An Approach to Developing Numeric Water Quality Criteria for Coastal Waters Using the SeaWiFS Satellite Data Record

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*Supporting Information

ABSTRACT: Human activities on land increase nutrient loads to coastal waters, which can increase phytoplankton production and biomass and associated ecological impacts. Numeric nutrient water quality standards are needed to protect coastal waters from eutrophication impacts. The Environmental Protection Agency determined that numeric nutrient criteria were necessary to protect designated uses of Florida’s waters. The objective of this study was to evaluate a reference condition approach for developing numeric water quality criteria for coastal waters, using data from Florida. Florida’s coastal waters have not been monitored comprehensively via field sampling to support numeric criteria development. However, satellite remote sensing had the potential to provide adequate data. Spatial and temporal measures of SeaWiFS OC4 chlorophyll-a (ChlRS-a, mg m⁻²) were resolved across Florida’s coastal waters between 1997 and 2010 and compared with in situ measurements. Statistical distributions of ChlRS-a were evaluated to determine a quantitative reference baseline. A binomial approach was implemented to consider how new data could be assessed against the criteria. The proposed satellite remote sensing approach to derive numeric criteria may be generally applicable to other coastal waters.

INTRODUCTION

Extensive modification of landscapes associated with increased human population, land development, and agricultural activities contributes to increased delivery of nitrogen and phosphorus to streams, rivers, estuaries, and ultimately to coastal waters.¹ Ecological impacts associated with anthropogenic nutrient enrichment are well documented for coastal ecosystems and include increased phytoplankton production and biomass, harmful algal blooms, decreased water clarity, degradation of submerged aquatic vegetation habitats, and hypoxia²⁻⁴. The Clean Water Act (CWA) requires states to identify designated uses of their waters and when necessary develop science-based water quality criteria to ensure protection of the designated uses. In 2009, the U.S. Environmental Protection Agency (EPA) determined that numeric criteria were needed for Florida waters to protect against impairment of designated uses caused by nutrient pollution. Numeric water quality criteria are concentrations or levels of a pollutant that, if achieved, provide an expectation that designated uses will be supported. EPA established a national strategy for development of numeric criteria calling total nitrogen (TN) and total phosphorus (TP) causal variables and chlorophyll-a a nutrient-related response variable.

In this work, we evaluate a reference condition approach for numeric criteria development that uses data from satellite remote sensing. We illustrate the approach using data for Florida coastal waters, which are marine waters up to 3 nautical miles (NM) from shore, but excluding waters within semi-enclosed basins, which are defined to be estuaries. These waters tend to be fully open to the Atlantic Ocean or Gulf of Mexico. A reference condition approach involves computing criteria based on water quality present in a water body that can be interpreted as supporting, or not impairing, the designated uses. The reference condition could be based on data collected in the past, when the water body was determined to be minimally impacted by nitrogen or phosphorus pollution (historical reference condition) or from a similar water body that was determined to be minimally impacted by nitrogen or...
phosphorus pollution (comparative reference condition). The State of Florida CWA section 303(d) listings did not include any coastal segments described as impaired for nutrients under Florida’s narrative standard. Therefore the historical reference condition could be based on existing water quality.

Karenia brevis is a harmful algal bloom dinoflagellate that frequently occurs within the coastal waters of Florida. However, nutrients from land have not been strongly implicated in bloom initiation. Nutrient export from land has been implicated in the maintenance phase of blooms when advected to near-shore waters. Acknowledging the potential for K. brevis blooms to increase coastal chlorophyll concentrations, we also evaluate an approach for addressing K. brevis blooms within the context of a reference condition approach to numeric water quality criteria development.

Water quality in Florida’s coastal waters has not been extensively monitored, potentially limiting application of a reference condition approach for criteria development. One possible solution is the use of remote sensing technologies. Satellite remote sensing currently uses low earth orbiting satellites to derive ocean color products on a global scale and at frequent revisit intervals. Remote sensing has most commonly been used for open ocean applications. However, these satellites are useful for applications in near-coastal waters.

EXPERIMENTAL SECTION

Coastal waters were subdivided into 76 coastal segments based on the Florida Department of Environmental Protection’s Water Body Identification System (WBIDs), which start at the land margin and extend seaward to 3 NM. Segment distance along the coast was typically between 6 and 14 NM depending on the State’s contour at a particular location. Coastal WBIDs located near an estuary pass were typically centered at the pass. This study included 17 coastal segments in the Florida Panhandle (FP) between the Alabama border and St. Joseph Bay, 20 segments on the West Florida Shelf (WFS) from Anclote Bay to Rookery Bay, and 39 Atlantic Coast (AC) segments from Biscayne Bay to the Georgia border (Figure 1). Areas within south Florida, including the Florida Keys, were omitted because comprehensive in situ monitoring of the area rendered a remote-sensing approach unnecessary, and significant bottom reflectance confound derivation of ChlRS-a. The area between St. Joseph Bay and Anclote Bay were also omitted because coastal seagrass coverage and extremely high colored dissolved organic carbon exports from rivers were expected to confound derivation of ChlRS-a.

Satellite ocean color data were obtained from the National Aeronautics and Space Administration’s (NASA) Ocean Color Web. The SeaWiFS provided daily images with pixels having a nominal 1.1 km spatial resolution. SeaWiFS data (reprocessing R2009) temporally spanned between September 14, 1997 and January 1, 2010. Imagery spatially covered between 31.0° N and 88.0° W. The SeaWiFS Data Analysis System (SeaDAS) version 6.1 was used to process data that...
met all standard quality control flags from level-1 to level-3 8-day composites.

SeaWiFS OC4 derived chlorophyll (ChlRS-a)\(^7\) and light attenuation (KdPAR)\(^6\) were validated against field chlorophyll (Chl-a) and light attenuation (KdPAR) measurements using the native resolution of the sensor. The OC4 was selected because it was a universal algorithm that could be applied to locations beyond Florida, and it was an algorithm packaged within the SeaDAS I2gen program so processing could be completed in SeaDAS by managers. Satellite match-ups were evaluated following Bailey and Werdell\(^{17}\) with a geometric completed in SeaDAS by managers. Satellite match-ups were evaluated following Bailey and Werdell\(^{17}\) with a geometric mean (Type II) linear regression\(^{18}\) between a 3 × 3 pixel extraction of satellite data centered at the corresponding field measurement location.

Field data used for satellite validation were from the following: the Northeastern Gulf of Mexico project (NEGOM), obtained from the NOAA National Oceanographic Data Center (NODC); the Ecology and Oceanography of Harmful Algal Blooms project (ECOHAB); the Fish and Wildlife Research Institute (FWRI); Mote Marine Laboratory; and SeaWiFS Bio-optical Archive and Storage System.\(^{19,20}\)

ChlRS-a values within coastal segments were extracted by matching segment polygon vertex coordinates with corresponding satellite image pixel and line values on 8-day composites within SeaDAS. The satellite image pixel and line locations were used to build a polygon using the 8-day array with Interactive Data Language (IDL, ITT VIS). Values from the 8-day array were then averaged if unmasked bins were completely contained within the coastal segment polygon using IDL’s region of interest (ROI, Figure S1 of the Supporting Information, SI). Averages were calculated from the beginning of the satellite mission (September 14, 1997) until January 1, 2010.

The relationship between bathymetry and satellite penetration depth were examined within each coastal segment to evaluate the potential for interference from bottom reflectance. Median depth of each coastal segment was calculated using 90 m resolution bathymetry data (NOAA National Geophysical Data Center). PAR integrated satellite penetration depths were calculated as the inverse of K\(_{dPAR}\). To assess the extent to which ChlRS-a varied with river discharge in various coastal regions of Florida, model II regression analyses were conducted on log\(_{10}\) transformed discharge and ChlRS-a. Daily discharge data were obtained from near coastal USGS gauges on dominant rivers. Discharge data were binned into 8-day averages that matched averaging periods for ChlRS-a.

Weekly K. brevis cell counts for the entire state of Florida were acquired from FWRI. Satellites detect K. brevis blooms when cell counts were above 50,000 cells L\(^{-1}\).\(^{21}\) Coastal segments with an FWRI count greater than 50,000 cells L\(^{-1}\) during an 8-day composite were flagged. In addition, the same segment was flagged one week prior to and after a bloom was detected to provide a temporal buffer as blooms were transported along the coast.

Criteria were defined as a specific concentration of ChlRS-a and a frequency with which that concentration may be exceeded in the future. Cumulative distribution functions were calculated for ChlRS-a in each coastal segment for coastal numeric criteria development. Criteria values were selected as the 90th percentile from the trailing 3-year 50th and 75th percentile values in each segment. No more than 50% and 25% of 8-day composite ChlRS-a values, within a trailing 3-year assessment period, are expected to exceed the criteria levels. The statistical significance of the proportion of 8-day composites exceeding the criteria could be evaluated using a binomial test. A time series of ChlRS-a in each segment was used to calculate criteria based on observations from the reference period (1997 to 2010). All data were used, including data flagged during K. brevis bloom events. Medians and upper quartiles (75th percentile) of ChlRS-a were computed for each segment within trailing 3-year periods, beginning with 1997–1999, 1998–2000, etc. Criteria values were calculated from the 90th percentile of the median and 75th percentile within each segment during the reference period using \(\hat{x} + t_{0.2,N,N} \cdot s\) where \(\hat{x}\) and \(s\) are the mean and sample standard deviation of the median or 75th percentile, and \(t_{0.2,N,N}\) is the Student’s t-statistic given \(\alpha = 0.2\) and \(N = 11\) 3-year periods evaluated. Once criteria values were determined, observations from within the reference period were tested against the criteria with a binomial test to ensure the data within the reference period did not exceed the criteria concentration or frequency.\(^{22}\)

RESULTS

Field data included >5500 Chl-a observations, which were reduced to 1947 after filtering for surface samples (0 to 2 m depth) and satellite overpass time (±3 h). Fewer KdPAR observations (429) were available for satellite match-up. Within the 3 NM limit, 62 Chl-a field observations were paired with ChlRS-a data and 34 KdPAR field observations were paired with K\(_{dPAR}\) (Figure 2 and Figure S2 of the SI). Within the 3 NM limit, 62 Chl-a field observations were paired with ChlRS-a data and 34 KdPAR field observations were paired with K\(_{dPAR}\) (Figure 2 and Figure S2 of the SI).

**Figure 2.** SeaWiFS observations of ChlRS-a compared to in situ Chl-a from stations within coastal segments (A) and for all the stations (B). Gray dashed line is 1:1 fit and black line is regression slope. Plots are presented in log space, but regression coefficients have been converted to linear space to represent a linear regression formula of \(y = \text{slope} \times x + \text{intercept}\).
determination of the cumulative distribution functions and calculation of criteria. Chl-a and KdPAR observations within the 3 NM boundary represented 6 and 16%, respectively, of the total available data for satellite match-ups. The relationship between Chl-a and ChlRS-a using all the Chl-a observations was stronger (R² = 0.81, RMSE = 0.24, p < 0.01, N = 1,941) with a higher slope (1.18). Using all the data for KdPAR resulted in a slope (0.76, R² = 0.46, RMSE = 0.14, p < 0.01, N = 429) similar to that obtained within the 3 NM limit. Data from outside a jurisdictional boundary could be used for criteria development if there was no expectation that water quality varied outside the boundary. However, in this case, we expect differences associated with the transition from optically complex (Case II) to open ocean (Case I) waters which is reflected in the apparent differences in the slopes discussed above. As a result, it was determined that only data within the 3 NM boundary would be used in this approach. Figures 2 and S2 of the SI indicate the value of collecting additional field observations within each coastal segment. To identify interference of bottom reflectance on ChlRS-a, the distributions of bathymetry and PAR integrated satellite penetration depth were examined within each coastal segment (Figure S3 of the SI). Differences in penetration depths were expected between the single OC4 bands (443, 490, 510, and 555) and the PAR integrated response since the PAR spectrum changes with depth in the water column due to different absorption rates at each wavelength. The red wavelengths attenuate rapidly with depth and the blue wavelengths penetrate deeper into the water column. PAR integrated satellite penetration depth was used here as a general indicator of the penetration depth from the four OC4 bands. Mean penetration depth was consistently shallower than median water depth within each FP coastal segment. The deepest penetration depths (90th percentile) were rarely greater than the shallowest water depths (10th percentile) in the FP. Similarly, AC exhibited little overlap between the deepest penetration depths and shallowest water depths. In the WFS mean penetration depth was deeper than the median water depth in 10% of the coastal segments. Coastal segments with median bathymetry shallower than 25 m exhibited bottom reflectance interference (Figure S4 of the SI) described by an exponential decay function (ChlRS-a = 1.17*exp(-0.14x), where x is the depth in meters; R² = 0.62, p < 0.01, N = 76).

Seagrass also impacts ChlRS-a, representing a special case of bottom reflectance. Although seagrass were not present in coastal waters in the FP, AC, and most of the WFS, they occur in the northern WFS between Cedar Key and Anclote Bay, and

Figure 3. Corrected ChlRS-a boxplots for all coastal segments between 1997 and 2009 with the minimum and maximum (black dots), the 10th and 90th (whiskers), the 25th and 75th (boxes) percentiles.
southwest Florida between Gullivin Bay and Florida Bay. These areas were not included in further analysis because the noise from the interferences was greater than the signal from chl-a.

Average ChlRS-a was low in the FP, higher in the WFS, and increased from low to high along the AC (Figure 3). Coefficient of variation within a segment was relatively uniform at 63% across most coastal segments. Higher values occurred near Panama City (segment 12) where C.V. was 142%. C.V. was also high (138%) near West Palm Beach where conditions fluctuated between low ChlRS-a to the south and higher values to the north. These means and C.V. described the reference condition between 1997 and January 1, 2010.

The 50th and 75th percentiles for each trailing 3-year period were calculated, resulting in 11 50th percentile and 11 75th percentile values for each segment (Figure 4A). Criteria values were selected as the 90th percentile from the 11 50th percentiles and 11 75th percentiles values. Criteria for the upper quartile (i.e., 75th percentile) averaged 2.37 and 3.10, respectively, could be used as criteria values. (B) Computed criteria values for all 76 coastal water segments. Insufficient data prevent computations for segments 35 and 72.

Figure 4. (A) Trailing 3-year cumulative distribution functions for ChlRS-a in segment 22 (outside Tampa Bay) for 1998 through 2009. The estimate of the 90th percentile of medians and upper quartiles (75th percentile), which are 2.37 and 3.10, respectively, could be used as criteria values. (B) Computed criteria values for all 76 coastal water segments. Insufficient data prevent computations for segments 35 and 72.
(MODIS), Medium Resolution Imaging Spectrometer (MERIS), possibly the Visible Infrared Imager Radiometer Suite (VIIRS), Pre-ACE, aerosols, clouds, and ecosystem (PACE) satellite, and the Ocean and Land Color Instrument (OLCI) on Sentinel-3. Multimission ocean color satellites are necessary to provide the future climate data record30 to continue the assessment process. Newer algorithms, such as the OC5,31 may perform better in coastal areas where turbidity is a major concern, such as within estuaries or near sediment-laden rivers. However, rivers in Florida were typically sediment starved such that chlorophyll-a along the WFS explained 87% of particulate backscatter.32 The OC5 may minimize effects of turbidity and bottom reflectance, but was not tested since it was not included in the SeaDAS l2gen program. Merging new missions, reprocessing events,33 newer algorithms,31,34 advanced atmospheric corrections, and the stability between ChlRS-a and Chl-a require further discussion, and could be considered during criteria triannual reviews.

It is recommended that compliance with ChlRS-a reference condition criteria values be assessed using similar satellite data and algorithms. This will mitigate problems associated with using the OC4 close to the coast, as interferences and overestimations are expected to be constant. Coastal segments could be considered impaired if a ChlRS-a assessment was identified as a statistically significant exceedance of the criteria value for either the medians or 75th percentiles. The exceedance could trigger appropriate actions under the Clean Water Act for remediation of impaired waters.

The approach for developing numeric water quality criteria evaluated in this study could potentially be used to compute criteria for any coastal waters of similar scale. Large field sampling programs, such as ECOHAB and NEOM, only provided a limited validation data set that was coincident with the SeaWiFS mission and within the 3NM limit. Preliminary analysis of field stations coincident with MODIS and MERIS suggested even less field data was available for validation within the 3NM limit due to later launch dates starting in 2002. There was less evidence of similar large field sampling programs looking into the future. Continued validation with field observations of existing satellites and new missions will be important.35

SeaWiFS ChlRS-a quantified a water quality baseline associated with use attainment and assessment data that could reveal changes that may cause loss of use. It would be necessary to have data and information available to demonstrate that water quality, during the reference period, was supportive of designated uses. Although coastal chlorophyll does change due to factors other than anthropogenic nutrient enrichment, such as coastal upwelling, we suggest a fixed quantitative baseline and an efficient procedure for detecting change as a valuable first step toward identifying water quality impairments resulting from nutrient pollution. Data quantifying nutrient fluxes to the coastal ocean would improve the prospects for relating ChlRS-a responses to anthropogenic nutrient pollution.

ASSOCIATED CONTENT

Supporting Information

Additional information is provided on region of interest coastal segment data extraction, \( k_{d(BR)} \) PAR validation regressions, optical penetration depth and bottom depth, \( K. brevis \) flagging, and river discharge. This material is available free of charge via the Internet at http://pubs.acs.org.

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