Satellite-based virtual buoy system to monitor coastal water quality

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1 Introduction

Coastal water quality plays a critical role in maintaining a healthy ecosystem and local economy. Timely information on the water quality state is a required component in every coastal ocean observing system (COOS). It allows for both the detection of anomaly events and the evaluation of long-term trends. To meet the needs of various stakeholders, the Gulf of Mexico Alliance (GOMA) proposed hundreds of locations in both the Gulf Coast estuaries and open GOM waters, to form a Gulf Monitoring Network (GMN) where water quality data as well as other physical and biogeochemical data are required (Fig. 1). These data include temperature, salinity, pH, dissolved oxygen, turbidity and water clarity, chlorophyll-a (Chla) concentrations, photosynthetically available radiation, current speed, etc. A variety of platforms including marine buoys, drifters, ships, and satellites together with customized sensors have been proposed to collect these data at various frequencies. However, implementing such a monitoring network faces significant challenges in technology, personnel, and funding availability.

On the other hand, modern satellite remote sensing has been providing synoptic and frequent information on several key water quality parameters. In the past few decades, the ocean color community has made significant progress in both sensor technology and algorithm development. Today, optical water quality data can often be derived, with sufficient accuracy on a regional basis, to assess coastal and estuarine water quality state (e.g., Ref. 2). However, effective interpretation and use of the satellite data require sophisticated skills and software that are often unavailable to the user community. Most often, these data are provided by the various COOS’s as imagery or scientific data formats [e.g., hierarchical data format (HDF), network common data form (netCDF)], and serve as layers that integrate with other variables. Interpretation of the imagery or the integrated maps is often straightforward with the aid of legends. However, temporal patterns at fixed locations such as trends or anomalies are not available, making it difficult to assess the current water quality state.

Realizing the difficulty in satellite data sharing and interpretation, the United States National Aeronautics and Space Administration (U.S. NASA) funded several Research, Education and Applications Solution Network projects to distribute and share satellite-derived information in user-friendly ways. One such project is the Ocean Color GIOVANNI (http://data.gsfc.nasa.gov/giovanni). It is an online interactive visualization and analysis tool, which allows the user to query available global ocean color data products, generated with standard NASA algorithms, at monthly intervals and medium resolution (4 and 9 km) at user specified locations or regions. With it, a time series analysis for the entire archive of Sea-viewing Wide Field-of-view Sensor (SeaWiFS) and Moderate Resolution Imaging Spectroradiometer (MODIS) collection, in both imagery and graphic formats, can be performed.
The Ocean Color GIOVANNI tool is an excellent template for the implementation of similar infrastructure to share satellite data at the GMN station locations. However, several obstacles need to be overcome in order to implement a customized data-serving tool. First, estuaries are typically small and the 4-km resolution data targeted for global ocean applications are insufficient for estuaries and other coastal waters. Indeed, there is always a compromise between coverage and resolution, and it is currently impossible to query the global ocean data set at 1 km or higher resolution due to lack of such a global database of map-projected data products at 1-km resolution and due to limited computing power. For high-resolution data products, only regional coverage is possible. Second, the data served through the Ocean Color GIOVANNI are standard NASA data products developed using globally optimized algorithms. The optical complexity of estuarine and coastal waters often calls into question the accuracy of such data (e.g., Ref. 3). Algorithm improvement is required for regional applications. It is well understood that regional algorithms may require design change (empirical or semianalytical) or algorithm coefficients adjustments in different regions, making it difficult to implement regional algorithms for a system designed primarily for large-scale studies covering the global oceans.

To facilitate the data analysis and interpretation need of the various users, and given the availability of satellite data and recent algorithm development, the objective of this work is to develop a customized data processing and sharing tool for key locations in estuaries and coastal waters. While many user needs can be met by querying the well-established Ocean Color GIOVANNI for large-scale studies using the standard NASA data products at coarse resolutions, this tool focuses on predefined small regions at higher spatial resolutions, thus making customized data products, derived using regionally tuned algorithms, available to satisfy more refined user requirements. The work combines information technology (IT) development, advances in remote sensing algorithms, and a customized web interface to maximize the value of satellite data for water quality monitoring.

2 Data and Method

Figure 2 presents a schematic flow chart to show the data processing and presenting streams. In 2010, a virtual antenna system (VAS) was established at the University of South Florida–College of Marine Science (USF–CMS), which provided the basis for the virtual buoy system (VBS). Through NASA Ocean Biology Processing Group (OBPG) data subscriptions, the VAS automatically downloads low-level satellite data collected by MODIS (1999–present for Terra and 2002–present for Aqua), Medium Resolution Imaging Spectrometer (MERIS) (2002–2012), and Visible Infrared Imager Radiometer Suite (VIIRS) (2011–present) in near real time (typically within 4 to 6 h of the satellite overpass) for predefined regions of interests (ROIs). These data have either global coverage (MODIS and VIIRS) or local coverage (MERIS full resolution, collected by a ground station in Canada). The data are processed immediately using both the NASA processing software SeaWiFS Data Analysis System (version 7.0) and in-house developed software to produce a suite of data products using both standard NASA algorithms and customized, peer-reviewed algorithms. The processing is controlled and monitored by the Simple
Scalable Script-based Science Processor (S4P) for each ROI, where a screen of control panels is displayed to show the status of each processing step (Fig. 2). S4P was originally tasked as a “foundation for several small- to medium-size systems for data mining, on-demand subsetting, processing of direct broadcast MODIS data, and Quick-Response MODIS processing.” Here, it has been adapted for VIIRS and other processing including Virtual Buoyos. If the processing is interrupted for any reason (e.g., power failure, temporarily unavailable of satellite data stream), it can be resumed through a simple click. The NASA standard data products produced by the VAS include:

- Sea surface temperature (SST, °C) from the multichannel nonlinear regression algorithm.
- Spectral remote sensing reflectance ($R_\text{rs}(\lambda)$, sr$^{-1}$) from a combination of the near-infrared and shortwave-infrared atmospheric correction algorithms.
- Chla (mg m$^{-3}$) using the default band-ratio algorithm.
- Diffuse attenuation coefficient at 490 nm [$K_d(490)$, m$^{-1}$] using a semianalytical algorithm.
- Normalized fluorescence line height (nFLH, mW cm$^{-2}$ μm$^{-1}$ sr$^{-1}$, for MODIS and MERIS only).
- Maximum chlorophyll index (mW cm$^{-2}$ μm$^{-1}$ sr$^{-1}$, for MERIS only).

The nonstandard data products include:

- Spectral Rayleigh corrected reflectance [$R_\text{rc}(\lambda)$, dimensionless].
- Red-green-blue (RGB) composite image using the $R_\text{rc}(\lambda)$ data in the red, green, and blue bands.
- Enhanced RGB (ERGB) composite image using the $R_\text{rs}(\lambda)$ data at 555 nm (R), 488 nm (G), and 443 nm (B).
- Floating algae index (FAI, dimensionless) to detect floating algae mats (Sargassum, Ulva prolifera, Trichodesmium, other cyanobacteria).
- Color index (CI, dimensionless) to remove sun glint and reveal ocean color patterns from MODIS measurements.

These data products are created for many ROIs in North America, East China, the Central Atlantic, and the Persian Gulf at resolutions from 250 m to 1 km in Google Earth (GE) compatible imagery format, while digital data are stored in HDF format for internal query. Figure 3 shows the coverage of the high-resolution products over the eastern GOM, where 250-m resolution data products from MODIS and MERIS are created and shared through GE compatible images.

In addition to the satellite data products, the VAS also downloads and displays other data types as separate data layers to overlay on the satellite images in Google Earth in near real time. These include ocean current vectors from the Hybrid Coordinate Ocean Model (HYCOM) at regional scale and from the Finite Volume Coastal Ocean Model (FVCOM) at local scale, and phytoplankton cell counts data from the Florida Fish and Wildlife Conservation Commission. The data are used to track ocean features and to validate satellite-observed blooms. Figure 4 shows an example of MODIS FAI image overlaid with the HYCOM-derived ocean current vectors. A Trichodesmium bloom is identified to the east coast of Florida on this image, while the ocean currents may be used to infer the bloom’s movement.

The VBS was established from the VAS using computer codes developed at USF–CMS using IDL (version 8.0) and Perl scripts to query predefined stations to produce time-series water quality data in both graphical and ASCII formats. The VB stations were designed to be at least 2 km away from shorelines to minimize the impact of land adjacency effect. For each small region, a query is performed of map-projected water quality data products from individual HDF computer files, which are stored by the VAS using a hierarchy structure sorted by years and regions. Through the web interface, each station’s time-series data are presented as monthly means for the entire period of the satellite mission and weekly means for the past two years, with simple statistics (climatology, linear trend) annotated on the graphics. The mean is calculated as an arithmetic mean of all valid pixels within 1 km of the station location for each time interval. Here, “valid” is defined as those data that pass the various quality controls defined by the “l2_flags” data field, including atmospheric correction failure, clouds, large sun angle or viewing angle. Note that these quality controls do not include negative water-leaving radiance, because many otherwise valid pixels in estuaries would be disqualified and discarded. Negative water-leaving radiance mainly occurred in the blue bands (412 and 443 nm); these bands were avoided in the customized inversion algorithms (e.g., Ref. 12). Also presented for each station are simple descriptions of the station (latitude, longitude, bottom depth, and whenever the information was available, bottom type).
how the data are derived, and what they mean. One difference between the VBS and the Ocean Color GIOVANNI system is that all data and statistics are computed and made available in both graphical and ASCII formats every Friday (for weekly data) and every first Friday of the month (for monthly data). Thus, upon a mouse click from a user, the most current results are immediately available to the user.

Not all data products from the VAS are suitable for time-series analysis, especially for estuaries. For example, the FAI and CI data only provide relative measures of algae mats and color patterns, respectively. The nFLH data for offshore, sediment-poor waters represent accurate measures of the biomass and therefore are useful to detect and trace blooms, but for estuarine waters they may be “contaminated” by high concentrations of suspended sediment and by land adjacency effect. Therefore, only the following data products are queried by the VBS: SST, Chla, turbidity or particulate backscattering coefficient at 700 nm \(b_{pp,700} \text{ m}^{-1} \), \(K_d(490)\) or seccchi disk depth (m), absorption coefficient of colored dissolved organic matter (CDOM) at 443 nm \(a_{443} \text{ m}^{-1} \), and bottom available light (BAL, %). Whenever new algorithms are available to improve the data quality, they are implemented to take the NASA standard \(R_{rs}(\lambda)\) as input to produce regional products. For example, Le et al. red/green band ratio algorithm and a hybrid algorithm were used to derive Chla and \(a_{443}\), respectively, for Tampa Bay (Fig. 5); the modified Lee et al. \(K_d\) algorithm was used to derive \(K_d(490)\) for the Florida Keys shallow-water (<30 m but >5 m) stations; the EOF-based algorithm of Craig et al. was used to derive the above products as well as \(a_{443}\) in the Big Bend region. Depending on the

Fig. 3 Examples of the S4P control panels for satellite data processing. Top: A main S4P panel showing several jobs running in green and waiting jobs in blue at various stations. The finished jobs are listed under the “OK” column. The failed jobs are shown in red. Bottom: A S4P SeaDAS level 3 processing station (i.e., one of the blue buttons in the top panel) with waiting work order highlighted in yellow. The contents of the work order can also be displayed.

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Fig. 4 (a) Coverage of the high-resolution (250 m) data products in the eastern GOM. The examples shown here are the MODIS and MERIS nFLH imagery for (from west to east): Mississippi Delta, Mobile Bay, Big Bend, Central West Florida Shelf, Florida Keys, SE Florida Shelf. The CWFS image shows a *Karenia brevis* harmful algal bloom (HAB) as indicated by the red color (high nFLH values). The same red color in the Mississippi Delta is mainly a result of high turbidity as opposed to an HAB, as nFLH is a reliable bloom index for sediment-poor waters only. (b) An example of the FAI image showing floating algae mats along the east coast of Florida overlaid with concurrent ocean current vectors.

Fig. 5 Field measurement stations in Tampa Bay (a), where water quality and bio-optical data have been collected to develop and validate customized algorithms for the VBS. The validation of two water quality products, namely Chla and $a_g443$, is presented in (b) and (c), respectively. Figures adapted from Le et al.2 and Le and Hu.17
region, the suite of data products may vary slightly due to the varying availability of customized algorithms.

The VBS was implemented to cover several regions, focusing mainly on the eastern GOM. This area was chosen because of continuous influence of hurricanes and harmful algal blooms and because of the existence of several National Estuary Programs (Fig. 1). Through the web interface, a map is provided for each region, with all predefined stations annotated. A mouse click on any station will display that station’s description and the water quality time series (Fig. 6).

3 Results

All data products can be accessed through the web link http://optics.marine.usf.edu via the menu under “Satellite Data Products” and “Virtual Data Products.” Figure 6 shows the VB stations in several regions: the central west Florida Shelf (WFS) (including Tampa Bay, Sarasota Bay, Charlotte Harbor), the Suwannee River estuary, and the Steinhatchee River estuary. In Tampa Bay, one station is sampled in each of the four bay segments (Old Tampa Bay, Hillsborough Bay, Middle Tampa Bay, and Lower Tampa Bay), and one additional station (TB04) is collocated with an existing Tampa Bay PORTS station for comparative purposes. In Sarasota Bay, only one station is sampled due to its small size. In Charlotte Harbor, one station is sampled in the upper, middle, and lower estuary, respectively. On the central WFS, the stations are sampled along several cross-shore transects at 10, 20, and 30 m bathymetric isobaths, respectively. An additional station (WF09) is collocated with an existing Coastal Ocean Monitoring and Prediction System (COMPS) station. In the Suwannee River estuary and Steinhatchee River estuary, stations are sampled along cross-shore transects. The distributions of the VB stations allow for time-series water quality data to be sampled along water quality gradients, thus maximizing coverage over a variety of conditions.

Figure 7 shows the web interface for the water quality display of a VB station. The top tabs allow a user to select the parameter of interest, while the graphs to the right show the monthly and weekly time series of the selected parameter. The descriptions of the station and how these data were generated and what they mean are all listed to the left. Also shown are the links to the ASCII data as well as the most current satellite imagery covering the station’s location.

Figure 8 presents several sample data products from different VB stations. Figure 8(a) shows that the BAL (in percentage of the surface light) at a coastal station in the Suwannee River estuary (SU08) is $\gg 20\%$ (red line) nearly all the time, suggesting that the bottom is not light limited for seagrass growth. Indeed, a healthy seagrass bed is found at this station [Fig. 8(b)]. The photo shows a moderately dense and healthy turtlegrass (Thalassia testudinum) bed with some drift red algae (Gracilaria and Laurencia spp.) in the center. The yellowish hue of the photo is due to high CDOM concentration in the water. Figure 8(c) shows that the water clarity (as represented by $K_d$) is improving over the 11-year period (2002 to 2012) (i.e., $K_d$ is decreasing), a result mainly attributed to weather anomalies during 2003 and 2004. The overlaid monthly climatology provides a measure of the “normal” conditions, thus enabling assessment of any anomaly events. In contrast to the optical water quality data, weekly mean SST at a station on the WFS [Fig. 8(d)] in the past 2 years shows a clear seasonal

![Fig. 6 VB stations in several estuaries and central west Florida Shelf (a), Suwannee River estuary (b), and Steinhatchee River estuary (c). A user can click on any of the stations to obtain the most current time-series water quality data through a web interface.](https://ebooks.spiedigitallibrary.org/journals/Optical-Engineering)
cycle that mimics the climatology, while small inter-annual changes can also be visualized.

There are many other examples to show the water quality time-series data and how they can be used to infer water quality conditions at a single station or in a region at multiple stations. Reviews of our web-visit statistics show that the user groups accessing these satellite-based data products range from government agencies, academic institutions, and private entities to the general public. With continuous improvement in data quality and data serving capacity, and with the increased demands of quality-controlled water quality data for estuaries and coastal waters, we expect to see increased usage of these customized data products through the VBS in the coming years.

4 Discussion

Data reliability or accuracy is one concern raised by many stakeholders when considering the use of satellite data as a proxy of coastal water quality. It is well known that although satellite data are generally accurate for open-ocean waters, in coastal waters their quality is often questionable due to algorithm artifacts (e.g., large uncertainties in atmospheric correction, failure of inversion algorithms due to optical complexity of the water column or shallow bottom). To overcome this difficulty, significant efforts have been dedicated to conduct field experiments (e.g., Fig. 7) to facilitate better algorithm development and validate the satellite data products. Currently, region-specific algorithms are available and used for Tampa Bay, Indian River Lagoon, and Florida Keys shallow waters. Uncertainties of these products are typically <35% for a large dynamic range. For SST, RMS uncertainties are <1°C for most cases and <0.5°C for some cases. Note that these uncertainty estimates are derived from individual data points (satellite versus in situ measurements), and they are due at least in part to the inherent differences between the two measurements (e.g., a satellite pixel represents a large area while a field measurement is from a point). In other words they serve as a measure of data scattering and should not be interpreted as a systematic bias. On weekly or monthly scales, the product uncertainties are usually much lower. However, even in these regions, not every water quality product has a corresponding regionally tuned algorithm. Under these circumstances, a cautious note on the provisional data quality is provided on the web page under the data's description.

Unlike imagery data products that provide spatially continuous information at all locations, the VBS is only focused on predefined discrete stations. At the price of losing the spatial context, the VBS has several advantages. First, the VBS provides long-term time-series data that are difficult or impossible to interpret from the imagery data products. Second, the VBS makes it much easier to incorporate updated algorithms. In fact, even within a particular region, different algorithms may be implemented at different stations for the same water quality parameter. In contrast, such an implementation may cause spatial discontinuity in satellite images due to an algorithm switch (e.g., atmospheric correction algorithm may switch from near-infrared to shortwave-infrared). Such image-based discontinuity would not impact the temporal patterns for a given VBS station as data derived from the stations come from the same algorithm. Finally, for the same reason, the VBS can focus on those locations where
applicable algorithms are available. For example, Barnes et al.\textsuperscript{21} found that the modified Lee et al.\textsuperscript{8} $K_d$ algorithm is valid only for waters with bottom depths $>5$ m in the Florida Keys. Because of this fact, VB stations can be planned to avoid waters $<5$ m.

Although our initial intention was to provide validated water quality data through the VBS mainly for the Gulf Coast estuaries and coastal waters, since its debut in early 2013 there have been several requests to extend its coverage to other coastal regions, even where the data quality is unknown or provisional due to lack of field validation. In response, several other ROIs were added with VB stations defined to cover water quality gradients. Figure\textsuperscript{9} presents two examples for coastal waters in the northern Persian Gulf and around Cape Cod (North America). The northern Persian Gulf might have experienced dramatic changes in the past decades due to climate variability and human activities (war, dam construction and destruction, river redirection, etc.), and the VBS may help track water quality events and trends in the region. There is a sewage discharge location in Massachusetts Bay [Fig.\textsuperscript{7}(b), red square], and it is important to know whether the sewage discharge has a direct impact on the nearby water quality. The VBS allows for continuous monitoring of the relative water quality patterns in these regions before field data are acquired and are used to tune the algorithms used to produce the products.

Indeed, the existing VAS makes it straightforward to extend the VBS to cover any coastal regions around the world, so long as the satellite data flow from NASA continues. Community efforts will lead to consistent data products from multiple sensors such as MODIS and VIIRS (e.g., Ref.\textsuperscript{26}). Even without field validation due to the absence of field-monitoring programs, the provisional satellite data through NASA standard algorithms (or algorithms validated in other similar coastal regions) may provide relative water quality patterns for the past decade to help make local management decisions. We expect to extend the VBS to help implement the GMN in the near future.

At the time of this writing the VBS has been implemented to meet the user needs of several groups. The established infrastructure makes it easy to add additional water quality parameters or new ways to present data more effectively for any VB stations. Figure\textsuperscript{10} shows a template for a possible design of water quality report card for the SU02 VB station in the Suwannee estuary. The report card will provide coastal managers and other user groups rapid information on the current water quality state in the context of historical baseline. Such a design or its modified version will be implemented for the VBS during the next processing update.

By no means will the VBS replace real buoys, as these buoys may collect and share meteorological or oceanographic data of many more types operationally at different
water depths. In contrast, the VBS currently can only produce a handful of water quality parameters for surface waters with weekly updates. However, the VBS infrastructure may be used to incorporate data collected by real buoys. Some of these buoys provide data in the ASCII format (e.g., National Oceanic and Atmospheric Administration National Data Buoy Center), so it may be pulled from the data providers and incorporated with the satellite-derived water quality data. Doing so will provide a complete suite of data, in both graphical and ASCII formats, to monitor the physical, biochemical, optical, and meteorological conditions of the coastal environments. This may be particularly useful once a resource is available to implement the GOMA GMN (Fig. 1) through real buoys such that the VB stations can be placed at the same buoy locations to provide complementary data and information to those collected by the buoys.

While the VBS may appear similar to the well-established and widely used Ocean Color GIOVANNI, there are several major differences between them. The VBS is focused on predefined small regions at higher spatial resolutions, thus making it easier to generate customized data products using regionally tuned algorithms. Indeed, the VBS differentiates itself from the Ocean Color GIOVANNI with at least the following characteristics: (1) higher spatial resolution; (2) customized algorithms tailored for specific regions; and (3) more water quality-oriented data products. In contrast, the Ocean Color GIOVANNI serves standard NASA data products at coarser resolution and these products are generated with unified algorithms optimized for the global oceans. In short, they were designed for different purposes, each with its own strengths and weaknesses.

5 Conclusion

Water quality monitoring programs require significant resources in instrumentation, personnel, and sustainable funding. Such resources are not available for most coastal regions. Satellite remote sensing provides several key water quality measurements. The VBS makes use of the timely information from satellite measurements to provide time series of water quality data at predefined regions and locations using regionally tuned algorithms. This capacity

Fig. 9. VB stations in the northern Persian Gulf (a) and coastal waters around Cape Cod (b). The red square [highlighted in the top left corner of (b)] outlines several stations centered at a swage discharge location.

Fig. 10. A template of water quality report card for a VB station (SU02 in the Suwannee estuary). The report card or its modification may be implemented for some VB stations during the next processing update for the VBS.
is based on a VAS, and therefore, not restricted to local coverage from a physical antenna. We expect to extend the VAS and VBS to cover other important coastal regions once the data products are validated or provisional data are demanded.

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References


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