate matter (SPM). Time-series of the three bio-optical water quality variables were generated from MEdium Resolution Imaging Spectrometer (MERIS) observations from 2003 to 2011. Bio-optical water quality in this estuary exhibited spatial and temporal variations that were correlated to river discharge and wind. Both annual mean and monthly mean bio-optical water quality variables were positively correlated to river discharge. Monthly mean bio-optical water quality variables were also positively correlated to wind speed and wind density (defined by the number of days with daily mean wind speed $> 3 \text{ m s}^{-1}$ in a month) over this estuary. These results indicate that bio-optical water quality dynamics in this estuary are vulnerable to changes in river discharge and river constituent loads and local weather conditions such as winter storms and hurricanes.

Key words: Bio-optical water quality, estuary, remote sensing, MERIS, Pensacola Bay

1. Introduction

Light in the water column is attenuated by phytoplankton, suspended particulate matter (SPM), and colored dissolved organic matter (CDOM). Thus, bio-optical water quality properties in estuaries are often described by concentrations of chlorophyll a (Chla), CDOM, and SPM. For example, many estuaries bordering the Gulf of Mexico are river-dominated and receive large inputs of freshwater, nutrients, dissolved and particulate organic matter, and contaminants from adjacent watersheds (Bianchi et al. 1997). These inputs can increase the water turbidity (Kirk et al., 1994), and contribute to decline in ecosystem health, such as loss of seagrass and increased occurrence of bottom-water hypoxia (US EPA 2001; Hagy and Murrell, 2007; Lewis et al., 2008; Tomasko et al., 2005). Therefore, effective management of estuarine ecosystems requires accurate knowledge of bio-optical water quality constituents and an understanding of the factors affecting their variation. However, knowledge of bio-optical water quality variations and their driving factors is often limited by incomplete or non-existent long-term bio-optical water quality records (Bricker et al. 2007).

Satellite remote sensing provides a powerful tool to observe physical and biological processes in the open oceans (Behrenfeld et al., 2001), however, its application in estuaries has

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4 been challenging due to the complex optical properties encountered (IOCCG, 2000). For
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6 example, the default blue-green band ratio algorithms such as OC3 for MODIS (Moderate
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8 Resolution Imaging Spectroradiometer) and OC4 for SeaWiFS (Sea-viewing Wide Field-of-view
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10 Sensor) generate high uncertainties in Chla estimates for coastal and estuarine waters because
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12 optical properties in these waters are dominated by CDOM or SPM (Gitelson et al., 2007; Le et
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14 al., 2013a; Werdell et al., 2009). Thus, different empirical algorithms have been developed for
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16 estuaries to retrieve Chla from MODIS and SeaWiFS using red-green or red-blue band ratio
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18 (Stumpf et al., 2003; Pan et al., 2009; Chen et al., 2007; Le et al., 2013b). In addition, other
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20 empirical algorithms, such as LUT (look-up table)-based algorithms (Lee et al., 1996; Liu &
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22 Miller, 2008), PCA (principal component analysis)-based algorithms (Fischer, 1985; Doerffer &
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24 Schiller, 1998), and band-ratio algorithms (D'Sa & Miller, 2003; Doxaran et al., 2005;
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26 Kowalczyk et al., 2005; Mannino et al., 2008; Tiwari & Shanmugam, 2011; Long & Pavelsky,
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28 2013 and references therein), have been developed to retrieve CDOM or SPM from satellite
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30 observations for coastal and estuarine waters.

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32 The Medium Resolution Imaging Spectrometer (MERIS) provided imagery from 2002 to
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34 2012 with moderate spatial resolution of 300-m and 15 spectral bands in the visible-NIR regions,
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36 which facilitates its potential use in small estuaries (Bézy et al., 2000). In addition, it has a
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38 channel centered at 709 nm for resolving constituents in optically complex waters. Numerous
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40 algorithms have been developed for MERIS to retrieve Chla for coastal, estuarine and inland
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42 waters. These algorithms include band-ratio (Gurlin et al., 2011; Matthews et al., 2010), three-
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44 band algorithm (Gitelson et al., 2008), neural network algorithm (Vilas et al., 2011), synthetic
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46 chlorophyll index (SCI) (Shen et al., 2010), and Maximum Chlorophyll Index (MCI) (Gower et
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48 al., 2005). The band-ratio algorithm may be the best application for MERIS imagery in different
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50 estuaries or lakes at present because of its simplicity and generally robust performance (Gurlin et
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52 al., 2011; Le et al., 2013c, Matthews et al., 2010). With regards to CDOM and SPM, few studies
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54 have evaluated the applicability of MERIS in estuaries. Thus, reliable, general-purpose retrieval
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56 algorithms for bio-optical water quality estimates from MERIS are still unavailable.

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58 Therefore, the purposes of this study were to (1) develop empirical algorithms to derive
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60 bio-optical water quality variables from MERIS, and (2) investigate their dynamics and their
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62 potential driving factors in Pensacola Bay, Florida. Herein, we first, characterize observed
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optical properties in Pensacola Bay. Next, empirical algorithms for bio-optical water quality variables were calibrated and validated using observed data and concurrent MERIS images. Then, nine-year time-series of bio-optical water quality variables were constructed, and their variations were investigated spatially and temporally relative to watershed and climate forcing. Finally, the implication of this work in estuarine environmental management is discussed.

2. Study area

Pensacola Bay is located in the northeast Gulf of Mexico, and is a river-dominated system of moderate size (370 km²), shallow depth (mean 3.4 m) and low tidal energy (Schroeder and Wiseman, 1999). Pensacola Bay is further divided into the Escambia Bay, East Bay, and the Lower Bay area that exchanges with the Gulf of Mexico through a narrow deep pass (Figure 1, Hagy and Murrell, 2007). Four main rivers flow into Pensacola Bay. The Escambia River flows into Escambia Bay, and the Blackwater River, Yellow River, and Big Coldwater Creek flow into East Bay. This estuary has moderate rates of primary production (~290 g cm⁻² y⁻¹) and is strongly influenced by seasonal and episodic freshwater flows (Hagy et al., 2006; Murrell et al., 2007). Seagrass coverage has declined and bottom-water hypoxia is frequent in this system (USEPA 2005; Hagy and Murrell, 2007). Approximately 43% seagrass coverage was lost from 1993 to 2003, and the seasonal hypoxia affects as much as 25% of the bottom area of the estuary (Lewis et al., 2008). Thus, knowledge of the bio-optical water quality dynamics and their influencing factors is very important for water quality management in this estuary.

3. Datasets and Methods

3.1 Observed bio-optical water quality

Surface (< 0.5 m depth) water samples (n=161) were collected approximately every two months from 15 stations in Pensacola Bay from September 2009 to December 2011 (Figure 1). Samples were processed on the day of collection using methods described by Mueller et al (2003). Bio-optical water quality and optical variables including Chla (mg m⁻³), SPM (mg L⁻¹), and light absorption from particles (a_p , m⁻¹), non-algal detrital particles (a_d , m⁻¹), phytoplankton (a_{ph} , m⁻¹), and CDOM (a_g , m⁻¹), were analyzed. Phytoplankton pigments were extracted with hot methanol and analyzed with a fluorometer to determine Chla concentration (Holm-Hansen and Riemann, 1978). SPM was determined gravimetrically. Samples were filtered through pre-

weighed and pre-combusted Whatman GF/F filters (550 °C for 4 h) and then dried (105 °C for 4 h) and weighted to obtain SPM. Spectra of absorption from particles ($a_p(\lambda)$) and non-algal detrital particles ($a_d(\lambda)$) were determined using the quantitative filter technique measured on a spectrophotometer (Kiefer and SooHoo, 1982). Phytoplankton absorption ($a_{ph}(\lambda)$) was calculated as the difference between $a_p(\lambda)$ and $a_d(\lambda)$. CDOM absorption ($a_g(\lambda)$) was measured from filtered seawater (0.7 μm nominal pore size) using a dual-beam spectrophotometer with 10-cm quartz cells. Spectra were normalized by subtracting from each wavelength the measured value at 700 nm CDOM absorption coefficient $a_g(\lambda)$ (Pegau et al., 2003). Absorption coefficients were calculated using:

$$a_g(\lambda) = 2.303/l \text{ } [[OD_s(\lambda) - OD_{bs}(\lambda)] - OD_{null}] \quad (1)$$

$$a_p(\lambda) = 2.303 A_f / \beta V_f \text{ } [[OD_{fp}(\lambda) - OD_{bf}(\lambda)] - OD_{null}] \quad (2)$$

where l (m) is the cuvette path length, $OD_s(\lambda)$ is the optical density of the filtrate sample, $OD_{bs}(\lambda)$ is optical density of a purified water blank, and OD_{null} is the apparent residual optical density where absorption is assumed to be zero. V_f is the volume of water filtered, A_f is the clearance area of the filter, $OD_{fp}(\lambda)$ is the optical density of the filter sample, $OD_{bf}(\lambda)$ is the optical density of the blank.

Remote sensing reflectance (Rrs) was derived using a hyperspectral surface acquisition system (HyperSAS, Satlantic Inc., Halifax, Nova Scotia). The HyperSAS logged spectral measurements of above-water radiance ($L_t(\lambda)$), sky radiance ($L_i(\lambda)$), and downwelling sky irradiance ($E_s(\lambda)$) from 350–800 nm (interpolated at 1 nm intervals). HyperSAS radiance sensors were mounted on the port side of the pilot house roof of a 25 ft boat to provide 40° nadir and zenith viewing angles (Mobley, 1999). During data acquisition, the boat was positioned so the radiance sensors were perpendicular to the sun's azimuth and to avoid boat shadow and wake. The irradiance sensor was mounted above the deck canopy for an unobstructed view of the sky. The HyperSAS above water Rrs spectra were corrected, following the surface correction algorithm of Gould et al. (2001), using the average absorption at 412 nm and derived spectral scattering shape (Gould et al. 1999). Only data collected on days without clouds and wind speed

less than 3 m s^{-1} were used to develop bio-optical water quality retrieval algorithms. Briefly, $R_{rs}(\lambda)$ was derived as:

$$R_r(\lambda) = R_{sky}(\lambda) * A + B \quad (3)$$

$$R_{rs}(\lambda) = R_t(\lambda) - R_r(\lambda) \quad (4)$$

where $R_{sky}(\lambda) * A$ accounts for the reflected sky light and the B term accounts for sunglint and reflected light. A p value is calculated (A) rather than assumed equal to Fresnel reflectance, and a residual offset is calculated (B). R_{rs} is calculated as the difference between $R_t(\lambda) = (L_t(\lambda) / E_s(\lambda))$ and R_r .

An AC-s (WET-Labs, Philomath, OR) was used to measure *in situ* vertical profiles of absorption (a) and beam attenuation (c) from 400-735 nm interpolated at 1 nm intervals. Temperature and salinity corrections were applied to the AC-s data using concurrent Seabird CTD vertical profile data (Sullivan et al. 2006). The AC-s a, c, and derived scatter coefficient (b) values were averaged over the surface of the water column to the secchi depth for use in deriving R_{rs}

3.2 Satellite data

Daily MERIS level-2 data for the period of January 2003–April 2012 were downloaded from the NASA GSFC website (<http://oceancolor.gsfc.nasa.gov/>). The 300m resolution data products included the spectral remote sensing reflectance, $R_{rs}(\lambda)$, in every spectral band, and various quality control flags (e.g., clouds, atmospheric correction warning, stray light, etc). $R_{rs}(\lambda)$ were extracted for locations and times that matched bio-optical water quality observations using computer routines written in the Interactive Data Language (IDL). The extracted $R_{rs}(\lambda)$ data were used to validate bio-optical water quality algorithms developed from field observation dataset, while the full nine-year $R_{rs}(\lambda)$ dataset was used to develop bio-optical water quality time-series from January 2003 to December 2011. During observation-satellite data matching, a time window of ± 1 d, and a median value from a 3×3 pixel box centered at the observation site was used to filter satellite sensor and algorithm noise. MERIS images were used for comparison with observed data if each 3×3 filter box contained at least four pixels after removal of quality control flags and the coefficient of variation (CV) was less than 0.4 (Le et al., 2013b). Pixels

over water of depth < 2m were masked to reduce issues arising from bottom reflectance (Chen et al., 2007).

3.3 Environmental data

Daily river discharge data were downloaded from the United States Geological Survey National Water Information System (USGS NWIS) for the period January 2003 to December 2011. River discharge data were retrieved from four USGS sites: Escambia River (USGS 02376033), Yellow River (USGS 02369600), Blackwater River (USGS 02370000), and Big Coldwater Creek (USGS 02370550). Monthly mean river discharge was calculated from the daily river discharge. Hourly wind speed data (January 2003–December 2011) were obtained from a National Oceanic Atmospheric Administration (NOAA) Pensacola Bay physical oceanographic real-time (PORT) station (30°24.2'N, 87°12.6'W). Hourly wind speed data were converted into daily and monthly means to identify the effects of wind on bio-optical water quality dynamics.

3.4 Algorithm development and data analysis

We separated the *in situ* dataset into two groups. One group without concurrent images was used for algorithm calibration, the other group with concurrent images was used for algorithm validation. Only observed Rrs wavelengths corresponding to MERIS bands were used. To reduce the contamination of the Chla signal by CDOM and non-algal detrital particles, the NIR-red band ratio (Rrs(709)/Rrs(665)) was used to calibrate the Chla retrieval algorithm. For CDOM, the NIR-green band ratio (Rrs(709)/Rrs(510)) was used to reduce the uncertainty from atmospheric correction at blue bands (i.e. 443 nm, 490 nm) and the effect from phytoplankton at red bands (i.e., 665 nm, 681 nm). For SPM, we tested different band ratios, and found that Rrs(709)/Rrs(681) had the best fit with SPM.

The accuracy of these algorithms were evaluated using average percent difference (APD) as an indicator of bias, relative root mean square error (*r*RMSE) as an indicator of accuracy, and the average unsigned percent difference (AUPD) as an indicator of total uncertainty (Zibordi et al. 2006). APD, *r*RMSE, and AUPD were calculated as

$$APD = \frac{1}{N} \cdot \sum_{i=1}^N \left(\frac{y_i - x_i}{x_i} \cdot 100\% \right) \quad (5)$$

$$rRMSE = \sqrt{\frac{1}{N} \cdot \sum_{i=1}^N \left(\frac{y_i - x_i}{x_i} \right)^2} * 100\% \quad (6)$$

$$AUPD = \frac{1}{N} \cdot \sum_{i=1}^N \left| \frac{y_i - x_i}{x_i} \right| \cdot 100\% \quad (7)$$

where x_i represents measured data, y_i represents derived data, and N is the number of samples.

The generated algorithms were applied to daily MERIS Rrs to create mean monthly and annual composites. To simplify the spatial and temporal analysis of the MERIS generated bio-optical water quality data, the data were averaged for East Bay, Escambia Bay, and Lower Bay (Figure 1). Monthly mean bio-optical water quality variables were calculated using all the pixels in each bay segment. To analyze potential influencing factors, Pearson correlation coefficients (r) for the annual and monthly bio-optical water quality time-series and the environmental forcing data (discharge and wind) were calculated in Matlab (Mathworks 2013a). Differences in spatial and temporal patterns were tested by ANOVA. Further, stepwise regression was used to detect the significant factors affecting bio-optical water quality variations in the three bay segments. All statistical analyses were judged significant at $\alpha = 0.05$.

4. Results

4.1 Variation of observed bio-optical water quality and optical properties

Observed bio-optical water quality and optical properties in Pensacola Bay exhibited spatial variations between bay areas and sample stations. Overall, Chla ranged from 1.1 mg m⁻³ to 28.0 mg m⁻³, with a mean ($\pm$ standard deviation) value of 5.5 $\pm$ 3.6 mg m⁻³. The highest Chla occurred at station PB02 in July 2011, the lowest value occurred at station PB09 in December 2011. SPM ranged from 0.5 mg L⁻¹ to 19.3 mg L⁻¹, with a mean value of 4.0 $\pm$ 2.6 mg L⁻¹. The highest SPM was observed at station PB13 in June 2010, and the lowest SPM was observed at station PB11 in May 2011. Escambia Bay had the highest mean Chla and SPM, whereas the Lower Bay had the lowest mean Chla and SPM (Table 1). Due to variation of bio-optical water quality, optical properties also presented spatial variation in this estuary. Escambia Bay had the highest $a_{ph}(443)$ (0.81 $\pm$ 0.29 m⁻¹) and $a_d(443)$ (0.30 $\pm$ 0.14 m⁻¹), followed by East Bay. The Lower Bay had the lowest $a_{ph}(443)$ (0.24 $\pm$ 0.14 m⁻¹) and $a_d(443)$ (0.20 $\pm$ 0.07 m⁻¹). For $a_g(443)$, East Bay had the highest $a_g(443)$ (1.5 $\pm$ 1.11 m⁻¹), followed by Escambia Bay, the Lower Bay had the

lowest $a_g(443)$ ($0.79 \pm 0.65 \text{ m}^{-1}$). However, except for SPM and $a_d(443)$, no significant difference in bio-optical water quality and optical properties was found in the three bay segments (Table 1).

The three bay segments had similar absorption budgets and $R_{rs}(\lambda)$ spectrums (Figure 2). CDOM dominated absorption in blue and green wavelengths. At 443 nm and 550 nm, CDOM contributed ~60% to the total absorption (without pure water absorption), whereas, non-algal detrital particles contributed ~30% and phytoplankton contributed ~10% to the total absorption. Phytoplankton dominated absorption in red wavelengths. At 670 nm, phytoplankton pigments absorption had average contribution of ~55% to total absorption, whereas, CDOM and detrital particles contributed ~20% and ~25% to total absorption, respectively. R_{rs} in the three bay segments had similar spectral characteristics. A large R_{rs} peak around 570 nm was observed due to the relatively low phytoplankton absorption and high backscatter from suspended sediments. A local absorption peak from phytoplankton caused the low reflectance around 670 nm. The distinct reflectance peak around 690 nm is the result of minima total absorption from water constituents and pure water, as well as the effect of chlorophyll fluorescence.

4.2 Algorithm performance and MERIS-derived bio-optical water quality time-series variation

Figure 3 presents the relationships between bio-optical water quality and R_{rs} band ratios from the observed dataset, as well as the comparison of measured and MERIS-derived bio-optical water quality variables. Strong relationships were yielded between band ratios and measured bio-optical water quality variables, with $R^2 > 0.7$ for the best fit of power functions (Figure 3 a&c&e). These algorithms had decent performance on satellite images. The NIR-red band ratio Chla algorithm yielded APD=11.6%, AUPD = 30.8%, and $rRMSE$ = 42.6% (Figure 3b) from concurrent MERIS images. The MERIS CDOM algorithm yielded APD = -10.9%, AUPD=20.1%, and $rRMSE$ = 25.0%, (Figure 3d). The SPM algorithm yielded APD = 25.4%, AUPD=49.8%, and $rRMSE$ = 58.2% (Figure 3f). These algorithms were subsequently applied to available MERIS images to derive bio-optical water quality variables and generate their time-series for Pensacola Bay.

Figures 4-6 show the MERIS-derived bio-optical water quality in Pensacola Bay. Spatial and temporal variations were apparent for Chla, CDOM, and SPM in annual mean distribution. Spatially, annual mean bio-optical water quality in upper bay segments was always higher than

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4 in lower bay segments. The highest mean Chla occurred near the river mouth, with mean > 12
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6 mg m^{-3} , decreasing to $\sim 6 \text{ mg m}^{-3}$ in the Lower Bay (Figure 4). A similar spatial pattern occurred
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8 with CDOM (Figure 5), decreasing from $\sim 2.0 \text{ m}^{-1}$ near the river month to $< 1.0 \text{ m}^{-1}$ in the Lower
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10 Bay. SPM exhibited similar but less spatial variation in this estuary, decreasing from $\sim 6.0 \text{ mg}$
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12 L^{-1} near the river mouth to $\sim 4 \text{ mg L}^{-1}$ in the Lower Bay (Figure 6). Annually, water quality in
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14 2003, 2004, and 2009 is obviously higher than in other years, the lowest water quality is
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16 occurred in 2011.

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18 The monthly mean bio-optical water quality time-series also showed clear spatial and
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20 temporal variability (Figure 7). Data gaps were apparent in the MERIS-derived time-series due
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22 to seasonal cloud cover mainly during spring and summer. The highest monthly mean Chla
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24 occurred in East Bay in October 2007, with a value of 17.1 mg m^{-3} . The lowest monthly mean
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26 Chla occurred in the Lower Bay in December 2007, with a value of 1.9 mg m^{-3} . CDOM had
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28 similar spatial and temporal variations with Chla. The highest monthly mean CDOM occurred in
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30 the Escambia Bay in March 2003, with a value of 2.7 m^{-1} . The lowest monthly mean CDOM
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32 occurred in the Lower Bay in December, 2007, with a value of 0.23 m^{-1} . The highest monthly
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34 mean SPM occurred in February 2010, with a value of 8.5 mg L^{-1} in the East Bay, and the lowest
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36 monthly mean SPM occurred in December 2007, with a value of 0.11 mg L^{-1} in the Lower Bay.
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38 Temporally, bio-optical water quality variables in winter and spring were always higher than in
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40 summer and fall months.

41 4.3 Relation of MERIS-derived bio-optical water quality with discharge and wind

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43 Monthly means and annual means of bio-optical water quality variables by bay segment
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45 were analyzed for correlations with river discharge and wind. Note that the monthly mean river
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47 discharge without available satellite data (e.g. May 2003) were not included to calculate annual
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49 mean river discharge. Monthly mean bio-optical water quality variables in the three bay
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51 segments were significantly correlated to river discharge (Table 2). Monthly mean Chla had
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53 strong correlations with river discharge in East Bay ($r = 0.66$, $p < 0.01$, $N=78$), and Escambia Bay
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55 ($r = 0.52$, $p < 0.01$, $N=78$). Chla in the Lower Bay had a weaker correlation with Escambia River
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57 discharge ($r=0.25$, $p=0.02$, $N=78$). A significant correlation was not observed between Chla in
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59 the Lower Bay and the river discharge flowing into East Bay. Monthly mean CDOM had the
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61 strongest correlation with river discharge, with $r \geq 0.69$ ($p < 0.01$, $N=78$) in the three bay
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segments. Monthly mean SPM had the $r = 0.56$ ($p < 0.01$, $N=78$), 0.52 ($p < 0.01$, $N=78$), and 0.38 ($p < 0.01$, $N=78$) for the correlations with river discharge in East Bay, Escambia Bay, and Lower Bay, respectively. Annually, bio-optical water quality variations were also significantly correlated to river discharge in the three bay segments (Figure 8).

Bio-optical water quality variations were also correlated to wind in this estuary. Monthly mean Chla, CDOM and SPM in East Bay and Escambia Bay were significantly correlated to wind speed (Table 2). They were also significantly correlated to wind density (number of days with daily wind speed > 3 m/s in a month) in Escambia Bay ($r > 0.29$, $p = 0.01$, $N=78$) and East Bay ($r = 0.27$, $p = 0.016$, $N=78$). Except CDOM ($r > 0.26$, $p < 0.023$, $N=78$), bio-optical water quality variables had no significant correlation with wind (i.e. wind speed and wind density) in the Lower Bay. No significant correlation was found for annual mean bio-optical water quality variables and wind in the three bay segments. Table 3 shows the stepwise regression using river discharge and wind to predict bio-optical water quality in Pensacola Bay. It reveals that river discharge and wind density were the two significant factors in the East Bay to influence bio-optical water quality variation, but in the Lower Bay, only river discharge significantly influenced the bio-optical water quality variation. In Escambia Bay, Chla variation was related to river discharge and wind density, CDOM variation was related to river discharge and wind speed, and SPM was only significantly affected by river discharge.

5. Discussion

5.1 Algorithm performance

Accurate estimation of bio-optical water quality from satellite observations in estuaries has been notoriously difficult due to the optical complexity of these waters and dynamic behavior of optical properties. In most estuarine waters, optical properties are often dominated by CDOM or detrital particles in the blue band, which results in high uncertainty from blue-green band ratio algorithms. Thus, the default algorithms developed for open oceans (i.e., OC3 and OC4) are not applicable in Pensacola Bay to retrieve bio-optical water quality. Another challenge using reflectance in the blue band for algorithm development is the presence of artifacts from atmospheric correction (Son and Wang, 2012). Thus, alternative empirical algorithms using the red/green or NIR/red band ratios were developed for estuarine waters to

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4 retrieve Chla. However, the red/green band ratio may only be appropriate for use in estuaries
5 where total absorptions at green and red wavelengths are related to Chla, such as in Tampa Bay
6 and Chesapeake Bay (Le et al., 2013b, Tzortziou et al., 2007); the NIR/red band ratio algorithm
7 may not be applicable to MODIS or SeaWiFS imagery because of low signal-noise ratios at their
8 NIR band (Le et al., 2013c). Most algorithms developed for CDOM and SPM rely on blue or red
9 band and their accuracies may be affected by atmospheric correction uncertainties or absorption
10 from phytoplankton (D'Sa & Miller, 2003; Doxaran et al., 2005; Kowalczyk et al., 2005;
11 Mannino et al., 2008; Tiwari & Shanmugam, 2011; Long & Pavelsky, 2013 and references
12 therein). These algorithms may not be applicable in this estuary (e.g., $rRMSE > 100\%$).
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22 Given the difficulties and uncertainties in the above approaches and the complex optical
23 properties in coastal waters, we developed Pensacola Bay specific Chla, CDOM and SPM
24 retrieval algorithms for MERIS. The results show that these algorithms developed from the
25 observed dataset had good performance, with $rRMSE$ of $\sim 40\%$ for Chla, $\sim 25\%$ for CDOM, and
26 $\sim 60\%$ for SPM. The $rRMSE$ are similar or better than satellite ocean color algorithms in clear
27 waters, which have average accuracies of about 35% (Hooker et al., 1992). The improved
28 performance of these algorithms was expected given that: (1) the blue wavelength was not used
29 in these algorithms, and thus the uncertainty from atmospheric correction was reduced; (2) the
30 NIR band at 709 nm was used in the algorithms construction, which minimizes the effect of
31 interactions among different water quality optical properties. For example, $Rrs(709)/Rrs(665)$
32 minimized the effect from CDOM and detrital particles on the Chla estimate; $Rrs(709)/Rrs(510)$
33 had a good relationship with CDOM because CDOM had relatively high contribution to total
34 absorption at 510 nm (Figure 2).
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46 We acknowledge that these algorithms still have relatively high $rRMSE$ and low R^2 on
47 satellite images because of several reasons. First, the difference in measurement times between
48 *in situ* and satellite overpasses may be an issue because we used the match-up window as $\pm 24h$.
49 However, observable changes may occur in the water column during that time. Second, there are
50 differences in the spatial scale of the satellite observations (representing on average $\sim 1 km^2$) and
51 the point measurements. Third, uncertainties from the imperfect atmospheric correction may
52 affect the satellite based algorithm performance. Other sources of uncertainties may be the
53 confounding effects from other water constituents. For example, Chla fluorescence or
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4 phytoplankton absorption at 681 nm may affect SPM retrieval accuracy. Nevertheless, the
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6 algorithms developed in this study have acceptable accuracy based on the fact that SeaWiFS
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8 default Chla data product showed RMS uncertainties of > 80% even in open ocean clear waters
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10 (Gregg & Casey, 2004).
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12 5.2 Effects of river discharge and wind on bio-optical water quality 13 14

15 A nine-year bio-optical water quality time-series was constructed from MERIS
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17 observation for Pensacola Bay. This time-series enabled the examination of bio-optical water
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19 quality dynamics and their potential influencing factors. The long-term bio-optical water quality
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21 exhibited significant spatial/temporal variation during the observation period, and these
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23 variations were mainly influenced by river discharge. Chla, CDOM, and SPM all had obvious
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25 spatial variation along the salinity gradient from the fresher upper bay segment to the saltier
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27 lower bay segment (Figure 4 & 5 & 6). This resulted from the upper bay segment bio-optical
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29 water quality variable being primarily driven by river discharge and constituent loads (Murrell et
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31 al. 2007), while the lower bay segment exchanges more rapidly with ocean water from Gulf of
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33 Mexico (Hagy and Murrell 2007)
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35 River discharge significantly influenced the inter-annual and monthly variability in bio-
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37 optical water quality. The annual and monthly mean of bio-optical water quality variables in the
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39 three bay segments had significant correlations with river discharge (Table 2, Figure 8). This is
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41 not surprising because large river discharge is accompanied by large loads of nutrient, dissolved
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43 organic carbon (DOC), and SPM from the watershed into the estuary and the nutrients stimulate
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45 production of phytoplankton biomass (Murrell et al. 2007). CDOM and SPM behave
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47 conservatively in this estuary, i.e. decreasing with increasing salinity (Le et al., 2015) suggesting
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49 they are mainly of terrestrial origin. This explains the high degree of correspondence between
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51 discharge and these variables at monthly (Table 2) and annual (Figure 8) time scales. Note that,
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53 the East Bay segment behaved differently in response to river discharge changing than the
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55 Escambia and Lower Bay segments (Figure 8), probably due to the differences in residence times
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57 of river discharge.
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59 Wind has been shown to affect water clarity through sediment resuspension in other
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61 waters (Chen et al., 2007, 2010; Le et al., 2013c; Kowalczyk et al., 2015; Zhou et al., 2016). In
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4 this study, we found that bio-optical water quality in Pensacola Bay was also correlated to wind
5 at short time scales (e.g., daily to monthly), which was demonstrated by the significant
6 correlations (Table 2) with wind speed (i.e. CDOM) and wind density (i.e. Chla, SPM). This
7 correlation likely occurs because high wind speed increases sediment resuspension, which
8 increases SPM in the water column and the release of nutrients and CDOM from sediments
9 (Chen et al., 2010). This indicates that bio-optical water quality in Pensacola Bay can also be
10 driven by local weather such as cold-air outbreaks and tropical storms that result in high winds.
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18 For example, the two arrows in Figure 7 show examples of the bio-optical water quality
19 related to increased wind in October 2007 and increased discharge in November 2009. These
20 months both had local wind density peaks, i.e. >10 days daily mean wind speed higher than 3 m
21 s⁻¹. Figure 9 further shows another example of the effects from wind on bio-optical water quality
22 on short time scales. Figure 9a, c & e presents the distributions of Chla, CDOM and SPM on
23 October 8, 2011 before a high-speed wind event occurred on October 9-11 (daily mean wind
24 speed were 5.1 m/s, 4.7 m/s and 3.2 m/s, respectively). Figure 9b, d & f presents bio-optical
25 water quality distributions on October 14, 2011 after the high-speed wind event. Figure 9g shows
26 the hourly mean wind speed (black dots) and daily river discharge (red square) from October 5 to
27 15, 2011. All the bio-optical water quality variables were increased. Chla increased from < 5 mg
28 m⁻³ on October 8 to ~8 mg m⁻³ on October 14, CDOM increased from ~ 0.5 m⁻¹ to ~ 1.0 m⁻¹, and
29 SPM increased from < 2.0 mg L⁻¹ to ~4.0 mg L⁻¹.
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41 Despite the high degree of correlation between river discharge, wind, and bio-optical
42 water quality documented in this study, the stepwise regressions (Table 3) indicated these factors
43 accounted for less than half of the variability in bio-optical water quality (except for CDOM in
44 the lower bay where $R^2 = 0.58$) in the three bay segments. Other potential driving factors
45 include seasonal variation in temperature, solar radiation, and leaf phenology of both terrestrial
46 plants and seagrasses that are known to affect Chla, CDOM, and SPM. Further, variation in end-
47 member boundary conditions in the adjacent Gulf of Mexico and local inputs of nutrients,
48 CDOM, and SPM from adjacent urbanized watersheds around the bay were not accounted for in
49 this study. Time-series of these other factors were not available for the present study but could
50 be incorporated in future work with satellite derived water quality time-series to better explain
51 the observed variability.
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5.3 Implication in estuarine environment management

The findings in this study provide important information for understanding the water clarity and hypoxia in this estuary, which are two important management endpoints. We observed that light in Pensacola Bay is primarily attenuated by CDOM, with an additional ~40% contribution from phytoplankton and SPM. Satellite observations showed that these optically significant bio-optical water quality parameters (i.e. Chla, CDOM, SPM) exhibited substantial temporal variations, which were primarily driven by river discharge and wind. Thus, substantial improvement in water clarity can only be brought about by addressing source reductions for all three of these optically active constituents. This is a challenge for management since CDOM is not typically targeted for reduction, and the source of CDOM is wetland and forested landscapes (Le et al. 2015).

Previous studies have concluded that Pensacola Bay is highly susceptible to hypoxia due the strong summer water-column stratification that occurs (Hagy et al. 2007). Here, we found that spring always had relatively high Chla, which may contribute to the maintenance of summer hypoxia because phytoplankton is considered to be the primary organic source which fuels the respiration causing hypoxia. The contribution from Chla to hypoxia in this estuary is supported by the inverse co-variation trend between bottom dissolved oxygen and surface Chla at station PB04 from 2002 to 2004 (Hagy et al. 2006). This result is similar to the significant correlation observed between Chla and hypoxia variation on the Louisiana continental shelf (Le et al. 2014). Thus, it is likely that hypoxia in Pensacola Bay could be reduced by reducing nutrient loads.

6. Summary

Despite the significant progress in the development of remote sensing algorithms for both open oceans and coastal waters in the past decades, applications for routine and long-term bio-optical water quality assessment in estuaries still remains a challenge. In this study, we developed regional algorithms for Chla, CDOM, and SPM in Pensacola Bay. Nine-year time-series were established from MERIS observations for the three bio-optical water quality parameters. The results revealed that bio-optical water quality exhibited clear spatial and temporal variations, which were mainly affected by river discharge and wind. We believe that these results will provide helpful information for local and state management agencies to guide

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4 decision-making with regard to numerical nutrient criteria or nutrient reduction. The approach
5 presented in our analysis may be extendable to other estuaries with similar optical complexity
6 and water quality issues.
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20 21 References 22

23
24 Behrenfeld, M. J., Randerson, J. T., McClain, C. R., et al. (2001). Biospheric primary production
25 during an ENSO transition. *Science*, 291, 2594-2597.
26
27

28
29 Bézy, J. L., Delwart S., & Rast, M (2000). MERIS – A New Generation of Ocean-Colour Sensor
30 onboard Envisat. EAS bulletin, ESA Directorate of Applications Programmes, ESTEC,
31 Noordwijk, The Netherlands, 103, 48-56.
32
33
34

35
36 Bianchi, T. S., Lambert, C. D., Santschi, P. H., and Guo, L (1997). Source and transport of land-
37 derived particulate and dissolved organic matter in the Gulf of Mexico (Texas shelf/slope): The
38 use of ligninphenols and loliolides and biomarkers. *Organic Geochemistry*, 27, 65-78.
39
40
41

42
43 Bricker, S., B. Longstaff, W. Dennison, A. Jones, K. Boicourt, C. Wicks, and J. Woerner. 2007.
44 "Effects of nutrient enrichment in the nation's estuaries: a decade of change." In *NOAA Coastal*
45 *Ocean Program Decision Analysis Series*, 328. Silver Spring, MD: National Centers for Coastal
46 Ocean Science.
47
48
49

50
51 Chen, Z., Hu, C., Muller-Karger, F.E., & Luther, M.E. (2010). Short-term variability of
52 suspended sediment and phytoplankton in Tampa Bay, Florida: observations from a coastal
53 oceanographic tower and ocean color satellites. *Estuarine, Coastal and Shelf Science*, 89, 62-72.
54
55
56
57
58
59
60
61
62
63
64
65

- Chen, Z., Muller-Karger, F. E., & Hu, C. (2007). Remote sensing of water clarity in Tampa Bay. *Remote Sensing of Environment*, 109, 249–259.
- Doerffer R., & Schiller, H. (1998). Determination of case 2 water constituents using radiative transfer simulation and its inversion by neural networks. Proceedings of Ocean Optics XIV, S. G. Ackleson and J. Campbell, Kailua-kona, ed., 1–13.
- Doxaran, D., Cherukuru, R. C. N., S. & Lavender, J. (2005). Use of reflectance band ratios to estimate suspended and dissolved matter concentrations in estuarine waters. *International Journal of Remote Sensing*, 26(8), 1763–1769.
- D'Sa, E. J., & Miller, R. L. (2003). Bio-optical properties in waters influenced by the Mississippi River during low flow conditions. *Remote Sensing of Environment*, 84(4), 538–549
- Fischer, J. (1985). On the information content of multispectral radiance measurements over an ocean. *International Journal of Remote Sensing*, 6(5), 773–786.
- Gitelson, A. A., Schalles, J. F., & Hladil, C. M. (2007). Remote chlorophyll-a retrieval in turbid, productive estuaries: Chesapeake Bay case study. *Remote Sensing of Environment*, 109, 464–472.
- Gitelson, A. A., Dall'Olmo, G., Moses, W. M., Rundquist, D. C., Barrow, T., Fisher, T. R., et al. (2008). A simple semi-analytical model for remote estimation of chlorophyll-a in turbid waters: Validation. *Remote Sensing of Environment*, 112(9), 3582–3593.
- Gould, R.W., Arnone, R.A., & Martinolich, P. (1999). Spectral dependence of the scattering coefficient in case 1 and case 2 waters. *Applied Optics*, 38, 2377-2383
- Gould, R.W., Arnone, R.A., & Sydor, M. (2001). Absorption, scattering, and remote-sensing reflectance relationships in coastal waters: testing a new inversion algorithm. *Journal of Coastal Research*, 17, 326-341

1
2
3
4 Gower, J., King, S., Borstad, G., & Brown, L. (2005). Detection of intense plankton blooms
5 using the 709 nm band of the MERIS imaging spectrometer. *International Journal of Remote*
6 *Sensing*, 26, 2005–2012.

10
11 Gurlin, D., Gitelson, A. A., & Moses, W. J. (2011). Remote estimation of chl-a concentration in
12 turbid productive waters — Return to a simple two-band NIR-red model? *Remote Sensing of*
13 *Environment*, 115(12), 3479–3490.

17
18
19 Hagy III, J.D., & Murrell, M.C. (2007). Susceptibility of a Gulf of Mexico estuary to hypoxia: an
20 analysis using box models. *Estuarine, Coastal and Shelf Science*, 74, 239–253.

23
24 Hagy III, J.D., Lehrter, J. C., Murrell, M. C. (2006). Effects of hurricane Ivan on water quality in
25 Pensacola Bay, FL USA. *Estuaries and Coasts*, 29, 919–925.

28
29
30 Holm-Hansen, O., Riemann, B. (1978). Chlorophyll a determination: improvements in
31 methodology. *Oikos*, 30, 438–447.

33
34
35 Hooker, S.B., Esaias, W.E., Feldman, G.C., Gregg, W.W., & McClain, C.R. (1992). An
36 Overview of SeaWiFS and Ocean Color. NASA Tech. Memo., vol. 104566. National
37 Aeronautics and Space Administration, Goddard Space Flight Center Greenbelt, MD.

40
41
42 International Ocean-Colour Coordinating Group (IOCCG) (2000): Remote Sensing of Ocean
43 Colour in Coastal, and Other Optically-Complex, Waters. Edited by Shubha Sathyendranath, pp.
44 140

47
48
49 Kirk, J.T.O. (1994). Light and Photosynthesis in Aquatic Ecosystems. Cambridge Univ.
50 Press, New York, 401 pp.

53
54
55 Kowalczyk, P., Olszewski, L., Darecki, M., & Kaczmarek, S. (2005). Empirical relationships
56 between coloured dissolved organic matter (CDOM) absorption and apparent optical properties
57 in Baltic Sea waters. *International Journal of Remote Sensing*, 26(2), 345–370.

Kiwakczuk, P., Sagan, S., Zablocka, M., & Borzycka, K. (2015). Mixing anomaly in deoxygenated Baltic Sea deeps indicates benthic flux and microbial transformation of chromophoric and fluorescent dissolved organic matter. *Estuarine, Coastal and Shelf Science*, 163, 206-217.

Le, C., Hu, C., English, D., Cannizzaro, J. P., Chen, Z., Kovach, C., et al., (2013a), Inherent and apparent optical properties of the complex estuarine water of Tampa Bay: What controls light. *Estuarine, Coastal and Shelf Science*, 117, 54-69.

Le, C., Hu, C., English, D., Cannizzaro, J. P., Chen, Z., Feng, L., Boler, & R., Kovach, C. (2013b). Towards a long-term chlorophyll-a data in a turbid estuary using MODIS observations, *Progress in Oceanography*, 109, 90-103.

Le, C., Hu, C., English, D., Cannizzaro, J., Chen, Z., Kovach, C., et al. (2013c). Evaluation of chlorophyll-a remote sensing algorithms for an optically complex estuary. *Remote Sensing of Environment*, 129, 75–89.

Le, C., Lehrter, J. C., Hu, C., Murrell, M. C., & Qi, L. (2014). Spatio-temporal chlorophyll-*a* dynamics on the Louisiana shelf from satellite observations and relationships with Mississippi River discharge and nutrients. *Journal of Geophysical Research: Oceans*, 119, 7449–7462..

Le, C., Lehrter, J. C., Hu, C., Schaeffer, B., MacIntyre, H., Hagy, J. D. and Beddick, D. L. (2015), Relation between inherent optical properties and land use and land cover across Gulf Coast estuaries. *Limnology and Oceanography*. doi:10.1002/lno.10065

Lee, Z. P., Carder, K. L., Peacock, T. G., Davis, C. O., & Mueller, J. L. (1996). Method to derive ocean absorption coefficients from remote-sensing reflectance, *Applied Optics*, 35(3), 453–462.

Lewis, M. A., Devereux, R., & Bourgeois, P. (2008). Seagrass distribution in the Pensacola Bay System, northwest Florida. *Gulf and Caribbean Research*, 20: 21–28.

1
2
3
4
5
6 Liu, C. C., & Miller, R. L. (2008). Spectrum matching method for estimating the chlorophyll-a
7 concentration, CDOM ratio, and backscatter fraction from remote sensing of ocean color,
8 *Canadian Journal of Remote Sensing*, 34(4), 343–355.
9

10
11
12
13 Long, C. M., & Pavelsky, T. M. (2013). Remote sensing of suspended sediment concentration
14 and hydrologic connectivity in a complex wetland environment, *Remote Sensing of Environment*
15 129, 197–209
16
17
18
19

20
21 Mannino, A., Russ, M. E., & Hooker, S. B. (2008). Algorithm development and validation for
22 satellite-derived distributions of DOC and CDOM in the US Middle Atlantic Bight, *Journal of*
23 *Geophysical Research*, 113(C7), C07051, doi:10.1029/2007JC004493.
24
25
26
27

28 Mobley, C.D. (1999). Estimation of the remote-sensing reflectance from above-surface
29 measurements. *Applied Optics*, 38, 7442-7455
30
31
32

33 Mueller, J. L., Bidigare, R.R., Trees, C., Dore, J., Karl, D., & Van Heukelem, L. (2003).
34 Biogeochemical and bio-optical measurements and data analysis protocols: ocean optics
35 protocols for satellite ocean color sensor validation. In: Mueller, J.L., Fargion, G.S., McClain,
36 C.R. (Eds.), NASA/TM-2003–21621. Revision 4, vol.2. Goddard Space Flight Cent, Greenbelt,
37 Md., pp. 39–64.
38
39
40
41
42
43

44 Murrell, M. C., Hagy J. D., Lores, E. M., & Greene, R. M. (2007), phytoplankton production and
45 nutrient distribution in a subtropical estuary: important of freshwater flow. *Estuaries and Coasts*,
46 30(3), 390-342.
47
48
49
50

51 Matthews, M.W., Matthews, S. Bernard, K. Winter, (2010). Remote sensing of cyanobacteria-
52 dominant algal blooms and water quality parameters in Zeekoevlei, a small hypertrophic lake,
53 using MERIS, *Remote Sensing of Environment*, 114 (2010), 2070–2087
54
55
56
57
58
59
60
61
62
63
64
65

- Pan, X., Mannino, A., Russ, M., Hooker, S., Harding, L. (2010). Remote sensing of phytoplankton pigment distribution in the United States northeast coast. *Remote Sensing of Environment*, 114, 2403–2416.
- Schroeder, W.W., & Wiseman Jr., W.J., 1999. Geology and hydrodynamics of Gulf of Mexico estuaries. In: Bianchi, T.S., Pennock, J.R., Twilley, R.R. (Eds.), *Biogeochemistry of Gulf of Mexico Estuaries*. John Wiley and Sons, Inc, New York, pp. 3-28.
- Shen, F., Zhou, Y. X., Li, D. J., Zhu, W. J., & Salama, M. S. (2010). Medium resolution imaging spectrometer (MERIS) estimation of chlorophyll-a concentration in the turbid sediment-laden waters of the Changjiang (Yangtze) Estuary. *International Journal of Remote Sensing*, 31, 4635–4650.
- Son, S., and M. Wang (2012), Water properties in Chesapeake Bay from MODIS-Aqua measurements, *Remote Sensing of Environment*, 123, 163-174.
- Stumpf, R. P., Culver, M. E., Tester, P. A., Tomlinson, M., Kirkpatrick, G. J., Pederson, B. A., et al. (2003). Monitoring *Karenia brevis* blooms in the Gulf of Mexico using satellite ocean color imagery and other data. *Harmful Algae*, 2(2), 147–160.
- Sullivan, J.M., Twardowski, M.S., Zaneveld, J.R.V., Moore, C.M., Barnard, A.H., Donaghay, P.L., & Rhoades, B. (2006). Hyperspectral temperature and salt dependencies of absorption by water and heavy water in the 400-750 nm spectral range. *Applied Optics*, 45, 5294-5309
- Tiwari, S. P., & Shanmugam, P. (2011). An optical model for the remote sensing of coloured dissolved organic matter in coastal/ocean waters, *Estuarine, Coastal and Shelf Science*. 93(4), 396–402.
- Tomasko, D.A., Corbett, C.A., Greening, H.S., & Raulerson, G.E. (2005). Spatial and temporal variation in seagrass coverage in Southwest Florida: assessing the relative effects of

anthropogenic nutrient load reductions and rainfall in four contiguous estuaries. *Marine Pollution Bulletin*, 50 (8), 797-805.

Tzortziou, M., Subramanian, A., Herman, J.R., Gallegos, C.L., Neale, P.J., Harding, L.W., 2007. Remote sensing reflectance and inherent optical properties in the mid Chesapeake Bay. *Estuarine, Coastal and Shelf Science*, 72, 16-32.

US EPA (US Environmental Protection Agency), 2005. National Coastal Condition Report. Office of Research and Development/Office of Water, Washington, DC, 204 pp.

Vilas, L. G., Spyarakos, E., & Palenzuela, J. M. T. (2011). Neural network estimation of chlorophyll a from MERIS full resolution data for the coastal waters of Galician rias (NW Spain), *Remote Sensing of Environment*, 115, 524–535

Werdell, P. J., Bailey, S. W., Franz, B. A., Harding, L. W., Feldman, G. C., & McClain, C. R. (2009). Regional and seasonal variability of chlorophyll-a in Chesapeake Bay as observed by SeaWiFS and MODIS-Aqua. *Remote Sensing of Environment*, 113, 1319–1330.

Zhou, Y., Zhou, J., Jeppesen, E., Zhang, Y., Qin, B., Shi, K., Tang, X., & Han, X. (2016). Will enhanced turbulence in inland waters result in elevated production of autochthonous dissolved organic matter? *Science of Total Environment*, 543, 405-415.

Zibordi, G., Mélin, F., & Berthon, J. F. (2006), Comparison of SeaWiFS, MODIS and MERIS radiometric products at a coastal site, *Geophysical Research Letter*, 33, L06617, doi:10.1029/2006GL025778.

Tables and captions

Table 1. Mean±standard deviation of water quality variables and absorption coefficients in the three bay segments. $p<0.05$ indicates the significant difference among the three bay segments (one-way ANOVA). N is the number of cruise.

	Chla	TSS	$a_d(443)$	$a_{ph}(443)$	$a_g(443)$
East Bay (N=14)	5.4±2.6	3.9±2.1	0.53±0.33	0.22±0.10	1.5±1.11
Escambia Bay (N=15)	6.1±3.6	5.1±2.2	0.81±0.29	0.30±0.14	1.4±1.1
Lower Bay (N=14)	4.1±1.9	2.8±0.82	0.24±0.14	0.20±0.07	0.79±0.65
p	0.19	<0.01	<0.01	0.05	0.07
F	3.57	5.2	15.9	3.2	2.8

Table 2. Correlation coefficients for monthly mean water quality variables and discharge, wind speed, and wind density in the three bay segments. Asterisk(*) indicates a non-significant correlation ($p > 0.05$).

	Escambia Bay			East Bay			Lower Bay		
	Chla	CDOM	SPM	Chla	CDOM	SPM	Chla	CDOM	SPM
Discharge	0.52	0.69	0.52	0.66	0.71	0.56	0.25	0.75	0.38
Wind speed	0.32	0.28	0.29	0.29	0.32	0.25	0.11*	0.32	0.14*
Wind density	0.31	0.40	0.29	0.27	0.27	0.27	0.20*	0.26	0.22*

Table 3. Stepwise regression results between water quality and environmental factors. Q_esc represents river discharge flow into Escambia Bay, Q_east represents river discharge into East Bay, W_D represents the number of days daily mean wind speed > 3 m/s in a month, W_S represents monthly mean wind speed.

	Equations	R ²	N	p
Escambia Bay	Chla=0.008×Q_esc+0.1×W_D+7.2	0.32	79	<0.01
	CDOM=0.002×Q_esc+0.16×W_S+0.68	0.50	79	<0.01
	SPM=0.005×Q_esc+3.99	0.31	79	<0.01
East Bay	Chla=0.04×Q_east+0.14×W_D+4.28	0.45	79	<0.01
	CDOM=0.0069×Q_east+0.02×W_D+0.54	0.50	79	<0.01
	SPM=0.016×Q_east+0.072×W_D+2.45	0.35	79	<0.01
Lower Bay	Chla=0.00475×Q_esc	0.07	79	0.02
	CDOM=0.0021×Q_esc	0.58	79	<0.01
	SPM=0.0045×Q_esc	0.21	79	<0.01

Figures and Captions

Figure 1. Sampling stations from September 2009 to May 2011 in Pensacola Bay. Water quality and optical properties were measured in most months from these stations. The color represents water depth. The dashed lines split the estuary into East Bay, Escambia Bay, and Lower Bay.

Figure 2. Average absorption spectra and remote sensing reflectance measured in (a) East Bay, (b) Escambia Bay, and (c) Lower Bay from September 2009 to May 2012.

Figure 3. (a) The relationship between measured Chla and observed Rrs(709)/Rrs(665), and (b) the comparison of measured and MERIS-derived Chla; (c) the relationship between measured CDOM and observed Rrs(709)/Rrs(510), and (d) the comparison of measured and MERIS-derived CDOM; (e) the relationship between measured SPM and observed Rrs(709)/Rrs(681), and (f) the comparison of measured and MERIS-derived SPM.

Figure 4. The distribution

of annual mean MERIS_derived Chla (mg m^{-3}) from 2003 to 2011 in Pensacola Bay.

Figure 5. The distribution of annual mean MERIS_derived a_{g_443} (m^{-1}) from 2003 to 2011 in Pensacola Bay.

Figure 6. The distribution of annual mean MERIS_derived SPM (mg L^{-1}) from 2003 to 2011 in Pensacola Bay.

Figure 7. (a)-(c) Chla, CDOM, and SPM monthly mean values in the three bay segments from Jan 2003 to Dec 2011, (d)-(e) presents monthly mean river discharge ($\text{m}^3 \text{s}^{-1}$), wind speed (m s^{-1}) and wind density (wind density represents the number of days when daily mean wind speed $> 3 \text{ m s}^{-1}$ in a month). The arrows point to examples of the water quality increased by wind in October 2007 and river discharge in November 2009.

Figure 8. (a) Annual mean river discharge flow into Escambia Bay and East Bay, (b)-(d) presents the relationships between annual mean water quality variables and river discharge in the three bay segments. For the Lower Bay, the relationships are between annual water quality variables and river discharge from the Escambia River.

Figure 9. (a) and (b) MERIS derived Chla on October 8, and October 14, 2011; (c) and (d) MERIS derived CDOM on October 8, and October 14, 2011; (e) and (f) MERIS derived SPM on October 8, and October 14, 2011; (g) hourly mean wind speed (black line) and daily mean river discharge (red square) from October 5 to October 15, 2011.