THE SPATIAL DISTRIBUTION OF SELECTED OPTICAL ACTIVE COMPONENTS IN THE GULF OF IZMIT USING BIVARIATE/MULTIVARIATE REGRESSION ANALYSIS

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ABSTRACT

Compared to traditional field-based (in-situ sampling) measurements, satellite-based remote sensing is an accurate, timely and costeffective approach to monitor the dynamics of water bodies using images at different spatial and temporal scales. With satellite-based remote sensing techniques, qualitative measurements obtained directly from satellite images are integrated with in-situ measurements, enabling the establishment of spectral statistical relationships between satellite data and water quality physical indicators such as suspended solids, turbidity and chlorophyll-a. In this study, the spatial distribution of three water quality parameters (Chlorophyll-a (Chl-a), Secchi disk and Conductivity (EC)) which are optical active components (OAC) in the Gulf of Izmit were evaluated using insitu water quality measurements, together with both field-spectroradiometer measurements and Sentinel-2 satellite imagery. In-situ water quality and field-spectroradiometer measurements were collected at the same date with the satellite overpass. Bivariate and multivariate regression models were established to analyse the correlation of in-situ water quality measurements with two different measurement datasets (i.e. satellite and spectroradiometer), and then the results were evaluated with two accuracy metrics Root Mean Square Error (RMSE) and Mean Absolute Error (MAE); and compared visually with the spatial distribution maps of the three water quality parameters generated by the ordinary Kriging interpolation method.

1. INTRODUCTION

Coastal areas, where approximately 40% of the world's population live, are among the most sensitive environments, as any change in these ecosystems resulting from anthropogenic activities could endanger the entire marine ecology (Gholizadeh et.al., 2016). Therefore the quality of water bodies is an important issue for the health of coastal ecosystems and is under the influence of human activities and climate change. As a result of the deterioration of water quality, water pollution events such as harmful algal blooms (Karlson et al., 2021), hypoxia (Lai et al., 2022) and mucilage (Sunar et al., 2022) occur. Field-based (insitu sampling) measurements that rely solely on frequent and/or long-term samples as a traditional approach cannot fully address the spatio-temporal variation of water quality in any watershed. Consequently, an integrated water conservation and reclamation approach is required for effective water quality monitoring, in which long-term field-based measurements can be used in conjunction with space technologies such as remote sensing. In other words, integrating traditional data collection with remote sensing technology today provides an effective monitoring approach for the dynamics of water bodies using images at different spatial and temporal scales (Hu et al., 2022; Zhu et al., 2022).

As known, the optically active constituents (OACs) (such as suspended sediments, colored dissolved organic matter (CDOM), chlorophyll-a (Chl-a) etc.) present in natural water bodies have inherent optical properties (IOPs) that affect the water's ability to absorb light. In order to determine underwater light dispersion, the photosynthetic process, and remote sensing reflectance, the IOPs of the individual OACs in the area are crucial (Shi et al., 2017). Many studies showed that water quality parameters can be retrieved with varying accuracy, as the spectral properties of water change depending on the interaction between solar radiation and OAC (Pizani et al., 2020). However, other water quality constituents, such as nutrient concentrations, dissolved oxygen levels, and microorganisms/pathogens, cannot be directly estimated by remote sensing data as they are not optically active; i.e. they may be estimated indirectly but still remains a big challenge (Sagan et al., 2020). In general, statistical regression models (bivariate and multivariate) that are often considered site-specific, are established to quantify measured reflectance – OAC relationships.

For monitoring the pollution and its effects on seas and coastal waters in Turkey, the Ministry of Environment, Urbanisation and Climate Change has conducted an Integrated Marine Pollution Monitoring Program (DEN-IZ) in cooperation with the Scientific and Technological Research Council of Turkey - Marmara Research Center (TUBITAK-MAM) since 2014. The scope of this program is to carry out in-situ measurements and analyses of water quality parameters at the designated stations in all seas (i.e. Black Sea, Marmara Sea and the Straits, Mediterranean and Aegean Sea), and then to report the results and evaluations periodically (Url-1). Gulf of Izmit, known as one of the most polluted marine ecosystems of Turkey and located in the east of the Marmara Sea, is one of the fragile coastal areas evaluated within the scope of the mentioned DEN-IZ program. In this study, the spatial distribution of the three OACs (Chl-a, Secchi disk and Conductivity) was evaluated using in-situ water quality measurements, together with handheld field spectroradiometer measurements and Sentinel-2 satellite imagery obtained simultaneously. For this purpose, the correlation of in-situ water quality measurements with two other different measurement datasets (satellite and spectroradiometer) was established with regression models and the results were evaluated with accuracy metrics.

2. STUDY AREA

The Gulf of Izmit, which is a semi-enclosed coastal ecosystem located in the east of the Marmara Sea, chosen as the study area, has an area of approximately 310 km², 60 km long and 2-10 km wide (Tugrul et al. 1989) (Figure 1). Due to salinity differences, stratification in the water column occurs throughout the year (Ergul et al., 2018).



Figure 1. The map of Gulf of Izmit and location of 17 in-situ sampling points in Sentinel-2 satellite image (© Copernicus).

Kocaeli province, located in the Gulf of Izmit, is known as a city with a giant natural harbor. The fact that the region has different natural potentials that are promising and that can attract many investors has led to the intense use of these coastal areas under many factors such as natural environment characteristics, human structure, industrial activities and transportation routes (Garipagaoglu and Uzun, 2014; Ergül et al., 2018). Hence, in the province, which has a current population of approximately 2 million people, a significant amount of uncontrolled sewage, industrial and agricultural wastes are discharged to the Gulf as a result of the increasing population and industrial activities since the 1980s (Figure 2).



Figure 2. Locations of main freshwater input source points and wastewater treatment plants in the eastern, central and western basins of the Gulf of Izmit (adapted from Ergül, 2016; Tolun et al., 2012).

3. MATERIALS AND METHODOLOGY

3.1 Materials

Sentinel-2 satellite image acquired on October 21, 2021 was used in the study. Sentinel-2 satellite images can be obtained free of charge by the European Space Agency in different processing levels such as Top-Of-Atmosphere (TOA) and Bottom-Of-Atmosphere (BOA). Its spatial resolution varies in different wavelength ranges (VNIR - SWIR spectral range) as 10 m, 20 m and 60 m. The spectral resolution of Sentinel-2 data, which has an open data access policy, is given in Figure 3.



Figure 3. The spectral resolution of Sentinel-2 data (©ESA).

In the study, BOA satellite image data was used together with 17 simultaneous spectroradiometer measurements and in-situ water quality measurements. The in-situ measurements are homogeneously distributed along the Gulf (Figure 1). The spectra of the points were measured by the hand-held ASD FieldSpec 4 with a spectral range of 325-1075 nm (Figure 4). 13 of the measurements were used in the regression models and 4 samples were reserved for accuracy assessment. The spectral values exhibit a similar tendency, with the exception of a few sampling locations.



Figure 4. Spectra of 13 in situ points measured with handheld ASD FieldSpec 4 and location of Sentinel 2 spectral bands.

3.2 Methodology

The methodology used consists of three main stages: i) surface analysis of three selected water quality parameters using the Kriging interpolation method; ii) establishing an empirical relationship (e.g. bivariate and multivariate regression) between the water-leaving radiance measured by the sensor (i.e. BOA reflectance values - individual or combinations of spectral bands) and in-situ water quality measurements; iii) the use of statistical accuracy metrics to evaluate the accuracy of the models accepted.

3.2.1 Kriging interpolation method: One of the geostatistical interpolation techniques used for modeling spatial data is the Kriging approach (Prusova et.al., 2012). This method is widely used in a water quality analysis to estimate the values of unmeasured water quality parameters and to analyze spatial distribution patterns of the parameters of interest. In this study, the ordinary Kriging interpolation method was applied for the surface analysis of the selected three water quality parameters and then compared with the results of the regression models (produced by satellite data and field spectroradiometer measurements) used to estimate these parameters.

3.2.2 Regression analysis: In this study, bivariate and multivariate linear regression analyses were performed for the aforementioned three OAC components. As a common statistical method, regression models are an efficient tool for investigating the relationship between variables, even when small sample size

variables are used (Razi and Athappilly, 2005). Linear regression models, also called simple bivariate regression, evaluate the linear relationship between two variables (i.e. dependent and independent variables) based on the least squares, and the best model has minimum square error between the observed and predicted parameters (Zare Abyaneh, 2014).

Multivariate linear regression (MLR), an extension of bivariate linear regression, is a common statistical modeling technique to explain a dependent variable with more than one independent variable. More clearly, MLR is used to predict a response variable (y) from multiple explanatory variables $(x_1, x_2, ..., x_n)$ to represent the linear relationship between many independent predictor variables (spectral bands) and a single dependent variable (a water quality parameter such as Chl-a) as a single functional formula (Shi, 2017).

As noted in the literature, correlations between in-situ water quality measurements and spectral reflectance values can be complex and nonlinear, especially for Case 2 water bodies (such as Gulf of Izmit), as these parameters respond differently to various spectral wavelengths (Gholizadeh et al., 2016; Hafeez et al., 2019; Topp et al., 2020). Therefore multivariate regression was also used in this study, assuming that there is no strong correlation between each independent variable, as the estimation of each OAC may depend on more than one independent variable (i.e. more than different bands or combinations). As a result, bivariate and multivariate linear regression analyzes were performed by using two different datasets; i) in-situ water quality measurements and satellite imagery and ii) in-situ water quality measurements and field spectroradiometer measurements. The best models in these two scenarios were evaluated using Root Mean Square Error (RMSE) and Mean Absolute Error (MAE).

3.2.3 Model performance evaluation: After the regression models are built, the goodness of fit of the model and the statistical significance of the estimated parameters need to be confirmed. Most commonly used p-value is the most important step to accept or reject a null hypothesis. More specifically, if the p-value is less than a common threshold (e.g. 0.05), the null hypothesis is rejected, indicating a relationship between the variables.

In order to evaluate the performance of the models used in regression analysis, R-squared (a measure to determine how well the model fits the dependent variables), Root Mean Square Error (RMSE - popular metric that shows how close the estimate is on average to the actual value, but also indicates the effect of large errors) and Mean Absolute Error (MAE - similar to the RMSE, the MAE is an indicator of how close the estimates are, on average, to the actual model) given in the Equations below were used and the accepted models for the selected parameters were tested using with in-situ measurements allocated as test data.

$$R^{2} = 1 - \frac{\sum_{i} (y_{i} - \hat{y}_{i})^{2}}{\sum_{i} (y_{i} - \overline{y})^{2}}$$
(1)

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y})^2}{n}}$$
(2)

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i|$$
(3)

where y_i is the measured value, \hat{y}_i is the estimated value and n is the number of measurements.

In general, the higher the R-squared, the better the model fits the data. On the other hand, the lower values of RMSE and MAE indicate higher accuracy of a regression model (i.e. the model estimates correctly).

4. RESULTS

First, the ordinary Kriging interpolation method was applied for the surface analysis of the selected three water quality parameters and spatial distribution maps produced are given in Figure 5. Four unused samples were considered for the accuracy assessment of each Kriging model and the results are given in Table 1.



Figure 5. The spatial distribution patterns of three selected water quality parameters produced by the ordinary Kriging interpolation method.

In Figure 5, it is clearly seen that the eastern basin (i.e. interior) and some parts of the central basin close to the eastern basin are more polluted (high Chl-a and low Sechi disc values) than other parts of the basin. The decrease in Chlorophyll-a values (primary production indicator) from the eastern basin to other regions is clearly evident and realistic in the Kriging model, because the interior basin has high pollutant load and low water circulation (Tuğrul and Morkoc, 1990). The eastern basin is influenced by industrial and domestic loads, particularly from the Kiraz (Kul-lar) and Kumla (Sarı) streams, and nutrient and chlorophyll-a levels confirm the findings (Figure 6) (Tan and Aslan, 2020).



Figure 6. Locations of Kiraz and Kumla streams connected to the interior basin.

Secchi disc visibility is likewise lowered where chlorophyll-a levels are high. In Figure 5, a sharp line in the Kriging interpolation method, especially in chlorophyll-a, is caused by the low number of in-situ measurements used in the model, so it does not fully reflect the real situation and a distribution as in Figure 7 is found to be more appropriate.

Although conductivity is considered an indirect indicator of pollution, it is a good parameter for determining water quality, as it presents a close relationship with the dissolved salt content in the water column of coastal water bodies, which is often associated with sewage discharge (Tolun et al., 2012; de Sousa et al., 2014; Eyuboglu and Eyüboğlu, 2020). Therefore, high EC values, which can generally be associated with the presence of domestic wastewater, confirm the high conductivity values, especially in the eastern and central basins (Figure 2).

In order to find the best estimator of the 3 selected water quality parameters in the Gulf of Izmit, bivariate and multivariate linear regression models were used. The best regression models selected for Chl-a, Secchi disk and Conductivity parameters in two different measurement datasets (i.e. Sentinel-2 Level 2A and field spectroradiometer) are given in Table 1. Again, four unused in-situ measurements were considered for the accuracy assessment of each model developed. The best regression models selected and the spatial distribution of the 3 parameters produced using these selected models are given in Figure 7.

Parameter	Variables	Data	Model	t	Significance (p-value)	F	Standard Error	R	R ²	RMSE	MAE
Chl-a	Kriging	•	•	•					_	4.237	2.328
	B4/B2	Spectroradiometer	Bivariate	5.40	0.0002	29.20	5.83	0.85	0.73	8.605	7.822
	B3 B4	Spectroradiometer	Multivariate	-0.03 0.79	0.125	2.57	9.49	0.58	0.34	3.863	3.313
	B3/B2	Sentinel-2	Bivariate	4.15	0.002	17.19	6.96	0.78	0.61	4.671	3.394
	B2 B3 B4	Sentinel-2	Multivariate	-3.03 1.14 0.14	0.028	4.90	7.59	0.79	0.62	3.068	2.353
Secci disk	Kriging	-	-	-					-	0.436	0.126
	B4	Spectroradiometer	Bivariate	-1.38	0.20	1.89	2.13	0.38	0.15	1.102	0.967
	B3 B4	Spectroradiometer	Multivariate	0.18 -0.61	0.44	0.88	2.23	0.39	0.15	0.744	0.545
	B4/B2	Sentinel-2	Bivariate	-5.79	0.0001	33.49	1.14	0.87	0.75	4.118	3.356
	B2 B3	Sentinel-2	Multivariate	6.34 -7.51	0.0001	30.65	0.90	0.93	0.86	1.373	1.262
Conductivity	Kriging		•	-					-	0.265	0.188
	B2+ B8A	Spectroradiometer	Bivariate	-3.25	0.008	10.58	0.36	0.70	0.49	0.285	0.227
	B2 B8A	Spectroradiometer	Multivariate	-1.06 -0.58	0.034	4.82	0.38	0.70	0.49	0.260	0.198
	(B3- B4)/B2	Sentinel-2	Bivariate	3.31	0.007	10.97	0.36	0.71	0.50	0.340	0.308
	B2 B3 B4	Sentinel-2	Multivariate	-2.26 1.64 -1.15	0.067	3.40	0.38	0.73	0.53	1.771	1.765

Table 1. The bivariate and multivariate regression models used for three water quality parameters on two different measurement datasets (the best predictive models selected are marked in bold).

As seen in Table 1, the multivariate regression model constructed using Sentinel-2 image (with bands B2, B3, and B4) estimated Chl-a concentrations with an R² value of over 60%. Also, this model has the lowest RMSE and MAE errors, i.e. 3.07 and 2.35, respectively. On the other hand, the spatial distribution of this model was found to be highly compatible with the Chl-a model produced by the Kriging interpolation method. Although the estimation of the spectroradiometer dataset for this parameter was higher with the bivariate model (i.e. R² \approx 73%), however, both accuracy measures were found to be high and their spatial distribution did not appear to be compatible with the surface model produced by the Kriging interpolation method (Figure 6).

For Secchi disk parameter retrieval, the multivariate model using the two spectral bands of the Sentinel-2 image (i.e. B2 and B3 bands) outperformed (i.e. high R^2 value; 86%) all models built with the spectroradiometer dataset. Although the multivariate model created with the spectroradiometer data set had the lowest RMSE and MAE accuracies, the R^2 values were found to be quite low (i.e. 15%).

Spectroradiometer dataset with bivariate model provided greater RMSE and MAE accuracies for the last parameter, Conductivity parameter retrieval, compared to Sentinel-2 image data, despite R² values being in almost the same range (i.e. 49% $\approx 50/53\%$).



Figure 7. The spatial distribution patterns of three selected water quality parameters produced by the best regression models selected.

When two figures (Figure 5 and Figure 6) showing the spatial distribution patterns of three selected water quality parameters were compared, it was observed that the results for Chl-a and Secchi disk characteristics were quite comparable. On the other hand, it was determined that the models' compatibility and comparability for the conductivity parameter were quite low, therefore further analysis is still required.

The results of this study demonstrate that improvements are still required for the generalization and transferability of the established models for other basins in the Marmara Sea with regard to the accuracy of the estimation of these three OACs. Additionally, it is thought that the variations seen for all parameters may also result from stratified formations that alter the distributions of water quality parameter along the water column of the Gulf of Izmit and from meteorological conditions that affect oceanographic features (Ergul, 2016).

5. CONCLUSIONS

In this study, bivariate and multivariate linear model accuracies of three OACs in the Gulf of Izmit were evaluated using satellite data. The findings show that pollutants in wastewater from residential and industrial regions, particularly in the inner and middle parts of the Gulf, have a negative impact on the water quality. The results of the established models were found to be relatively consistent with in-situ measurements of water quality parameters, but it is thought that more extensive field measurements and different satellite datasets across the Gulf should be used to improve the results.

Despite its potential, there are several issues in water quality monitoring using space-borne remote sensing that need to be addressed before the developed prediction models can be adapted for operational use in the Marmara Sea; i) since the Gulf of Izmit is a coastal inland body of water, it contains optically active components at various concentrations, making it difficult to utilize, compare, and apply the prediction models created in other basins in the Marmara Sea; ii) since the optical properties of these waters are complex and change over time, the seasonal and annual fluctuations of these parameters need to be evaluated using a wider range of in-situ data collection.

As a continuation of this study, the models created in October 2021 will be tested with additional in-situ measurements and spectroradiometer data performed in October 2022, and their utility and compatibility of the models will be evaluated in order to reduce the aforementioned problems.

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