

SYNOPSIS

Project Number: CIMP-001

Start: 01/09/2002

End: 08/31/2003

Title: Monitoring the Water Quality Parameters of Mayagüez Bay

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Focus Category: Water Quality Monitoring

Congressional District: N/A

Descriptors:

PROBLEM AND RESEARCH OBJECTIVES:

Mayagüez Bay is located in the west coast of Puerto Rico and the major sources of contamination come from rivers, industrial effluents, and city sewage. Rivers collect contaminants that are mainly originated from agriculture and industrial activities. There are three major rivers discharging directly into the Mayagüez Bay: the Guanajibo, Añasco and Yaguez Rivers. The United States Geological Survey (USGS, 1999) reported that these rivers exhibited fecal coliform contamination; however, the Guanajibo River is the one that showed the highest level of fecal coliform. A tuna factory is also located in the Mayagüez Bay and its activities affect significantly the water characteristics of the bay. Another important source of contamination is the sewage pipe that continuously dumps treated water into the bay.

The interaction of physical, chemical and biological processes affect the marine organisms in coastal areas. The dynamics of these processes are operating over different spatial and temporal scales and its variability is highly affected by seasonal changes. For instance, the seasonal rainfall in tropical areas induces temporal and regional patterns in river discharge, which includes fluctuations in nutrient concentration, turbidity, heavy metals and others. Water turbidity limits the penetration of light and consequently affects the biological productivity. Land use and heterogeneous landscape of Puerto Rican coastal waters may affect the plankton communities at different spatial and temporal scale. Large variations in weather and topographic conditions combined with human activity produce significant changes in the amount and composition of river discharge. Agriculture and cattle activities increase the concentration of nutrients, like phosphates and nitrates, which eventually could be transported to coastal regions. Intense urban development, especially in coastal areas, accelerates soil erosion and increases the sediment load from rivers. These sediments are deposited within the coastal zone, or remain suspended and transported to oceanic waters. The Añasco, Yaguez, and Guanajibo rivers supply sediments derived from igneous rock environments onto the narrow insular shelf of Mayagüez Bay. Sediments in water column affect the light penetration and provoke that remote sensing algorithms cannot work properly in coastal

areas. Therefore, one of the major contribution of this research is to develop some statistical and mathematical tools that help the SeaWiFS remote sensing algorithms to properly measure the chlorophyll *a* concentration on coastal waters, and consequently to monitor the water quality parameters of Mayagüez Bay. The following specific objectives have been established to accomplish the main target:

- 1) Identify a time series model for each of the selected water-quality parameters to estimate the pollution deposition at the mouth of each river based on upstream observations.
- 2) Conduct sampling field to collect water-quality parameters and bio-optical properties over the Mayagüez Bay.
- 3) Design a neural network model to improve the estimates of Chlorophyll *a* and other water quality parameters from SeaWiFS measurements in coastal waters.

METHODOLOGY:

This research was planned for three years. The research activities described here correspond to the second year. This methodology includes estimation of water quality parameters at the mouth of the Guanajibo and Yaguez Rivers and conducting sampling field in the Mayagüez Bay. Parameter estimations are compared with actual observations to validate the statistical model. The Añasco River was studied during the first year of this project, and the correlation of satellite reflectance with water contaminants will be studied in the third year. The implemented methodology during the second year is divided in three main parts: (1) Parameter Estimation, (2) Sampling Field and (3) Chlorophyll *a* estimation. A detailed description of the first part is given in the working paper entitled “A Stochastic-Dynamic Model to Predict Fecal Coliforms at the Mouth of the Añasco River” (Ramirez and Gilbes, 2003). The detailed description of the second and third parts is given in the working paper entitled “Bio-Optical Evidence of Land-Sea Interactions in the Western Coast of Puerto Rico” (Gilbes et al., 2002).

1. PARAMETER ESTIMATION.

The proposed estimation scheme includes four major tasks: (1) An adaptive estimation procedure is introduced to reconstruct the monthly time series. (2) Seasonal time series models are identified to represent the behavior of water quality parameters at each water quality station. (3) Spatial interpolation algorithm is used to estimate water quality parameters at the mouth of the Guanajibo River.

1.1 Reconstruction of time series.

The studied water quality data were obtained from the US Geological Survey at the following web page: www.usgs.gov. The available water quality stations on the studied rivers are the following:

Guanajibo River:

- Station 50133600 located near San German (18.12° N, 67.06° W).
- Station 50136400 located near Rosario (18.16° N, 67.08° W).
- Station 50138000 located near Hormigueros: HW100 (18.14° N, 67.15° W).

Yaguez River:

- Station 50138800 located near Mayaguez: HW106 (18.25° N, 67.13° W).

The available data period spans from 1973 to 2001 and these data were collected on a bimonthly basis from 1973 to 1996 and in a quarterly basis after 1996. Potential outliers were identified and studied. The ones that revealed evidences of incorrect observations were removed from data; otherwise, the potential outliers were kept on the data set. The available water quality data were not systematically obtained and have some missing values. One of the most efficient techniques to represents stochastic processes is the time series model. Unfortunately, time series models require observations at equal time intervals. Since our water quality data is not given on a regularly periods of time, an adaptive estimation technique was developed to estimate the missing values and consequently to generate a time series at equal time intervals.

Cross-correlation between Añasco and Guanajibo rivers were used to identify regression models. The first seven years of monthly data for each parameter (i.e., 84 monthly values) were estimated using multiple regression models. The first 84 values of each parameter were used to identify a Seasonal Autoregressive Integrated and Moving Average (SARIMA) model (Brockwell and Davis, 2002). A SARIMA model is a seasonal time series model that was used to reconstruct the monthly time series. An adaptive estimation procedure was implemented to reconstruct the time series. The adaptive procedure consists on assuming that the first 84 values were observations and then a SARIMA model was developed to predict the next missing value. Once a missing value is predicted it is assumed to be an additional observed value. Thus recorded observations and estimated missing values were used again to fit a new SARIMA model to predict the next missing value. This process was repeated over and over until the time series were completed. Once a time series was complete the initial 84 values were removed and the backward adaptive forecast procedure was used to estimate the removed values. The developed time series was called reconstructed time series. Figure 1 shows the original values of oxygen dissolved (mg/l) in the Guanajibo River at the Rosario station. Figure 2 exhibited the reconstructed time series for oxygen dissolved in Rosario station. Figure 3 shows the superposition of the observed and reconstructed time series for oxygen dissolved at Rosario station.

1.2. Time Series Models.

A SARIMA model was identified for each one of the reconstructed time series. Some of the water quality parameters exhibited unstable variability and therefore mathematical transformations were applied to stabilize the variance. A SARIMA model expresses the seasonal, the trend, and the stochastic components into a single time difference equation. This model includes autoregressive components and consequently performs predictions based on his passed data. Prediction errors based on the autoregressive component are obtained and the linear combinations of errors are included in the model. In that sense, the SARIMA model modifies its coefficient depending on previous errors, i.e., SARIMA learns on its previous errors to derive accurate predictions.

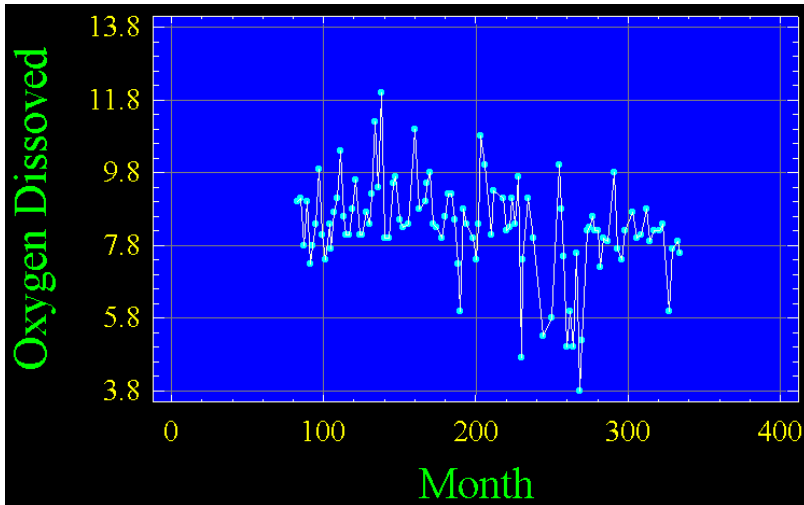


Figure 1. Observations of Oxygen Dissolved (mg/l) at Rosario Station (1979 – 2000)

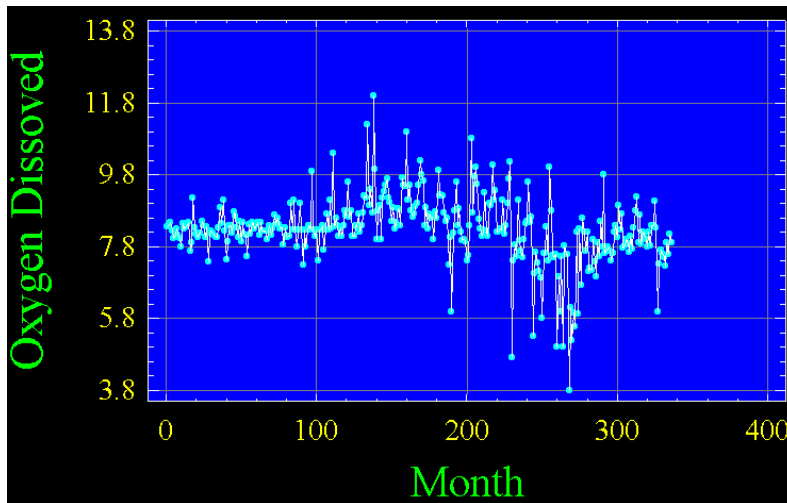


Figure 2. Reconstructed of Oxygen Dissolved (mg/l) at Rosario Station (1979 – 2000)

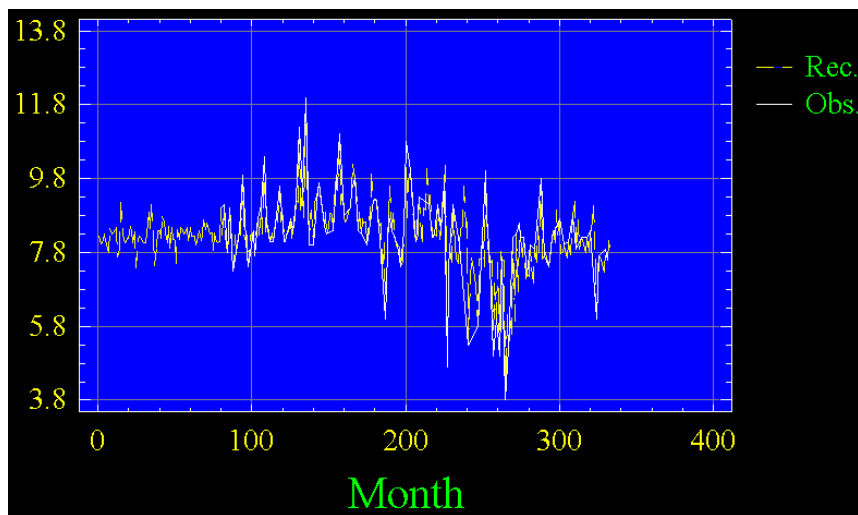


Figure 3. Superposition of observations and reconstructed time series Oxygen dissolved (mg/l) at Rosario Station (1979 – 2000)

The reconstructed time series exhibited a strong seasonal component, and therefore, a 12 difference was applied to remove the seasonal component. The remaining part of the stochastic process exhibited a stationary behavior and consequently a stochastic model was identified for each one of the time series. Coefficients involved in the time series models indicated that they are statistically significant and also the autocorrelation function on residuals resembles a white noise processes.

Arbitrarily the oxygen-dissolved variable was used for illustration purposes. The identified SARIMA model for the oxygen dissolved in the Guanajibo River at the Rosario station has the following structure:

$$(1 - B^{12})(1 - \phi B)x_t = (1 + \theta B)(1 - \Theta B^{12})a_t \quad (1)$$

where x_t represents the oxygen dissolved in Guanajibo River at Rosario station during the month t , ϕ is the autoregressive coefficient, θ is the moving average coefficient, Θ is the seasonal moving average coefficient, B , is the back-shift operator, and a_t is a sequence of random noise. Parameter estimation is exhibited on Table 1.

Table 1. Parameter estimation.

Parameter	Estimate	Std. error	t	p-value
ϕ	0.959861	0.022475	42.70	0.00000
θ	0.757672	0.055058	14.98	0.00000
Θ	0.931493	0.014196	65.61	0.00000

The SARIMA models can be used to predict one year ahead the water quality parameters at each one of the water quality stations. For instance equation (1) was used to predict the oxygen dissolved in Guanajibo River at Rosario station for the year 2001 and the values at the Internet were used to compute the prediction error and validate the accuracy of the model. Table 2 shows the observed, and predicted values as well as the prediction errors. It should be noted that equation (1) was developed using data up to time 2000. The observed values during year 2001 were incorporated into the model to predict the year 2002. Observations for the year 2002 are not available at the Internet by the time that this report was made. Table 3 shows the prediction for oxygen dissolved (mg/l) in Guanajibo River at Rosario station for the year 2002.

Table 2. Oxygen Predicted and Observed in Guanajibo River at Rosario station for the year 2001.

Month	1	2	3	4	5	6	7	8	9	10	11	12
Observed		8.6			8.4				8.1			
Predicted	7.60	7.72	7.83	7.70	7.50	7.78	7.58	8.22	8.04	8.85	8.19	8.41
Error		0.88			0.90				0.06			

Table 3. Predicted Oxygen in Guanajibo River at Rosario station for the year 2002.

Month	1	2	3	4	5	6	7	8	9	10	11	12
Predicted	7.72	8.38	8.20	8.99	8.43	8.57	7.89	8.04	8.10	7.97	7.76	7.98

1.3 Spatial Interpolation.

An artificial neural network (ANN) model was designed to model the spatial relationships among the quality parameters from the three water stations of the Guanajibo River. An adaptive neural network model was designed to increase extrapolation accuracy. Thus, at a given point in time an ANN was trained with a window size of 8 and a spatial extrapolation was compute to estimate the water quality parameter at the mouth of the Guanajibo River. One unit increased the time and again a new window of size 8 was used to estimate the water quality parameter at time $t+1$. This process was repeated over and over until the last estimate was computed.

The Levenberg- Marquardt algorithm was used as the learning rule to accelerate the convergence process (Hagan, 1996; Ramirez and Montes, 2002). The number of neurons in the hidden layer was estimated using a cross-validation technique, to avoid over-fitting problem.

Let X_t, Y_t , and Z_t be the known water quality parameters at time t for the San German, Rosario, and Hormigueros stations, respectively. Let W_t be the unknown water quality parameter at the mouth of the Guanajibo River at time t . Let d_{ij} be the Euclidian distances between the i^{th} and j^{th} stations. The training sets for estimating W_t can be obtained by defining the input matrix \mathbf{P}_t and the target vector \mathbf{T}_t as follows:

$$\mathbf{P}_t = \begin{bmatrix} d_{yz} Y_{t-L} & d_{yz} Y_{t-L+1} & \cdots & d_{yz} Y_t \\ d_{xz} X_{t-L} & d_{xz} X_{t-L+1} & \cdots & d_{yz} X_t \end{bmatrix}, \quad t = L+1, L+2, \dots, n \quad (2)$$

$$\mathbf{T}_t = [Z_{t-L} \quad Z_{t-L+1} \quad \cdots \quad Z_t] \quad t = L+1, L+2, \dots, n \quad (3)$$

where L is the window size, and $\hat{\mathbf{p}}_t$ is a vector to evaluate the trained neural network. Thus, after performing this evaluation the neural network obtains the required spatial interpolation. The required information to perform prediction is:

$$\hat{\mathbf{p}}_t = \begin{bmatrix} d_{yw} Y_t \\ d_{xw} X_t \end{bmatrix} \quad t = L+1, L+2, \dots, n \quad (4)$$

2. FIELD SAMPLING.

Field data was collected during two cruises to the Mayagüez Bay in August 20-22 of 2002 (rainy season), and February 25-27 of 2003 (dry season). Samplings during the dry and wet seasons were performed from inshore to offshore waters, covering the Añasco, Yagüez, and Guanajibo Rivers, and the regions affected by the dumping of the tuna factory and the sewage pipe. Figure 4 shows the location of the stations. Twenty-four (24) stations were sampled with an optical package, in which 12 stations had ancillary data.

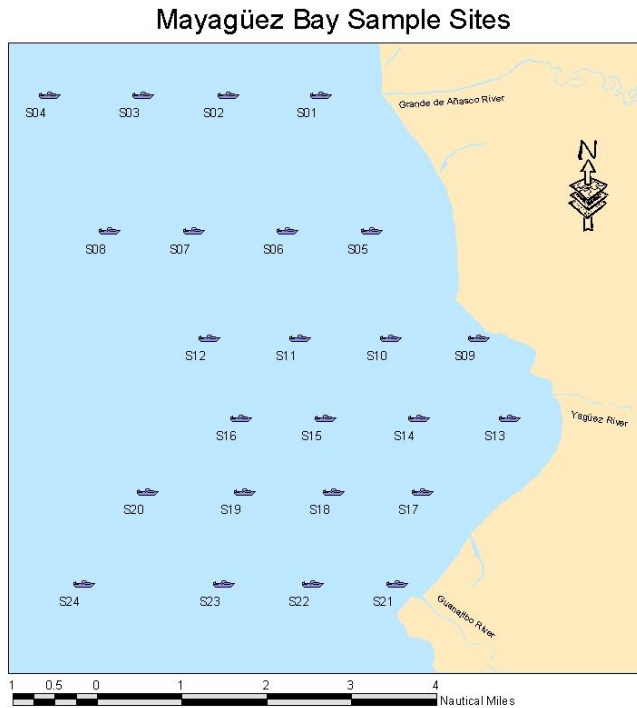


Figure 4. Sampling stations at Mayagüez Bay.

An optical package with several instruments was used to measure profiles of different water properties. A CTD (Seabird SBE-19 with pump) measured temperature and salinity. A small fluorometer (Model WetStar from Wet Labs) measured chlorophyll fluorescence. The spectral transmittance, $c(\lambda)$, and spectral adsorption, $a(\lambda)$, were measured over nine wavelengths with the AC-9 meter (from Wet Labs). The backscattering coefficient, $b_b(\lambda)$, at six wavelengths was measured with the HydroScat-6 (from Hobi Labs). Upwelling radiance, $L_u(0^-, \lambda)$, and downwelling irradiance, $E_d(0^-, \lambda)$, were obtained using a submersible radiometer (Model OCR-200 from Satlantic). Water-leaving radiance, $L_w(\lambda)$, and the above-surface downwelling irradiance, $E_d(0^+, \lambda)$, were measured using the GER 1500 portable spectroradiometer. The remote sensing reflectance, $R_{rs}(\lambda)$, was calculated from the ratio between $L_w(\lambda)$ and $E_d(0^+, \lambda)$.

The optical measurements from the profilers were compared with water samples measurements collected at several depths. Concentration of phytoplankton chlorophyll-*a* was obtained using the fluorometric method by Welschmeyer (1994). Total particulate absorption spectra, $a_p(\lambda)$, for samples collected on Whatman GF/F glass-fiber filters were measured with an integrating sphere attached to a GER 1500 portable spectroradiometer using the method developed by Mitchell and Kiefer (1984) and the optical-path elongation factor β from Bricaud and Stramski (1990). Methanol-extractable pigments were removed by slowly passing hot methanol through the filter pad (Roesler et al., 1989). The absorption spectrum of this pad were measured to determine the detritus absorption coefficient, $a_d(\lambda)$. The difference between the particulate and detritus spectra,

before and after the methanol extraction, is considered to be the *in vivo* phytoplankton absorption, $a_{ph}(\lambda)$. Optical absorption spectra of the colored dissolved organic matter, $a_g(\lambda)$, were determined with a Perkin Elmer double-beam spectrophotometer following the method described by Bricaud et al. (1981).

3. ESTIMATION OF CHLOROPHYLL *a*

The developed time series models will be used to predict one year ahead the levels of the water quality parameters at the mouth of the rivers based on data from the USGS stations. The probability models will be used to predict the stochastic behavior of such parameters at the mouth of the Añasco, Guanajibo and Yaguez rivers. Statistical models will estimate nutrients at the rivers' mouth and these estimates will be compared with the *in-situ* observations during the sampling campaigns.

3.1 Validation of Redfield Ratios.

Field measurements of nutrients and phytoplankton Chlorophyll-*a* were compared with the Redfield ratios in order to validate their theoretical relationship in Mayagüez Bay. The weight ratio of Carbon to Nitrogen is equal to 5.7 according to Redfield (1958). However, the weight ratio between Carbon and Chlorophyll has been reported between 10 and 75. The large variability in this ratio has been attributed to changes in species composition and population dynamics. We performed several statistical analyses with our nutrients and Chl-*a* data in order to determine the C:Chl ratio. These analyses will strength our forecasting capabilities of the models and will help to better understand the biological and chemical dynamics of the Mayagüez Bay. Table 4 shows the calculated values for the carbon to chlorophyll ratio based on the field data. The rainy season shows higher ratios than the dry season at the surface, while similar values were found at deep waters. More data are necessary to corroborate these results.

Table 4. Ratio values between Carbon and Chlorophyll-*a* in Mayagüez Bay.

Station	Dry Season	Rainy Season
S1s	15	64
S1p	16	26
S4s	N/A	41
S4p	N/A	7
S5s	34	28
S5p	34	19
S9s	43	36
S9p	26	33
S13s	26	13
S13p	40	16
S19s	N/A	63
S19p	N/A	57
S21s	17	66
S21p	8	21
Mean at Surface	27	44
Mean at Deep	25	26
Overall Mean	26	35

3.2 Estimation of chlorophyll a due to river discharge.

Now with the Redfield weight ratio of C:N of 5.7 and the calculated ratios of C:Chl (26 for dry season and 35 for rainy season) we can better estimate the amount of Chl-*a* produced at the mouth of the rivers based on the nutrients from the models of river discharge. The measured Chl-*a* will be compared with this Chl-*a* that comes from rivers and the amount of Chl-*a* that is originated from other sources will be estimated.

PRINCIPAL FINDINGS AND SIGNIFICANCE

A computer program was developed to estimate the level of the water quality parameters at the mouth of the Añasco River. The complete set of equations includes 48 time series models. The necessary equations were evaluated first, and the results were used as inputs for the ANN algorithm to estimate the water quality parameters at the mouth of the river. The oxygen dissolved was arbitrarily selected to exemplify the present results. Figure 5 shows the ANN estimates of the oxygen dissolved (mg/l) at the mouth of the Guanajibo River.

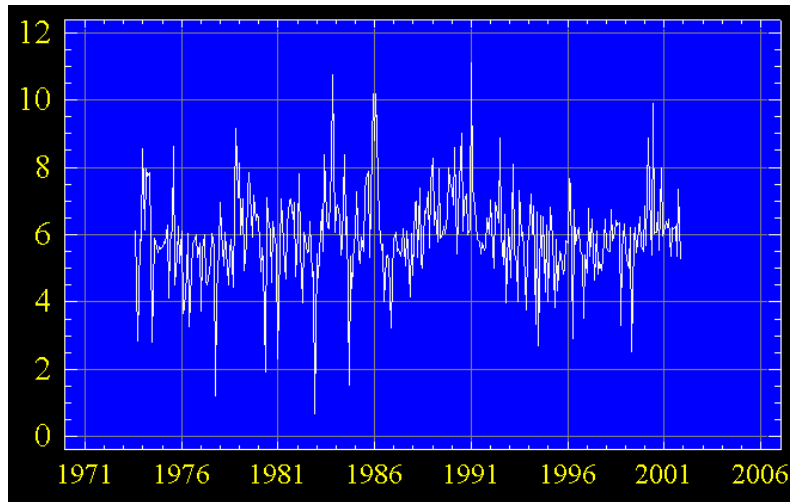


Figure 5. Estimates of Oxygen Dissolved at the mouth of the Guanajibo River.

The first contribution of this research is to develop an adaptive algorithm to estimate the missing values for a given time series. The second contribution is to design an ANN model to estimate the water quality parameters at the mouth of the Guanajibo River. Estimates at the Yaguez River cannot be obtained by the described procedure, since upstream information is not available for this River.

Mayagüez Bay is a highly dynamic environment that shows large spatial and temporal variability of bio-optical properties. Trends in Chl-*a* concentrations measured in this bay during recent years are similar to those measured in the past by Gilbes et al. (1996). A clear Chl-*a* peak in October (Figure 6) is due to the high river discharge during the rainy season that goes from August to November. Stations 1, 13, and 21 are the closest to the rivers mouth and they show the higher concentrations of Chl-*a*.

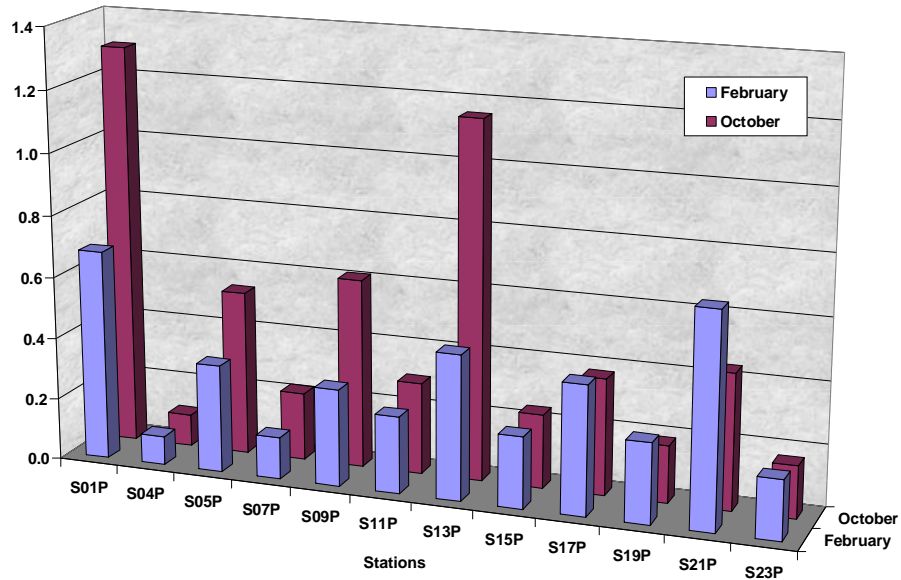


Figure 6. Chlorophyll-*a* concentrations in surface waters of Mayagüez Bay.

The effect of river discharge on the bio-optical properties of Mayagüez Bay is perhaps more clearly presented with the data collected by the bio-optical rosette. For example, a contour map of Chl-*a* fluorescence is presented in Figure 7, showing the higher concentrations closed to the rivers, especially in the rainy season.

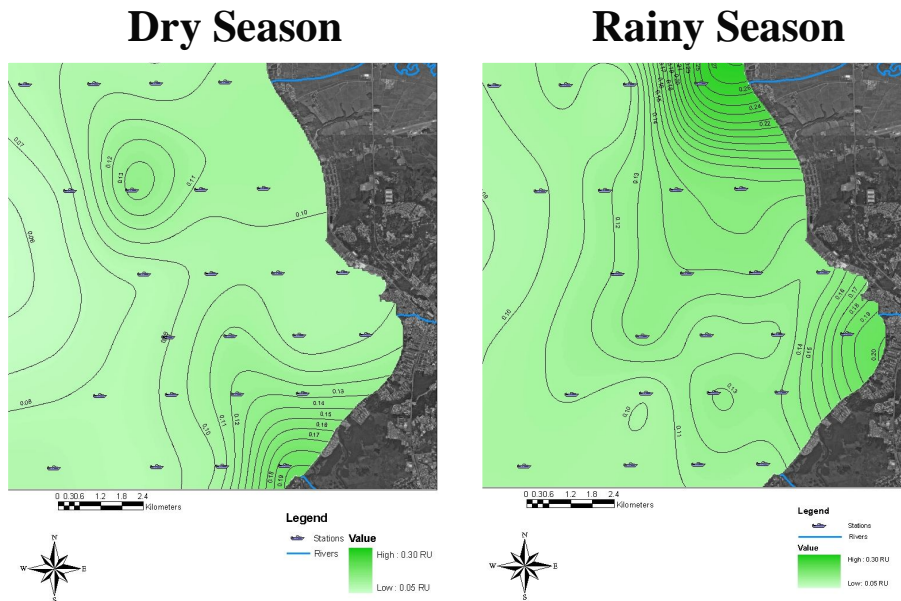


Figure 7. Chlorophyll *a* fluorescence as measured with the bio-optical rosette.

Profiles of bio-optical data are another evidence of the effect of river discharge (Figure 8). Lenses of low salinity and high optical properties (absorption, attenuation, and backscattering) are clearly identified on the top of the water column.

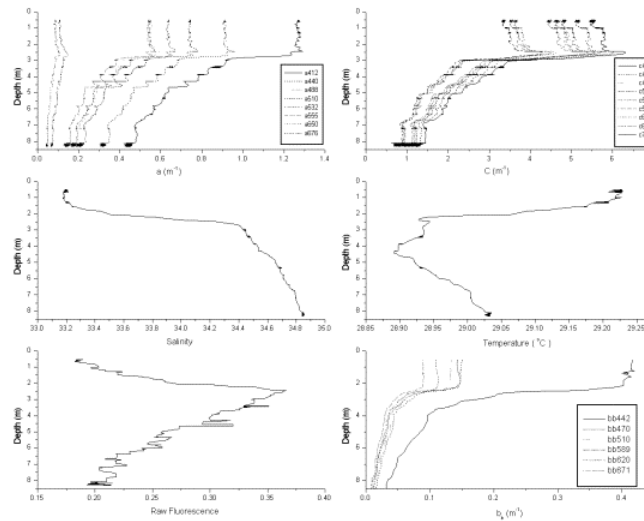


Figure 8. Profiles of water optical properties as measured in one station with the bio-optical rosette.

Changes in bio-optical properties are highly correlated with the river input of suspended sediments. The distribution of suspended sediments follows the seasonality and magnitude of river discharge (Figure 9). During the rainy season (October) the northern stations of the bay show the higher concentrations and during the dry season (February) the southern stations have the higher concentrations. Recent observations demonstrate that this is due to the combination of the bathymetry, wind effect and anthropogenic activities.

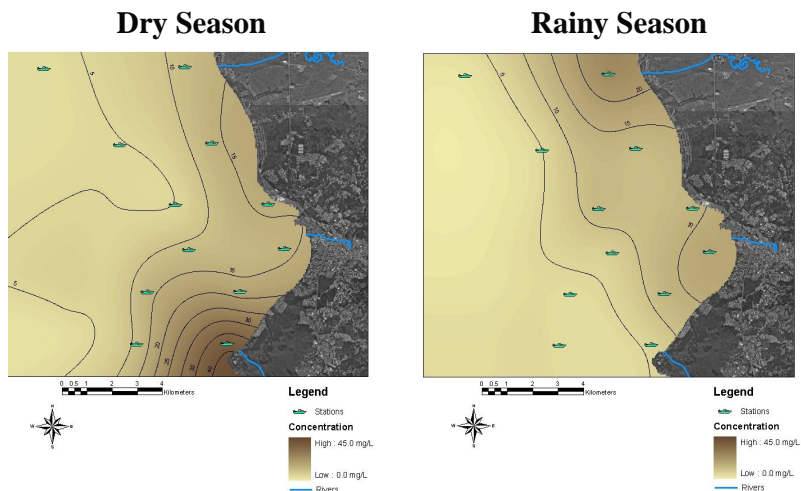


Figure 9. Suspended sediments at surface waters of Mayagüez Bay.

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Publications

This is a list of all publications resulting from work completed during previous budget period.

1. Articles in refereed Scientific Journals

Author (last name, first name)	Ramirez-Beltran, Nazario D.
Other authors (first name, last name)	Fernando Gilbes
Year	2003 (to be submitted)
Title	A Stochastic-Dynamic Model to Predict Fecal Coliforms at the Mouth of the Añasco River
Name of Journal	Water Resources Research
Volume (number)	
Page numbers	
Supporting Section 104 Project No.	(to be filled by the Institute Office)

Author (last name, first name)	Gilbes, Fernando
Other authors (first name, last name)	Roy A. Armstrong, Richard L. Miller, Carlos E. Del Castillo, Marcos Rosado, and Nazario D. Ramirez
Year	2003 (to be submitted)
Title	Bio-Optical Evidence of Land-Sea Interactions in the Western Coast of Puerto Rico.
Name of Journal	Caribbean Journal of Science
Volume (number)	
Page numbers	
Supporting Section 104 Project No.	(to be filled by the Institute Office)

Author (last name, first name)	Rosado, Marcos
Other authors (first name, last name)	Fernando Gilbes, Roy A. Armstrong, Jorge R. Garcia, and Richard L. Miller
Year	2003 (to be submitted)
Title	Spatial and Temporal Variability of Bio-Optical Properties in the Western Coast of Puerto Rico.
Name of Journal	Caribbean Journal of Science
Volume (number)	
Page numbers	
Supporting Section 104 Project No.	(to be filled by the Institute Office)

2. Book Chapters

Author (last name, first name)	
Other authors (first name, last name)	
Year	
Title of the Chapter	
Name of the Editor(s)	
Title of the Book	
Publisher	
City	
State	
Page numbers	
Supporting Section 104 Project No.	(to be filled by the Institute Office)

3. Dissertations

Author (last name, first name)	Rosado, Marcos
Year	2003
Title	Bio-Optical Algorithms for Mayagüez Bay
MS or Ph.D. dissertation?	Ph.D.
Department	Marine Sciences
College	Arts and Sciences
University	University of Puerto Rico at Mayagüez
City	Mayagüez
State	Puerto Rico
Number of pages	N/A
Supporting Section 104 Project No.	(to be filled by the Institute Office)

4. Water Resources and Environmental Research Institute Reports

Author (last name, first name)	
Other authors (first name, last name)	
Year	
Title	
Name of WRERI	
University	
City	
State	
Number of pages	
Supporting Section 104 Project No.	(to be filled by the Institute Office)

5. Conference Proceedings

Author (last name, first name)	Gilbes, Fernando
Other authors (first name, last name)	Roy A. Armstrong, Richard L. Miller, Carlos E. Del Castillo, Marcos Rosado, and Nazario D. Ramirez
Year	2002
Title of Presentation	Bio-Optical Evidence of Land-sea Interactions in the Western Coast of Puerto Rico.
Name of Editor(s)	N/A
Title of Proceedings	Ocean Optics XVI Proceedings
Publisher	Office of Naval Research
City	Santa Fe
State	New Mexico
Page number	N/A
Supporting Section 104 Project No.	(to be filled by the Institute Office)

Author (last name, first name)	Rosado, Marcos
Other authors (first name, last name)	Gilbes, Fernando, Armstrong, Roy and Lee-Borges, Jesus
Year	2002
Title of Presentation	Validation of Bio-Optical Algorithms in the Western Coast of Puerto Rico.
Name of Editor(s)	N/A
Title of Proceedings	Ocean Optics XVI Proceedings
Publisher	Office of Naval Research
City	Santa Fe
State	New Mexico
Page number	N/A
Supporting Section 104 Project No.	(to be filled by the Institute Office)

6. Other Publications

Author (last name, first name)	Ramirez-Beltran, Nazario D.
Other authors (first name, last name)	William Lau, Amos Winter, Joan Castro, and Nazario Escalante,
Year	2003
Title	Empirical Probability Models to Predict Puerto Rico Monthly Rainfall Process
Other information needed to locate publication	17 Conference on Hydrology, 2003 AMS Annual Meeting
Page numbers (if in publication)	Paper number: JP3.22 (7 pages)
Number of pages (in monograph)	
Supporting Section 104 Project No.	(to be filled by the Institute Office)

TRAINING ACCOMPLISHMENTS

A total of 9 students participated in the development of this project. Each student was trained on at least one of the following tasks: (1) data collection (2) data analysis, (3) parameter estimation, (4) computer programming, (5) mathematical optimization, (6) collection of water samples in Mayagüez Bay, and (7) Performing water quality analyses on chemical laboratory.

Field of study	Academic Level				Total
	Undergraduate	MS	Ph.D.	Post Ph.D.	
Chemistry					
Engineering					
Agricultural					
Civil	1				1
Chemical	1				1
Computer	1				1
Electrical					
Industrial	1				1
Mechanical					
Geology	2				2
Hydrology					
Agronomy	1				1
Biology					
Ecology					
Fisheries, Wildlife, and Forestry					
Computer Science					
Economics					
Geography					
Law					
Resources Planning					
Social Sciences					
Business Administration					
Other (specify) Marine Sciences			2		2
Totals	7		2		9