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Research Article

Comparison of Grain Size Trend Analysis and Multi-Index Pollution Assessment of Marine Sediments of the Gülbahçe Bay, Aegean Sea

Ezgi Talas[1,*], Muhammet Duman [1,2]

[1] Dokuz Eylül University, The Graduate School of Natural and Applied Sciences, Izmir, TÜRKIYE
[2] Dokuz Eylül University, The Institute of Marine Sciences and Technology, Izmir, TÜRKIYE

* Corresponding author: E. Talas

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Abstract

In this study, 46 elements plus total carbonate and total organic carbon contents were measured in 48 sea bottom sediments to determine the pollution levels in the study area and their source to understand better the natural and anthropogenic processes in the study area. Also current flows and sediment transport pathways inferred using multidisciplinary methods by interrelation between grain size trend analysis, shallow seismic and acoustic doppler current profiler analysis to unravel the hydro-sedimentary processes in a micro-tidal environment. Four main factors that were affecting the study area were identified as lithogenic factor (50.6%) anthropogenic factor caused by untreated domestic waste (13.2%), anthropogenic factor caused by marine traffic/port activities (9.3%) and anthropogenic factor caused by small-scale industrial activities (with 6.9% of the total variance). The main source of metals in the study area were determined as untreated domestic waste discharges (total organic carbon and sulfur), maritime traffic/harbor activities (copper and zinc), and discharges of other wastes caused by urbanization. The main metal element that poses the most significant risk for benthic organisms was determined as nickel in the study area. All environmental indices showed non to moderate pollution existing in Gülbahçe Bay. It has been observed that most prominent feature of the distribution of elemental concentrations and assessment of pollution indices were that the pollutants carried inwards to Gülbahçe Bay from Izmir Central Bay with inflows, following the sediment transport directions.

Keywords: Pollution indices, PCA, STA, *Posidonia oceanica* habitat map, Gülbahçe Bay (Aegean Sea)

Introduction

Sediments can be transported from terrestrial environments to marine environments by many different parameters such as rivers, streams, etc (Zhao et al., 2016; Li et al., 2019). These parameters carry both the clastic sediments and pollutants such as metal particles and organic pollutants that were produced by anthropogenic activities (Li et al., 2007). The heavy-metal particles accumulate within clay minerals that absorb metal ions in their structure in aquatic environments. They follow a fine-grained (mud=silt+clay) sediment trend and accumulate the deposition zones that are rich by fine sediments (Herut and Sandler, 2006). Thus, can cause critical risks to the durability and stability of marine ecosystems.

The pollution assessment indices are the most widely used statistical method to identify and classify the level of chemical pollution in aquatic environments by researchers and government authorities by worldwide. Most of these indices have used metal accumulation levels in sediment, water or biota samples to estimate the environmental and biological risks in study areas (Kowalska et al., 2018). The Principal Component Analysis (PCA) is another most widely used multivariate statistical analysis methods to identify the sources of trace metal particles in marine sediments by researchers (Garcia et al., 2023). The grain size trend analysis (GSTA) is a statistical technique that uses the relative changes in grain-size shape and distributions that are naturally formed according to affecting environmental parameters to reveal the pattern of sediment transport (McLaren et al., 2007). Interpreting granulometric parameters of sediments can be very informative about sediment formation, transportation features, deposition of clastic sediments, and factors which they were affected by along these processes in aquatic environments. It could also be used to identify the element accumulation pathways. These multidisciplinary methods can be used to understand different parameters and their sources that shape main effects in environment in deep.

Posidonia oceanica (L.) Delile is a marine phanerogam endemic to the Aegean and Mediterranean Seas that were called as the lungs of the seas as they are the main source of oxygen in seawater with their ability to mass photosynthesis in marine ecosystems. These meadows form widely distributed habitats that provide a nursery for other marine organisms so they represent a key ecosystem in shallow water or tropical coastal areas (Pasqualini et al., 1998; Demir et al., 2016; Okuş et al., 2004, 2006, 2010). *P. oceanica* grows up on the sandy sea bottom with the help of its horizontal rhizomes and catches solid materials in the water column with its leaves. Thus, causes water clarification by reducing turbidity. They also act as a barrier against coastal erosion and severe wave movements or currents by stabilizing the sea bottom surface. *P. oceanica*'s rhizomes can adsorb radioactive materials, synthetic chemicals and heavy metals, because of this they can be used as biological indicators for monitoring the quality of coastal waters (Pasqualini et al., 1998; Lionello et al., 2006; Demir et al., 2016). The existence of the *Posidonia oceanica (L.) Delile* meadows affects the both water flows and sediment trend parameters thus, affecting metal accumulation parameters in aquatic environments.

During this study, a data set with 51 variables that were determined by different geotechnical and geochemical analyses was used to determine and classify the factors and sources of these factors, which were effective in the study area such as anthropogenic, lithological, natural, etc. The results were compared with multi-index pollution assessment outcomes to determine the severity of environmental contamination in the study area. The source of pollutants in the area and the effect of hydro-sedimentological parameters that shaped the transport trend of the pollutants, that caused the severity of contamination by metal accumulation and risk for benthic organisms, and the regions that were most affected by these parameters were determined.

Geological Setting

The Gülbahçe Bay is located at the west of Türkiye and part of Izmir Gulf which is one of the largest gulfs situated in the northeast of the Aegean Sea (Fig.1A). The Izmir Gulf is a naturally formed gulf divided into three main regions according to its bathymetric features; inner, central, outer gulf and Gülbahçe Bay (Fig.1B). The Gülbahçe Bay can be classified as a separate region because it is relatively isolated from these other areas. The Aegean Sea has been under the influence of the Alpine mountain formation belt, the Hellenic arc system, and the Taurus mountain formation belt until the last geological period (McKenzie, 1972; Le Pichon and Angelier, 1979; Okay and Satır, 2000). The geological formations around the Izmir Gulf range from Precambrian aged units to overlying Neogene and Quaternary aged units (Emre et al., 2005) as given in Fig.1B.

Materials and Methods

Sample and Data Collection

This study was conducted on 48 sea bottom sediment samples from the Gülbahçe Bay (Fig.1C) to understand anthropogenic and hydro-sedimantologic parameters. Surface samples were obtained during the Scientific and Technological Research Council of Türkiye (TÜBİTAK) 1001-Funding Program (Project no: 115Y180) cruise in 2016. The research project was carried out by the Institute of Marine Sciences and Technology of Dokuz Eylül University.

During the study, the differential global positioning system (DGPS-Ashtech ProMark 500 RTK GPS rover and rover/base system) was used to determine sampling locations. All samples were collected within a grid system that was parallel to the coast.

The 48 sea bottom surface sediment samples were collected within a 2000m mesh range out of region to determine the sedimentary and geochemical parameters that generally affect the study area. The sediment samples were obtained by a stainless steel Van Veen grab sampler in shallow water and by a box corer in deeper areas.The first ~2 cm of sea bottom sediment (fluff layer) was sampled for chemical laboratory analyses because they have the best chance to imply anthropogenic effects as they categorize recently deposited sediments. The sediments under the fluff layer were collected for geotechnical grain size analysis, results were interrelated with fluff layer grain size results for fine (Mud=Silt+Clay) grain percent and coarse (Gravel+Sand) grain percent.

The location map of Izmir Gulf (Fig.1A) was created by the raster elevation products of Global Multi-Resolution Terrain Elevation Data 2010 (USGS/EROS Archive, 2010). The bathymetric relief and contour map (Fig.1B and Fig.1C) were created by digitized depth data from the IHO-S57_TR300221 vector map (IHO, 2009). The geological map (Fig.1B) was created by digitization of image of the Editor of GeoScience MapViewer and Drawing website of General Directorate of Mineral Research and Exploration (MTA) (Akbaş et al., 2011; Emre et al., 2013).

The base map of Gülbahçe Bay was created by multispectral data of Landsat 8 Operational Land Imager (OLI) and Thermal Infrared Sensor (TIRS) Images (USGS/EROS Archive, 2019). The four-band (Band 7,4,2,8) of the *LC08-L1TP-181033-20190823-20200826-02-T1* image was processed with ESA-SNAP Image Processing Software; the images were layer stacked and HPF resolution was merged to create a raster image layer that was used as a base layer to create grid maps. The SURFER Ver.21 Software was used to create maps in the study. The oceanographic data processed with OCEAN DATA VIEW SOFTWARE 2023 (Mieruch-Schnülle and Schlitzer, 2023).

Laboratory analysis

The fluff layer sediment samples were used for chemical analysis (multi-element, total organic carbon and total carbonate analyses). They transported inside the cooler box and dried in a freeze-dryer (Labconco) before they were homogenized and sieved through 63 µm mesh for grain size (Mud=Silt+Clay fractions) correction and also percent of the fine/coarse sediment contents recorded for comparison to non-fluff layer sediments samples which used for grain size analysis from the same station.

The total organic carbon (TOC) in samples was calculated through measured total organic matter content (TOM) according to Muller, 1967 method. The TOM content was measured with the spectrophotometric method modified after Walkley-Black (1934) estimation of soil organic carbon by the chromic acid titration method (Hach, 1988). The precision of this method is ±0.017% organic matter in sediment samples.

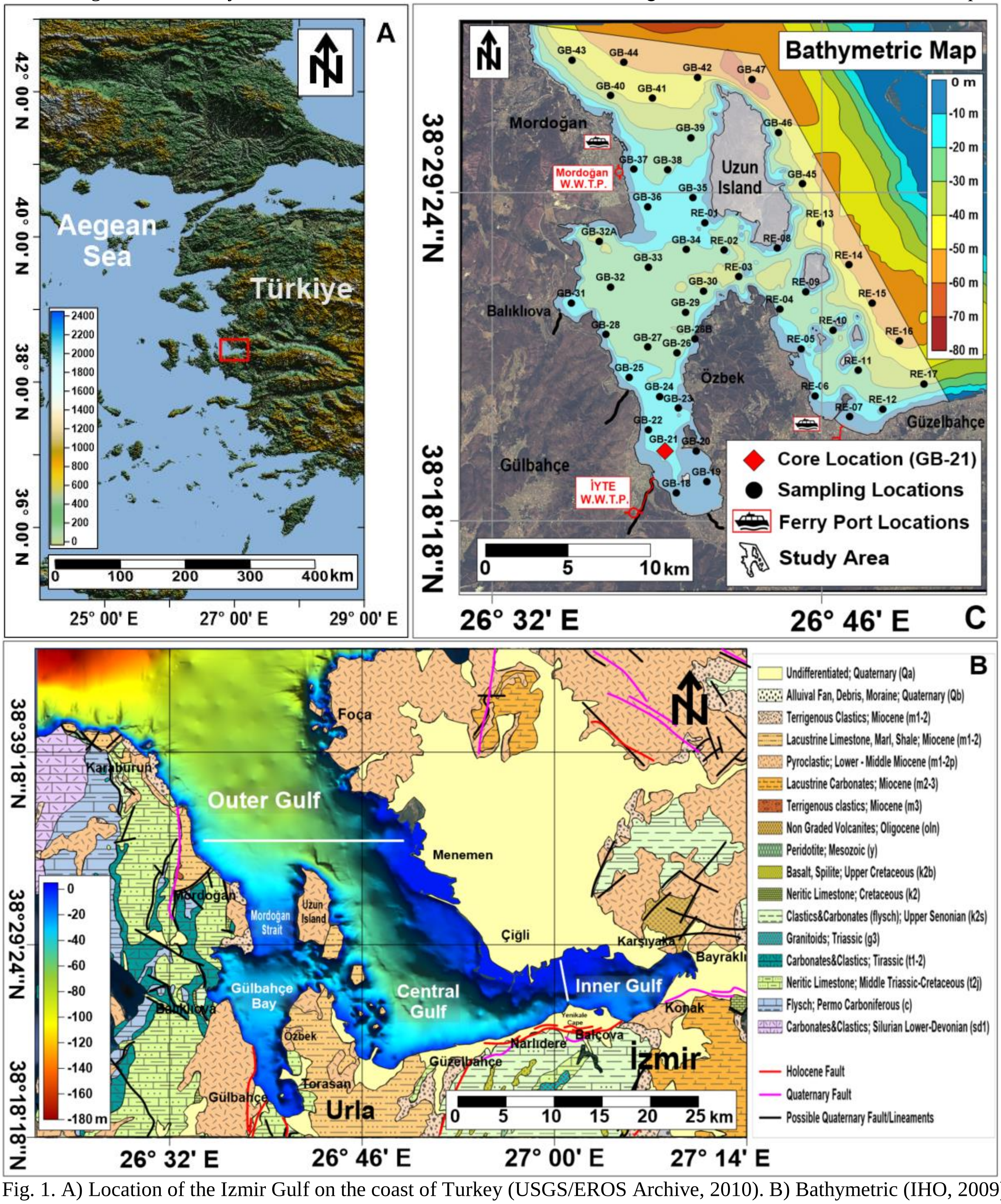

Fig. 1. A) Location of the Izmir Gulf on the coast of Turkey (USGS/EROS Archive, 2010). B) Bathymetric (IHO, 2009) and geological map (Akbaş et al., 2011; Emre et al., 2013) around the study area. C) The surface sediment sampling locations and one core location on bathymetric map.

A 0.5 g of prepared fluff layer sediment sample from each sampling location used in analysis and final solution read using 610 nm absorbance with a spectrophotometer.

The Piper (1977) method was used for determination of the total carbonate ($CaCO_3$) in the samples. This method is a combined version of carbonate determination methods by Carver (1971), and Grimaldi et al. (1966). The results of this analysis are accurate to within approximately 1% in carbonate-rich sediments. A 0.5 g of prepared fluff layer sediment sample from each sampling location used in analysis.

The inductively coupled plasma emission/mass spectrometry (ICP-ES/MS) analysis method uses a high temperature of the inductively coupled plasma causes changes in the conditions forming the analysed sample, and it allows the dissociating of the components of the sample almost completely into atoms and separating many elements in the periodic table down to their individual ions. These single ion concentrations can be measured with the detector connected to the emission/mass spectrometry system and the exact amounts of the elements in the sample can be found in ppb, ppm or percentage (Evans, 2005).

Through this method, the amounts of 45 elements (Ag, Al, As, Ba, Be, Bi, Ca, Cd, Ce, Co, Cr, Cu, Fe, Hf, Hg, In, La, Li, Mg, Mn, Mo, Na, Nb, Ni, P, Pb, Rb, S, Sb, Sc, Se, Sn, Sr, Ta, Te, Th, Ti, Tl, U, V, W, Y, Zn, Zr) were determined in sediment samples of study area. A 5 g of prepared fluff layer sediment sample from each sampling location were sent to the Bureau Veritas Commodities Canada Ltd. Mineral Laboratories (AcmeLabs) for ICP-ES/MS analysis with service code: MA200 plus AQ200-Hg) with multi-acid digestion (HNO_3, $HClO_4$, HF and HCl) was used for this study. The data quality was checked using certified reference sediment sample (Standard STD OREAS262 and STD OREAS25A-4A).

Grain size analyses are used for classifying sediments according to their grain size distributions by percentages of gravel (>2 mm.), sand (2 mm-63µm), silt (63 µm-20 µm) and clay (<20 µm) sediment with the determination of the particle size and its weight in the total mass in percent value (Duman et al., 2012).

The classification of sediments was determined by four-step geotechnical analysis. The particle-size analyses were carried out on 48 sea bottom surface sediment samples which sampled from under the fluff layer. A 500 g to 1 kg sample was firstly washed through ASTM No.200 sieve (<75 µm) to separate the coarse and fine fractions. After washing, prepared samples were tested according to the particle size analysis-dry sieve method (ASTM D421, ASTM D422, AASHTO T87, AASHTO T88; Bowles, 1992) and particle-size analysis-hydrometer method (ASTM D421, ASTM D422, AASHTO T87-86 (1990) and AASHTO T88-90; Bowles, 1992).

For specific gravity of sediment analysis, 200 g of dry sediment (dried at 50°C) sample was sieved through ASTM Sieve No 10 (2 mm) sieve to separate shells in the sample before being tested according to specific gravity of sediment analysis (ASTM D854 and AASHTO T100; Bowles, 1992).

In this study, sediment grain size analyses were performed with classical geotechnical grain size analysis method, and the proportions of sand, silt and clay were determined according to Folk (1980).

Geochemical and Geostatistical Analysis

During this study, different environmental assessment indices were applied to geochemical data to evaluate the pollution status of Gülbahçe Bay. The equations and categorizations of the contamination indices used in this study are given in the supplementary section Table S1 and Table S2, respectively.

The Normalized Total Organic Content (TOC_N) was an index suggested by Molvær et al. (1997) that was described as a normalization of total organic carbon (TOC) according to fine sediment (<63 µm) percent to determinate the environmental condition of area (Carroll et al., 2003).

The Contamination Factor (C_f) was an index suggested by Håkanson (1980) that indicates the metal accumulation rate in the sediment of the location, which is based on the linear ratio between the mean value of the concentrations of a particular metal in the samples taken from the entire region to the preindustrial local concentrations of same metal in the area. This index used to determine the pollution levels according to local contaminant concentrations and it was also main index that based on to calculate the C_{deg}, mC_d, PLI and PI_{Nem} indices. In this study, to calculate the C_f, the GB-21/125-128 cm sediment sample's element concentrations used as preindustrial local (Ref._1) background concentrations (Table 1). The GB-21 core sample with 128 cm length was taken from the Gülbahçe Bay (Fig.1C). The C_{deg} index was proposed by Håkanson (1980) and used to determine the pollution degree of the study area by using seven specific metal concentrations (As, Cd, Cu, Cr, Hg, Pb, Zn) and one other pollutant (Håkanson, 1980 used PCB), which can be considered as markers for anthropogenic effect. In this study, the organic pollutant (polycyclic aromatic hydrocarbons-PAH or environmental poisons like PCB, DDT, etc.,) determination in sediment was not one of the experiments were performed thus PCB parameters was not involved in the calculation.

Table 1. The local, global reference values and detected concentration of metals in study area (in mg/kg).

	As	Cd	Cr	Cu	Hg	Ni	Pb	Zn	References
Local Referans (Ref._1)	12	0.07	85	16.1	0.08	42	32.3	121	Core_ GB-21/125-128
Global Referans (Ref._2)	13	0.3	90	45	0.4	68	20	95	Turekian and Wedepohl (1961)
Ref._TEL	7.24	0.68	52.3	18.7	0.13	15.9	30.2	124	TEL – PEL Guid. (Macdonald et al., 1996)
Ref._PEL	41.6	4.21	160	108	0.7	42.8	112	271	
Ref._ERL	8.2	1.2	81	34	0.15	20.9	46.7	150	ERL – ERM Guidelines (Long et al., 1995)
Ref._ERM	70	9.6	370	270	0.71	51.6	218	410	
*****This study samples (min./max., mean±std.dev.)***	*9.0/39.0 17.5±5.6*	*0.1/0.6 0.09±0.08*	*23.0/309.0 89.31±48.2*	*6.0/33.0 17.38±6.9*	*0.1/0.7 0.2±0.1*	*19.1/130.3 59.4±29.3*	*14.2/38.6 25.5±6.0*	*24.0/196.0 65.9±29.7*	

The mC_d suggested by Abrahim and Parker (2008) because that Håkanson' (1980) C_{deg} method which based on eight specific parameters and was limited by the number of parameters. Thus, they modified the C_{deg} as mC_d (Table S1 and Table S2). The PLI index that been suggested by Tomlinson et al. (1980) and PI_{Nem} index that been proposed by Nemerow (1991) other pollution indices widely used by researchers which were based on C_f (Table S1 and Table S2).

The enrichment factor (EF) was a geochemical approach based on the assumption that under natural conditions, there is a linear relationship between the amount of an element with reference element ratio inside an environmental material (such as atmospheric dust, ice, aquatic sediments, etc.). This ratio is used to determine the enrichment level of the element inside the environment and its allows to determine if the enrichment was natural or it was caused by other effects such as anthropogenic effects (Zoller et al., 1974; Idris, 2008; Qingjie et al., 2008; Kowalska et al., 2018). The preindustrial global (Ref_2) reference concentrations by Turekian and Wedepohl's (1961) used as global reference (Table 1). Also, aluminium (Al) used as reference element in EF calculations because Al represents the aluminosilicates which are the main group of clay and mica minerals generally found in the fine marine sediment fractions (Herut and Sandler, 2006). The enrichment factor values of As, Cd, Cr, Cu, Hg, Ni, Pb and Zn elements were used to calculate the modified pollution ındex (MPI) for this study. The geoaccumulation index (I_{geo}) was introduced by Muller (1969) to compare the preindustrial concentrations of the metal ratios in the sediments with the current concentrations (Zhang et al., 2009). The Igeo is used to define and determine the metal pollution ratio by measuring pollution levels from sediments in water. The Ref._2 used for preindustrial global background concentrations to calculate the I_{geo}.

The anthropogenic pollution in marine environments can cause adverse biological effects on resident living (benthic) organisms. The sediment quality guidelines (SQG) are used to determine potential problem areas for benthic populations that can be greatly affected by sediment contamination (Long et al., 1995). MacDonald et al. (1996) used the relationships between contaminant exposure and biological effects (percentile of the effects data set) for each analyte to derive threshold effect level (TEL) and the probable effect level (PEL). Long et al. (1995), similarly, derived the effects range-low (ERL) and effects range-median (ERM) values from the biologic effects data set. The incidence of adverse effects within each range was quantified by dividing the number of effects entries by the total number of entries and expressed as a percent (Long et al., 1995). The TEL-PEL and ERL-ERM reference values were given in Table 1. A similar in-situ study has been not conducted to investigate the adverse biological effects on benthic organisms by contaminated sediments for Türkiye's aquatic areas. Because of this, the SQGs values that are stated by Long et al. (1995) and MacDonald et al (1996) were used in this study. The toxic risk index (TRI) is a general index used to determine the level of risk the environment carries for benthic organisms (Table S1 and Table S2).

The principal component analysis (PCA) is a multivariate statistical technique which is capable of discerning patterns in data sets. The PCA reduces the dimensionality of complex and dense datasets, increasing interpretability while preserving as much statistical information as possible. The PCA creates new variables that are linear functions of variables in the original dataset, that successively maximize variance and differ the uncorrelated values with each other (Jolliffe and Cadima, 2016b).

The factor analysis can be used to define the chemical elements that shows similar geochemical patterns of distribution or behavior in sedimentary environments. This method is based on the concept that geochemical elements tend to coexist in certain mineral assemblages that form the paragenesis community in different environments and conditions; and thus, can be used to identify the common feature distinguished by the factors for each variable (Albanese et al., 2007). During this study, STATISTICA Ver.12 software program was used to determine the factor analysis. This program used an analysis based on Principal Component Analysis of Thurstone (1931) and correlation matrix has been determined based on log10. The Varimax Normalization rotation system was chosen to determine the factors.

When sediments are transported in the aquatic environments, the increase of the effective energy of the fluid or prolongation of it in the duration of action causes the sediment to mature texturally (Kaya, 2005). Folk and Ward (1957), developed a geostatistical method to determine characteristics of the sediment, especially about the transport conditions of the sediments, based on the dimensional and structural properties of the sediment particles that make up the sediment formations. They used the Krumbein Phi (ϕ) Scale (1934) to calculate mean, sorting, skewness, and kurtosis values to determine granulometric parameters of the sediments, which were the characteristics that shaped the sediment transportation and deposition features. In this study, Folk and Ward (1957) logarithmic method of the related parameters and their classifications used to calculate the mean grain size, sorting, skewness and kurtosis parameters which can be used to determine the sediment transport pathways.

In this study, a two-dimensional approach model of Gao et al. (1991) was used to determine point-to-point transport vectors by averaging the vectors of neighboring stations to create the grain size trend model (Gao and Collins, 1992; Poizot and Méar, 2010). The sediment samples of the study were taken in a regular grid with grid mesh size 2000m in the general study area. Also, a semi-variogram map created by mean grain size (Phi) values was used to determine the characteristic distance parameter (Dcr). The Fotran GSTAST (Gao and Collins,

1992) software was used to calculate sediment sorting, mean size, skewness and kurtosis values for each sample before the GisedTrend plugin software tool to perform a GSTA approach provided by Poizot and Méar (2010) of the QGIS geographical information system was used to compute sediment trend vectors. In this study, two trend types; Finer (F)-Better sorted (B) and more negatively (-) skewed (FB-) sediments, and alternatively, Coarser (C)-Better sorted (B) and more positively (+) skewed (CB+) sediments were investigated. The coastline, islands, and other land surfaces in the study area were defined as barrier with a shape file when the sediment trend vectors field was computed.

Results

The grain size parameters, $CaCO_3$ and TOC contents, of Gülbahçe Bay were determined and given in Table 2.
The spatial distributions of $CaCO_3$ and TOC contents of bottom sediments are given on Fig.2. The sediment classification according to Folk (1980) ternary diagrams were used to determine the sediment classes in the study area, also the spatial distribution of sediment mean size fraction (in phi), sorting coefficient (σ_g), skewness (S_k) and kurtosis (K_g) parameters are given in Fig.3. The statistical parameters of determined metal concentrations in study area given in Table 1 and their spatial distribution maps given in Fig.10.

Discussion and Conclusion

Assessment of Sediment Grain Size Parameters and GSTA Model

The most common sediment grain size in Gülbahçe Bay determined as the silt fraction with a rate of 51.4%. Silt fractions followed by sand with a rate of 38.0%, clay with 11.2% and finally gravel with 2.1% (Table 2). The overall grain size distribution of sea bottom sediments varies from mud to sand throughout the study area (Fig.3).

A deposition zone has been determined that starts from the north of the study area and descends to the northwest of Özbek through between the east of Mordoğan and the west of Uzun Ada which contains more than 40 % sand-size fractions. This zone follows through the coastline to the west of Torasan. A mud zone has been observed that formed between the smaller islands, which divides two sand zones at the east of Urla. The sea bottom surface sediments contain silt-sized fractions higher than 50% through the Balıklıova and Gülbahçe coastlines in the west of the study area. Also, it was determined that silt content has been higher than 60% in the eastern part of Uzun Island, which is in the Izmir Central Gulf (Fig.3).

Table 2. The sediment grain size, $CaCO_3$ and TOC parameters of Gülbahçe Bay.

	Min.	Max.	Mean	Std. Dev.
Gravel (%)	0.00	46.39	2.10	6.91
Sand (%)	1.30	84.88	38.00	24.90
Silt (%)	16.41	90.46	51.41	20.93
Clay (%)	2.38	28.82	11.20	5.94
Mean G. Size (in ϕ)	2.09	8.62	5.40	1.84
Sorting-σ_g (in ϕ)	1.92	4.10	2.97	0.63
Skewness-S_k) (in ϕ)	-0.23	0.76	0.16	0.23
Kurtosis-K_g (in ϕ)	0.63	2.56	1.04	0.38
Shell (%)	0.22	27.93	8.25	7.20
$CaCO_3$ (%)	7.29	63.75	36.64	13.80
TOC (%)	0.86	5.49	3.09	1.13

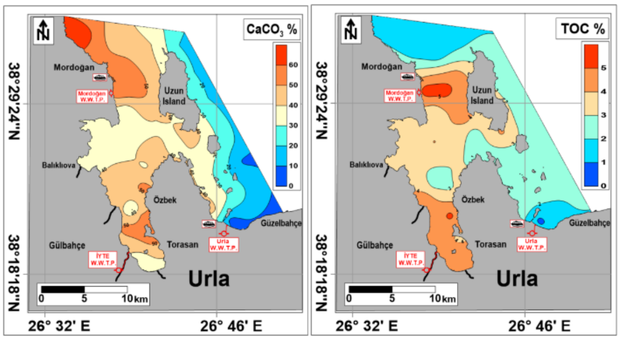

Fig. 2. The $CaCO_3$ and TOC content distributions of Gülbahçe Bay.

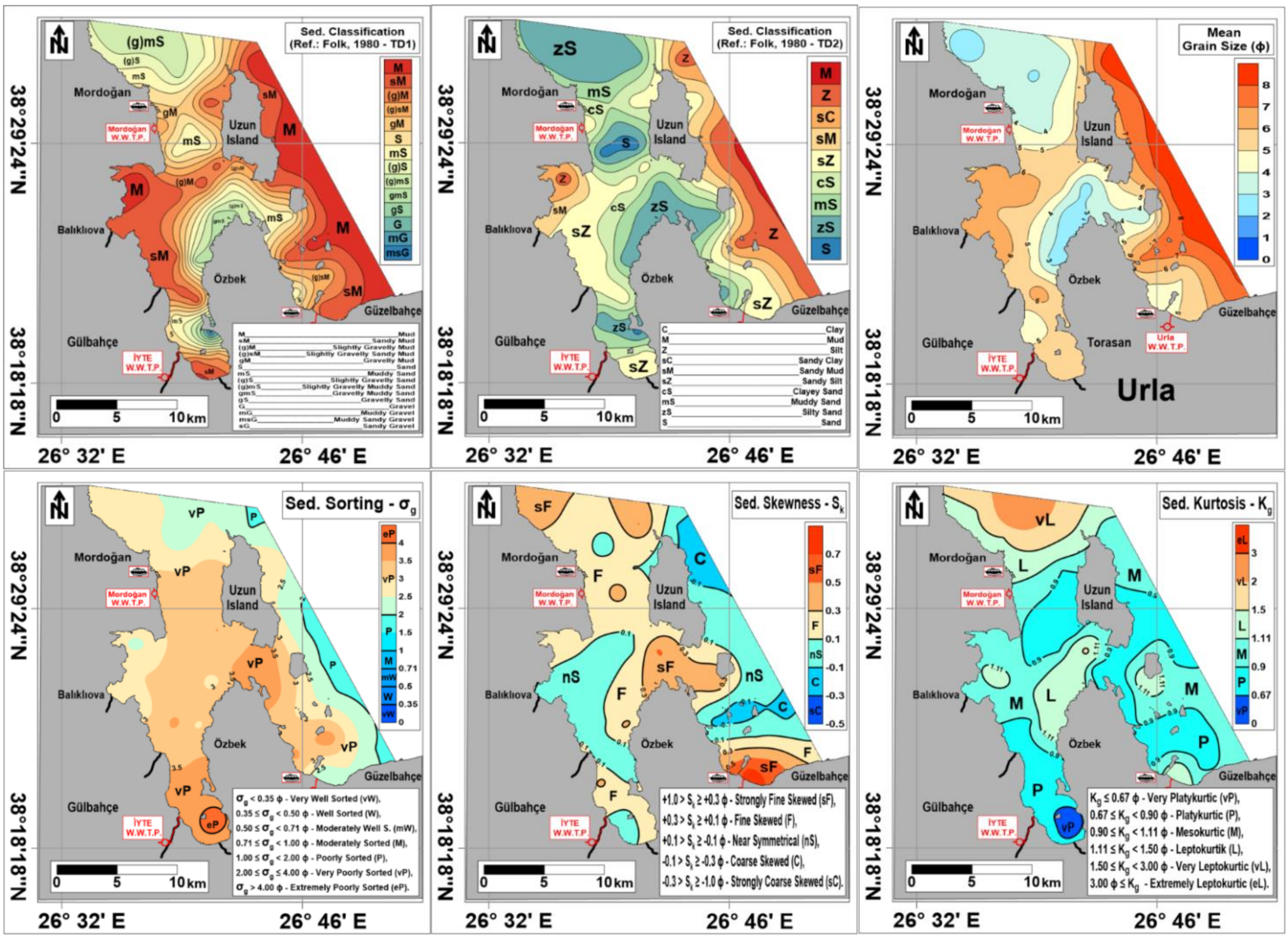

Fig. 3. The sediment grain size class distribution according to Folk (1980) ternary diagrams, the spatial distribution of sediment mean size fraction, sorting coefficient (σ_g), skewness (S_k) and kurtosis (K_g) parameters distributions of Gülbahçe Bay.

Within the scope of this study, the sediment transport model was created by the sediment transport vectors in the study area (Fig.4). The direction and magnitude of sediment transport are characteristic with arrows and dimensions in the model presented in Fig.4. An overview of the sediment transport model presents the dominant and main elements of the transport models given in Fig.4. The ADCP and shallow seismic profiles were collected during the survey of Gülbahçe Bay within the scope of the TÜBİTAK 115Y180 Project. The *Posidonia oceanica* habitat boundaries were determined from seismic data in the area. The distribution of *Posidonia oceanica* habitat is given in Fig.4. The distribution of salinity values in study area and salinity and temperature profiles with NE-SW orientation given in Fig.5. It has been determined that the temperature and salinity values are higher in the southern end of Gülbahçe Bay, where the depth is less than 15 m. This low-density water layer flows from sought to the north in the shallow water up to 20m depth in the study area. Another water flow has been detected with lower temperature and salinity in the part deeper than 20m deep (Fig. 5). It has been observed that the sediments in the zone close to the coastline are generally transported in the northeast direction due to the surface waves and currents formed under the influence of the north and west winds (Fig. 4) in Gülbahçe Bay. However, there is a more complex sediment transport process under the influence of different currents in the region which were located between the south of Uzun Ada and the smaller islands, where the sea bottom depth has been changed from 10 m to 40 m.

The ADCP profile that was taken in the NE-SW direction in the east of Uzun Island was given in Fig.6. According to this profile, there is a surface flow zone with low density and strong magnitude with the north-west orientation that was observed from the northeast of Uzun Island to the southwest throughout of profile line.

This current forms a surface flow zone that continues from 30 m of depth in the north throughout to 15 in the southeast. The deep water inflows from Izmir Central Gulf towards between the islands. This deep inflow water has a high salinity, low magnitude and high density with the north-east orientation. However, this dense deep water flow was intersected between the islands by current outflows with moderate magnitude and less density and the south-west orientation.

The NW-SE-oriented outflows which have been developed under the effect of Coriolis flow move from Gülbahçe Bay to the south of Uzun Island and the northwest of Hekim Island. These outflows cause the transportation of coarse-grained sediments from the northeast of Özbek throughout the southwest of Hekim Island in the opposite direction of the FB- oriented sediment transportation.

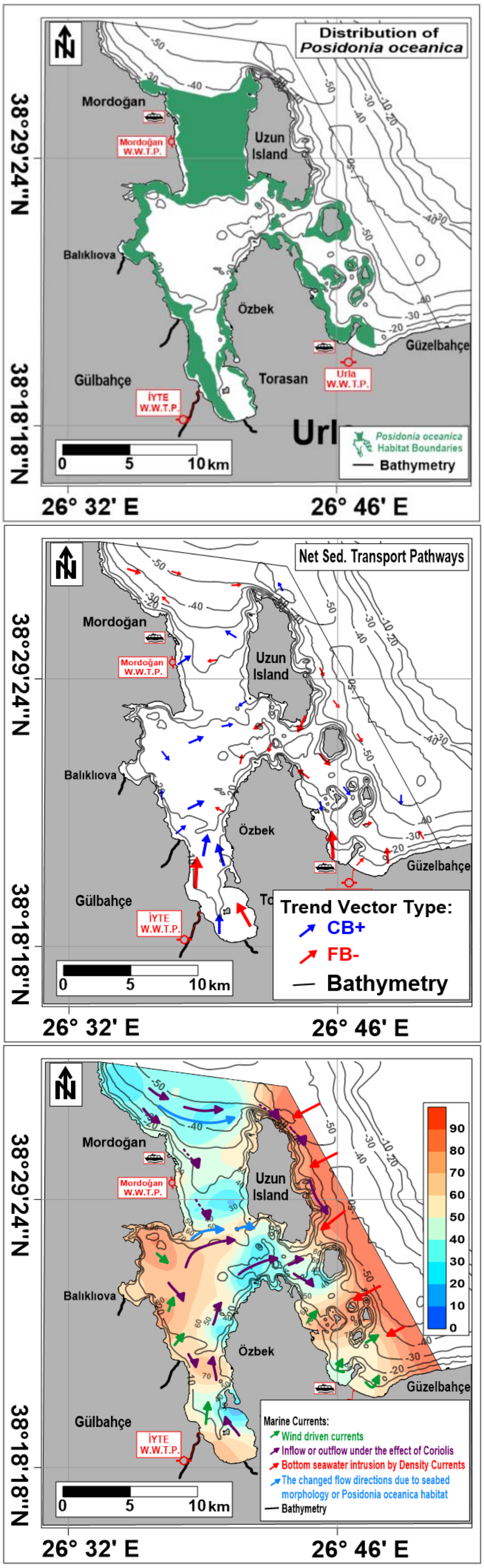

Fig. 4. The spatial distribution of *Posidonia oceanica* habitat borders, the net sediment transport pathways (GSTA-calculated sediment trends) and the marine currents that effecting the study area on fine (<63µm) sediment distributions map.

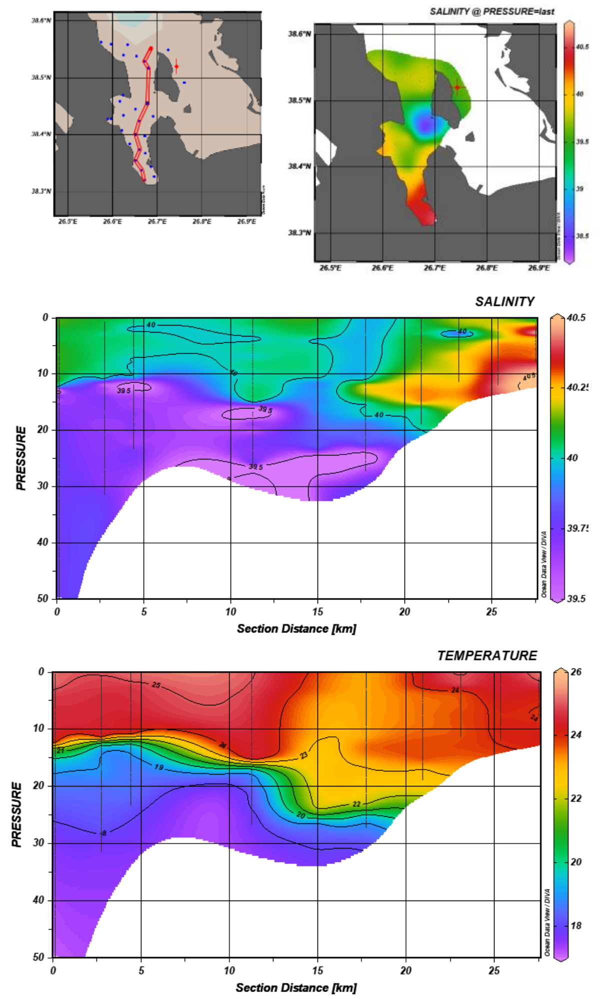

Fig. 5. The surficialdistribution of salinity values in study area and salinity and temperature profiles with NE-SW orientation.

On the other hand, the high-density deep flow with a north-east orientation penetrates inwards from Izmir Central Gulf to the southeast of Uzun Island and/or the south of Hekim Island and forms a fine-size sedimentation zone with mud between the islands by characterized with FB- oriented sediment transportation (Fig. 4). The ADCP and shallow seismic profile taken from the west of Uzun Island in the NW-SE oriented was given in Fig.7. It has been observed that there is a *Posidonia oceanica* habitat on the Mordoğan Strait which starts from 30m depth in the north and continues to 20m depth in the south. A presence of the recent sediment deposition up to approximately 2 m consisting mostly of fine-grained sediment has been detected in the northeast of Mordoğan towards the open sea in the deeper part of the bay on more than 30 m depth of the sea floor. An erosion/transport zone with a thickness of up to 2 m and consisting of coarse-grained sediment accumulation has been observed, at the SE end of the profile line, on the bottom of Mordoğan strait's slope in the inner side of Gülbahçe Bay where the sea floor is deeper than 20 m. Due to both the seafloor morphology and the density of the *Posidonia oceanica* habitat, it is difficult to observe the sediment transport that affects the ridge between Mordoğan and the east of Uzun Ada (Fig.7).

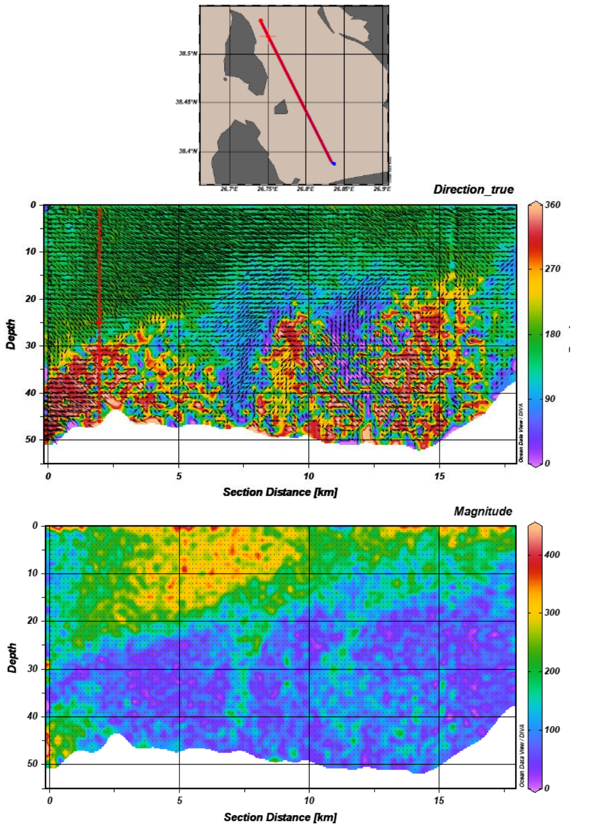

Fig. 6. The ADCP profile that was taken in the NE-SW direction in the east of Uzun Island.

A high-magnitude current with high salinity and south-east orientation has been detected that has been thought to be the causes the nurture of the habitat on the Mordoğan strait. Above this flow, it was determined that there is a low saline current with south-west oriented and lower magnitude that was thought to have been developed under the influence of Coriolis, that moves towards inward from the north to the south of the bay (Fig.7).

At the top of the water column, there has been determined a north-east oriented surface current with high salinity but less density that was moving outward from the inside of the bay (Fig.7). It has been determined that the coarse-grained (>63 µm) sediment content was denser on the Mordoğan Strait's sea floor. However, it was not possible to determine the sediment transport trends precisely due to the density of the *Posidonia oceanica* habitat.
The SW-NE-oriented ADCP and shallow seismic profile had been taken from south of the Mordoğan Strait in the inner part of Gülbahçe Bay was given in Fig.8. According to this profile, it has been determined that the *Posidonia oceanica* habitat ends at around the depth of 20 m on the slope towards the inner part of the bay from the Mordoğan Strait. The presence of a recent deposition that consisting of fine-grained sediment accumulations up to 5 m in thickness has been detected on the sea floor towards the southwest of the Mordoğan Strait's slope.

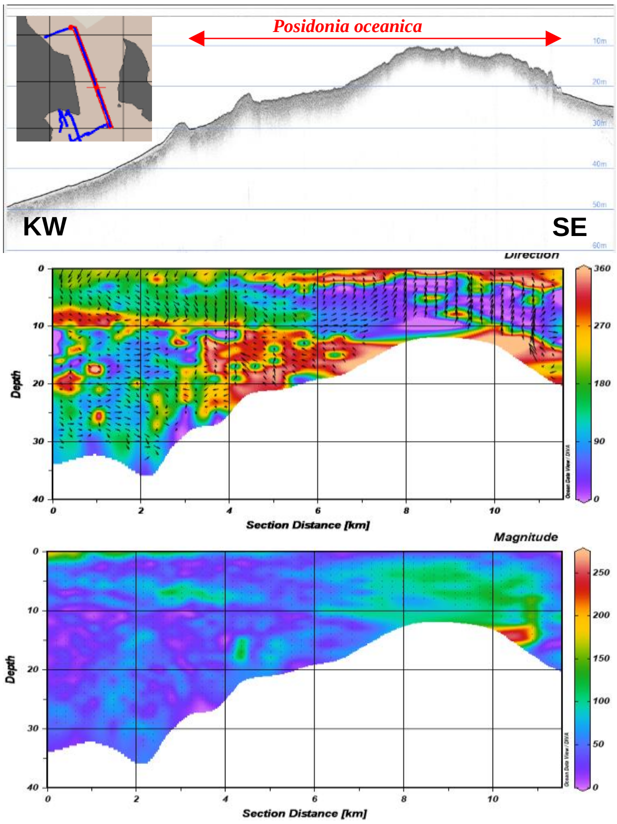

Fig. 7. The ADCP and shallow seismic profile taken from the west of Uzun Island in the NW-SE orientation.

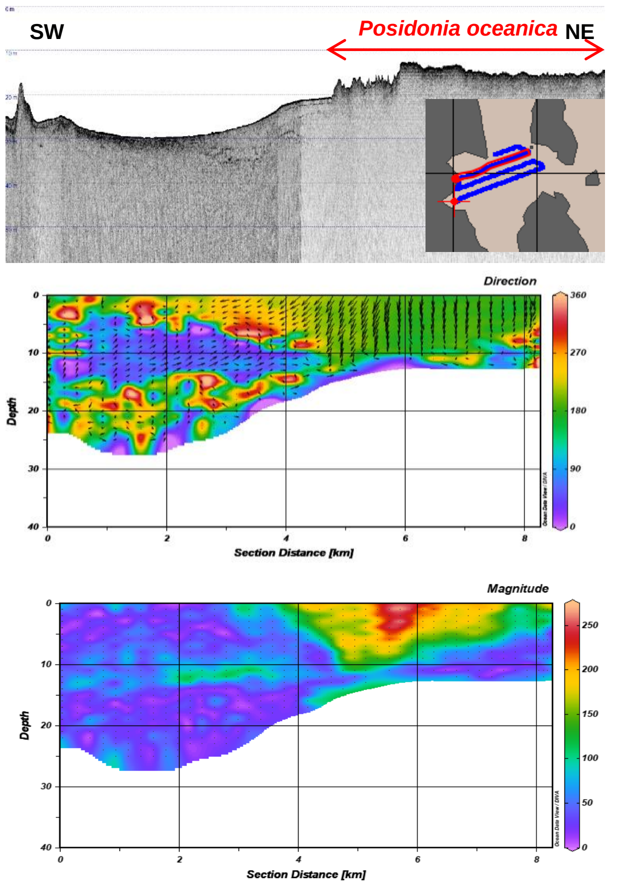

Fig. 8. The SW-NE-oriented ADCP and shallow seismic profile had been taken from south of the Mordoğan Strait in the inner part of Gülbahçe Bay.

It was observed that there are three types of currents in the water column on the front of the coastline of the east of Balıklıova (Fig.8). The first of these currents that had been observed was a surface water flow with north-east orientation, which was developed under the influence of surface winds and has been seen in the entire study area in zones that are closer to the coastline.

The second one has been developed under the Coriolis effect and was the low-density water flow with the south-west orientation. It has been observed that there are small turbulent-like currents of less magnitude in the water branch at a depth of more than 15 m, at the bottom. It is thought that these currents are irregular currents formed as a result of the encounter of the north-east oriented surface flow trying to enter the bay on the slope and the south-west oriented water flow trying to get out of the bay (Fig.8).

It has been observed that the low-density water flow with the south-west orientation that had developed under the Coriolis effect moves outward from the east of Balıklıova throughout to the southwest of Uzun Ada, instead of heading north due to the existence of Posidonia oceanica habitat and sea floor morphology. Thus, causes the sediment transport to proceed in the direction of CB+ sediment transport (Fig.4).

Assessment of Total Carbonate and Total Organic Carbon Contents

It has been observed that the $CaCO_3$ content in surface sediments has been denser more than 30% on the inner side of the study area, in the zone through the northeast of Mordoğan to the southwest of Uzun Island. Two different zones were determined in the study area; the first is between the northeast of Mordoğan and the west of Uzun Ada where the $CaCO_3$ amount is over 50%. The second zone is between the east of Gülbahçe and the west of Özbek where the $CaCO_3$ amount is over 40%. The intense presence of clastic and carbonate rocks around Gülbahçe Bay causes total carbonate enrichment in the sediments in the study area. The east side of Uzun Island is under the effect of intensive current flows that cause an erosional zone. Because of this, dense $CaCO_3$ accumulation was not observed in the erosional zone (Fig.2).

The concentration of organic carbon within marine sediments has been caused by the accumulation of organic matter in the marine environment. The inputs caused by various domestic and industrial pollutants' accumulation, the metabolic wastes of aquatic organisms, and bacterial degradation products can cause enrichment of the organic matter that causes eutrophication thus causing an increase in the deaths of organisms and increasing the percentage of TOC.

It has been observed that the content of TOC was over 3% in most of the study area, especially where the denser population was located (Fig.2). The TOC increased in the east of Mordoğan and the inner southern part of the Gülbahçe Bay by up to 6%. These zones are under the effect of mostly domestic discharges caused by residential areas and some small urbanization activities. Thus, the TOC accumulation was identified as one of the results of the anthropogenic effects in the area.

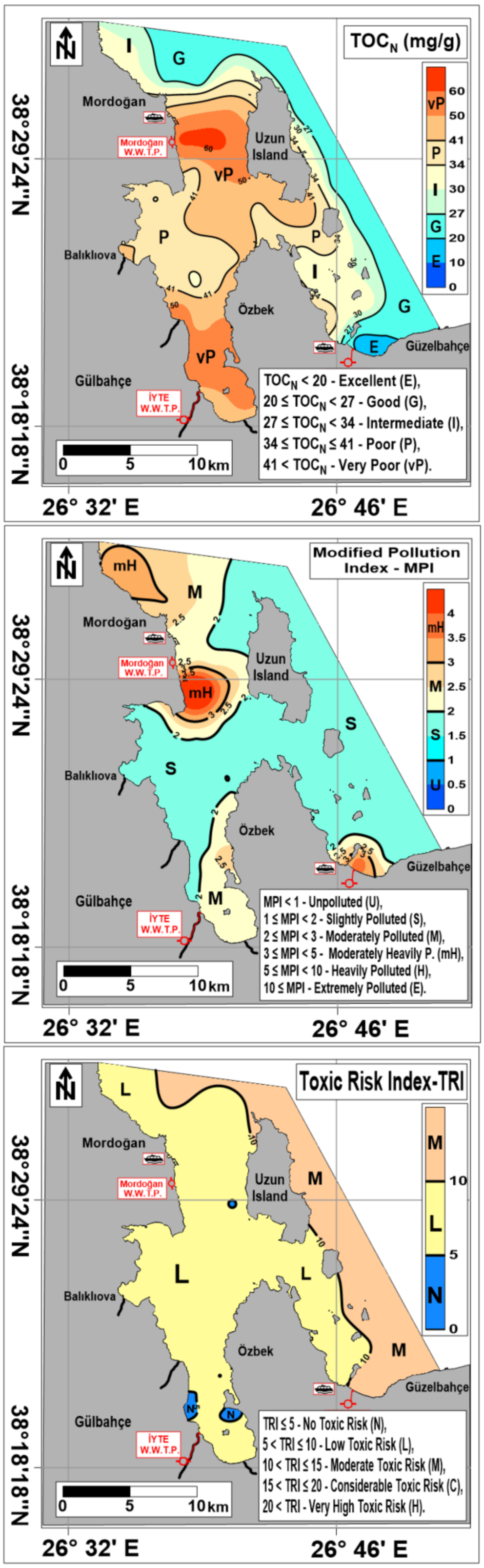

Fig. 9. The distributions of sediment quality according to TOC_N index, distributions of MPI and TRI in the study area.

The normalized total organic content (TOC_N) confirms the TOC ratio values. According to the TOC_N index, the sediment quality ranges from moderate (27-34 mg/g) to

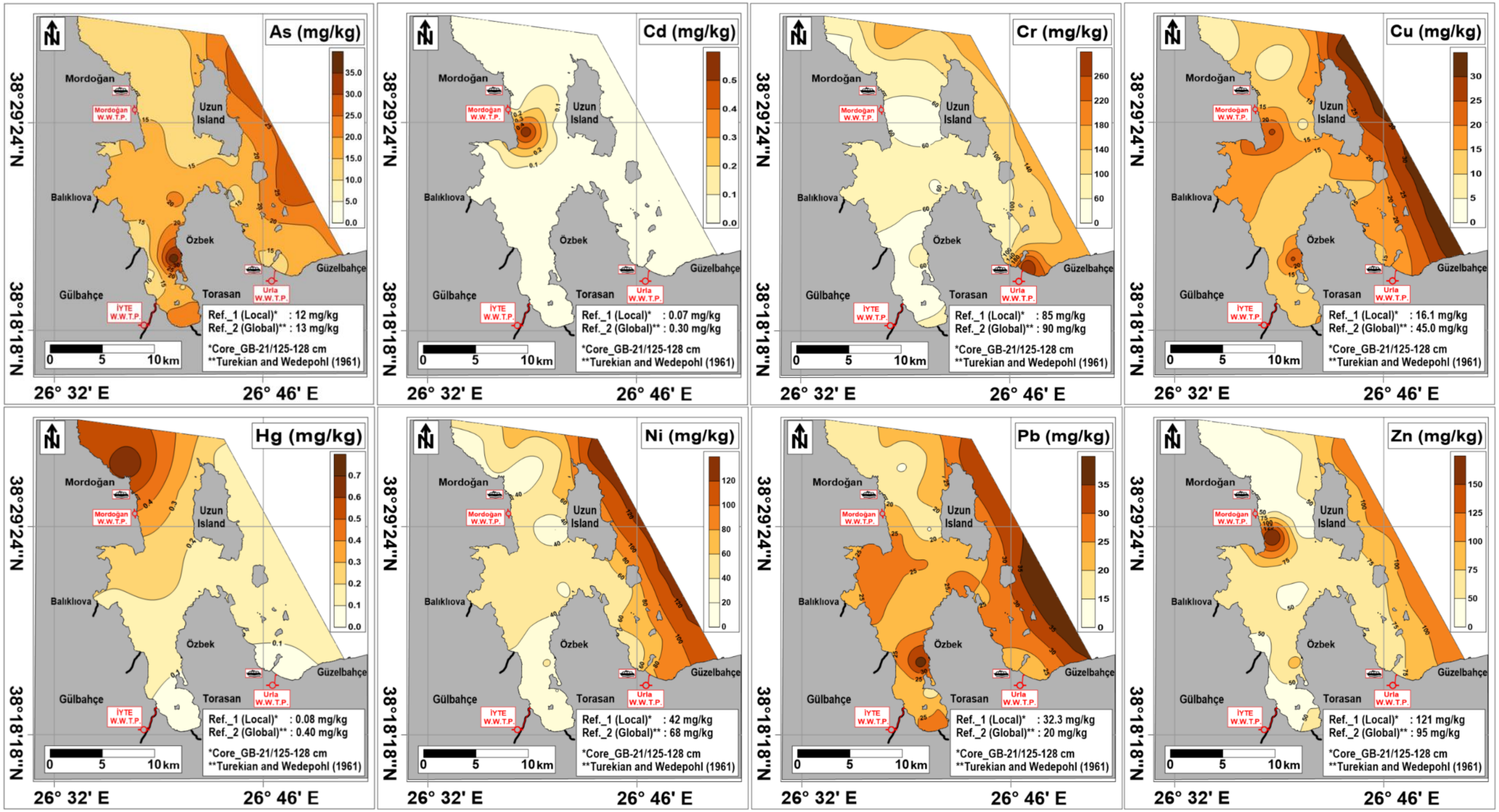

Fig. 10. The spatial distribution of the As, Cd, Cr, Cu, Hg, Ni, Pb and Zn contents of sediment samples.

very poor (greater than 41 mg/g) in the study area (Fig.9) where has been densely populated areas are close to the coastline (Mordoğan, Balıklıova, Gülbahçe, Torosan, Özbek and Urla).

Assessment of environmental effects of metal concentrations

The spatial distribution of the As, Cd, Cr, Cu, Hg, Ni, Pb and Zn contents of sediment samples is given in Fig.10. The determined metal mean concentrations in the study area were Cr>Zn>Ni>Pb>As>Cu>Hg>Cd in the descending order.

It has been observed that the distribution of elemental amounts in Gülbahçe Bay is generally denser in three zones. The first of these is the zone in the east of Uzun Island, which continues from north to south and can be clearly distinguished in the Cu, Pb and Zn element distribution maps. This zone is located where the study area intersects with Izmir Central Bay and it has been thought that the reason for the high element values in this zone is due to the intense marine traffic in this zone (Fig.10).

The amount of elements with lithogenic origin such as Ni has been determined as more densely concentrated in the region of the east of Uzun Island that intercepts with the sedimentation basin where fine-grained sediments accumulate due to the morphology of the seafloor. Also, it has been determined that the Cu, Pb and Zn concentrations are more prominent due to marine traffic in the zone where Mordağan harbor has been located, and dense accumulation was observed as continues towards the south of Uzun Island (Fig.10).

The second zone where element distributions were observed densely was the southern inner part of Gülbahçe Bay and the area around it (Fig.10). Particularly, it was observed that the amount of As, Pb, Cu, S and TOC were higher in the zone front of the coastline where populated areas by humans are denser, like from the southwest of Torosan towards the west of Özbek. It has been thought that this pollution was caused by the discharges of untreated domestic waste and the discharges of resulted by small industrial activities into the sea.

The third zone has been identified by the accumulation of Hg being denser in the northern side of the Mordoğan. It has been known that there are mercury mines that closed in this region. The mercury concentration in the sea was thought to be caused by the remnants of the accumulation of Hg particles in the older sediment that related to these closed mines (Fig.10).

The contamination factor (C_f) ranking, which is calculated according to local reference values, were identified as Hg (2.5)>As (1.5)>Ni (1.4)>Cd (1.3)> Cu (1.1)>Cr (1.1)>Pb (0.8)>Zn (0.5) in the Gülbahçe Bay. According to C_f, study area was moderately contaminated by Hg>As>Ni>Cd>Cu>Cr; and Pb>Zn showed lower contamination.

The determined contamination degree (C_{deg}) shows moderate degree of contamination with value of 10.1 in Gülbahçe Gulf while the modified contamination degree (mC_d) shows very low degree of contamination with value of 1.3 in the same area. The area is polluted according to pollution load index (PLI) with value of 1.2 and slightly polluted domain according to Nemerow pollution index (PI_{Nem}) with value of 2.

The metal ranking in Gülbahçe Bay was observed as As>Pb>Cr>Ni>Zn>Hg>Cu>Cd according to the enrichment factor (EF) and geoaccumulation factor (I_{geo}) values (Fig.11A and Fig.11D). According to EF, study area was significantly contaminated by As, Cd, Cr and Zn in 3% of area; moderately contaminated by Pb>As in more than 50% and Hg>Cr>Ni>Cu in more than 20% of area of area. The study area minimally contaminated by Cd>Cu>Ni>Zn>Cr>Hg in more than 70% of area (Fig.11B). Up to 3% of Gülbahçe Bay was moderately contaminated by As and Cr according to the I_{geo}. The uncontaminated to moderate level contamination by As>Pb>Ni>Cr was determined less than 30% of area while up to 3% of area Cd, Hg and Zn shows uncontaminated to moderate level contamination. More than 50% of area uncontaminated by elements. The copper is only element inside uncontaminated level according to I_{geo} in all of the area (Fig.11C).

According to TOC_N, the sediment quality was determined as poor in general of the area. According to MPI, most of the area has been moderately polluted. Lastly, according to TRI, there is a low risk for benthic organisms caused by element pollution. In summary, moderate pollution was determined in Gülbahçe Bay according to pollution indices evaluations.

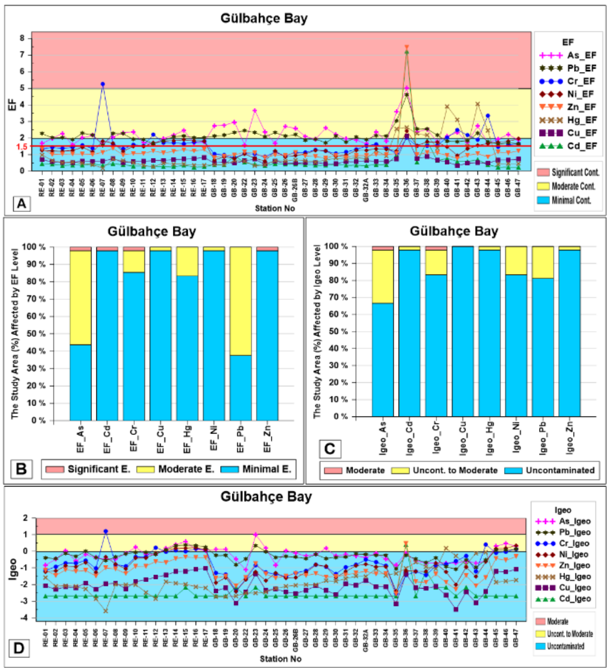

Fig. 2. The EF and I_{geo} distributions according to samples and percent of the area have been affected by their levels.

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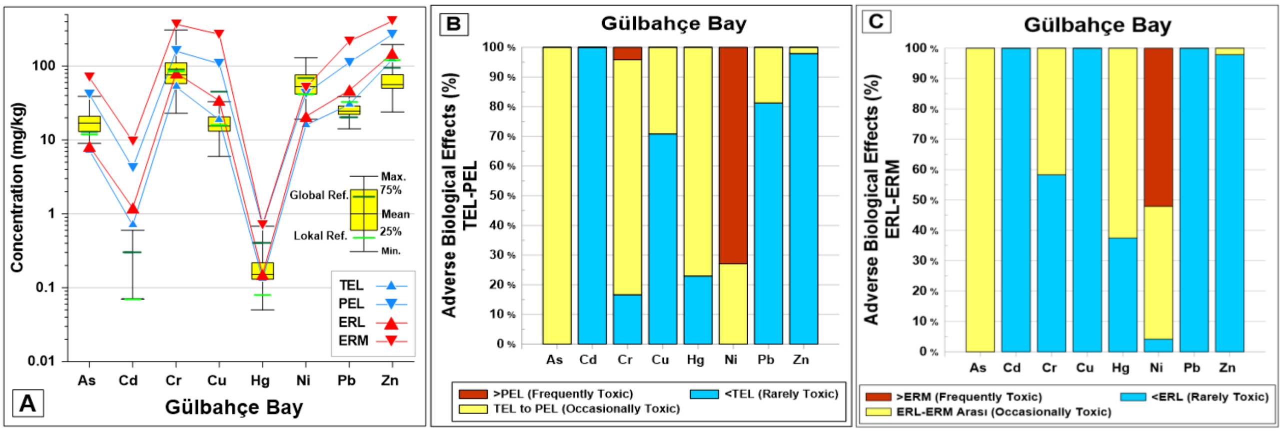

Fig. 3. The comparison diagrams of metal concentration ranges to TEL-PEL-ERL-ERM levels, percent of the area had been affected by adverse effects of TEL-PEL and ERL-ERM levels.

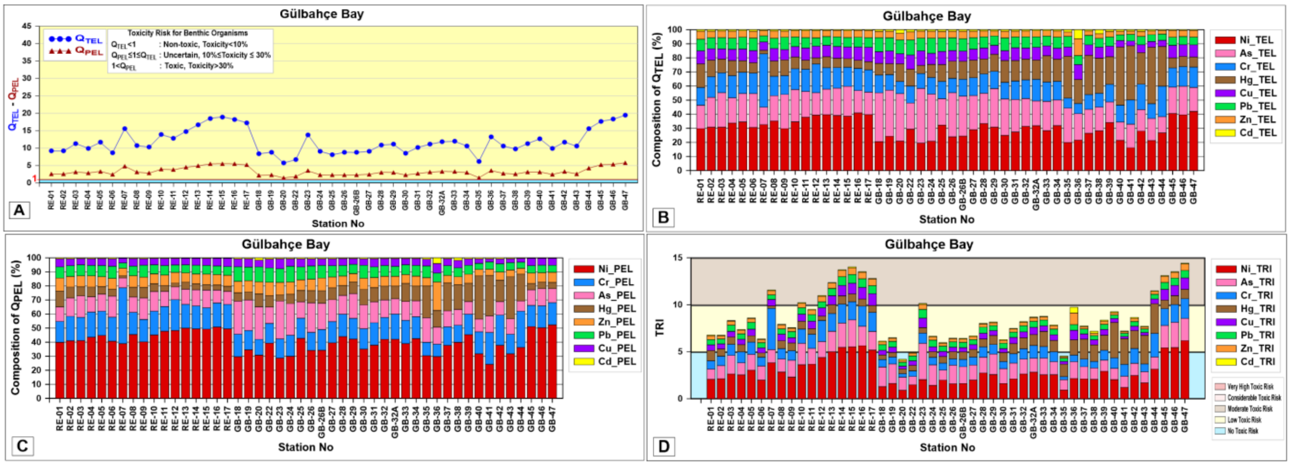

Fig. 4. The Q_{TEL}-Q_{PEL} values' spatial distribution at the study area, and the element compositions that constituted the Q_{TEL}, Q_{PEL} and TRI indices.

Table 3. The elements effects' risk range for each element according to SQGs and the percentage of the study area affected by each element.

	As		Cd		Cr		Cu	
	the area under the risk (in %)	probability of risk (in %)	the area under the risk (in %)	probability of risk (in %)	the area under the risk (in %)	probability of risk (in %)	the area under the risk (in %)	probability of risk (in %)
Minimal Effects Range (ppm<TEL)	0	2.7	100	5.6	16.7	3.5	70.8	9.0
Possible Effects R. (TEL<ppm<PEL)	100	12.9	0	20.1	79.2	15.4	29.2	21.9
Probable Effects Range (ppm>PEL)	0	46.8	0	70.8	4.2	52.9	0	55.9
Rarely Toxic (ppm<ERL)	0	5.0	100	6.6	58.3	2.9	100	9.4
Occasionally T. R. (ERL<ppm<ERM)	100	11.1	0	36.6	41.7	21.1	0	29.1
Frequently T. R. (ppm>ERM)	0	63.0	0	65.7	0	95.0	0	83.7

	Hg		Ni		Pb		Zn	
	the area under the risk (in %)	probability of risk (in %)	the area under the risk (in %)	probability of risk (in %)	the area under the risk (in %)	probability of risk (in %)	the area under the risk (in %)	probability of risk (in %)
Minimal Effects Range (ppm<TEL)	22.9	7.8	0	3.3	81.3	5.8	97.9	3.8
Possible Effects R. (TEL<ppm<PEL)	77.1	23.6	27.1	8.4	18.8	25.8	2.1	27.2
Probable Effects Range (ppm>PEL)	0	36.7	72.9	9.4	0	58.4	0	64.4
Rarely Toxic (ppm<ERL)	37	8.3	4.2	1.9	100	8.0	97.9	6.1
Occasionally T. R. (ERL<ppm<ERM)	62.5	23.5	43.8	16.7	0	35.8	2.1	47.0
Frequently T. R. (ppm>ERM)	0	42.3	52.1	16.9	0	90.2	0	69.8

Ascertaining the potential risk areas for organisms by metal concentrations using SQGs

The comparison diagrams for the range of metal concentration of the study area to the SQG reference values (TEL, PEL, ERL and ERM), local and world references are given in Fig.12.

The Ni concentrations are higher than SQG reference values reference values throughout the Gülbahçe Bay, the Cd Cu, Pb and Zn concentrations are close to the TEL reference value and lower than the PEL-ERL-ERM reference values. The As, Cr, and Hg concentrations higher than TEL-PEL-ERL reference values and lower than ERM reference value (Fig.12). The elements' affect risk ranges according to SQGs and the percentage of the study area affected by each element are given in Table 3. For example, the accumulation of nickel is within the Frequently Toxic Range (ppm<ERML) in 52.1% area of study area, and has a 16.9% probability of adversely affecting benthic organisms. While in 72.9% of the study area, the amount of nickel is greater than the PEL reference value (within the Probable Effect Range) and the probability of adversely affecting benthic organisms is 9.4% in this zone. According to SQG, the main element ranking that negatively affects benthic organisms and poses a significant risk for living organisms in the area was determined as Ni>Hg>Cr>As>Cu>Pb>Zn>Cd in the Gülbahçe Bay (Table 3). The Q_{TEL}-Q_{PEL} values' spatial distribution at the study area, and the element composition that constituted the Q_{TEL}, Q_{PEL} and TRI indices given in Fig.13

The risk quotient based on TEL (Q_{TEL}) values ranges from 5.7 to 19.5 while the risk quotient based on PEL (Q_{PEL}) values shows a similar approach to Q_{TEL} and ranges from 1.5 to 5.8 in study area (Fig. 13). Both indices show that the study area, generally, was under the toxic risk with more than 30% possibility. Both indices indicate that the toxicity level caused by heavy metals is above the acceptable toxicity level for living benthic organisms. TRI values that were determined in the study area range between 4.2 (non-toxic) to 14.4 (moderately toxic). The distribution of TRI values in the study area shows that most of the study area under the low toxic risk (Fig.9).

Determination of the sources of element accumulations

During this study, 51 geochemical variables that were determined by different analyses were used for application of the PCA with varimax normalized rotation of standardized component loadings to identify four significant factors (>2.5 in eigenvalue) that explained 79.98% of the total variance (Table S3).

The primary factor (Factor 1) in the region was explained as the lithogenic factor with 50.6% of total variance. This factor (Fig.14) was defined with a positive correlation of fine sediment (<63µm), Al, As, Ba, Bi, Co, Cu, Fe, In, K, Li, Mg, Mn, Ni, Pb, Rb, Sb, Sc, Sn, Ti, Tl, V and W. This factor was classified as lithogenic factor because the $CaCO_3$ and TOC variables showed a negative correlation while the fine sediment variable showed a very high positive correlation, and the soil elements of lithogenic origin and heavy metals that tended to be absorbed by fine sediments showed a low positive correlation. This factor increases in the eastern side of Balıklıova and in the zone where the study area intersects with Izmir Central Gulf where there are deposition zones by fine sediments in the study area that reaches its highest values confirming this assessment (Fig.14). The distribution of the Lithogenic Factor in the study area also shows that Gülbahçe Bay is also affected by the pollution present in Izmir Gulf. It was observed that this factor become evident in the zone from southwest of Uzun Island to the west of Urla harbor, where the area is under the influence of the high-density undercurrent that tends inwards from Izmir Central Gulf to Gülbahçe Bay. The effects of W.W.T.P. discharge channels have been not observed in this factor's data.

The secondary factor (Factor 2) in the region was explained as the anthropogenic factor with 13.18% of total variance. This factor was determined with very high and moderate positive correlations of TOC, As, Be, Hg, Mo, Na, Nb, Re, S, Ta, Th, U and Zr variables. Due to the TOC, As, and S variables showing a high positive correlation, Factor 2 was named as anthropogenic factor that was determined to represent the parameters of domestic waste originating from the density of the residentially populated area around Urla, Gülbahçe, Torasan and Özbek (Fig.14). The İ.Y.T.E W.W.T.P. discharge channel's negative effect has been observed in this factor's data.

The third factor that was determined as effective in Gülbahçe Bay is Factor 3 which was represented by 9.30% of the total variance. Factor 3 was defined by a very high (>0.7) level of negative correlation of Ag, Cd, P, S and Zn, and a low (<0.4) negative correlation of coarse sediment, Cu, Sn, Mo, Na and Pb. The investigation of element correlation parameters of Factor 3 shows that these element concentrations are caused by sea traffic (Cu, Sn and Zn) or by the pollutants carried to the sea as a result of small-scale maintenance/repair activities of the boats in the areas where the small yacht and fishing ports are located. The spatial distribution map of factor 3 in the area shows that this factor is concentrated in the zones where the small yacht and fishing ports were located in the study area where maritime traffic routes were more frequent. Therefore, this factor was named as anthropogenic factor caused by marine traffic/port activities (Fig.14). When this study was conducted, the Mordoğan W.W.T.P was under construction and has been not actively operated. The Mordoğan W.W.T.P was activated in the summer of 2022. The effect of Mordoğan W.W.T.P was not observed in this study. Still, we think this study is essential because it shows the environmental condition of Gülbahçe Bay before the activation of Mordoğan W.W.T.P.

The fourth factor that was determined as effective in Gülbahçe Bay is Factor 4 which was represented by

6.86% of the total variance. This factor was defined as an industrial factor. Factor 4 was identified by the fact that Cr and Ce variables show very high positive correlations, and other variables such as coarse sediment, As, Cu, Hg, La, Ni, Pb and Zn show moderate and low positive correlations. The variable values that were composed of factor 4 show almost similar properties with variables such as Al, Fe, La and Ti, which were known to be of lithogenic origin, in the same factor composition. This shows that although this factor was caused by the anthropogenic effects due to the small-scale industrial activities in the vicinity of Gülbahçe Bay, this negative affect is very low (Fig.14). The Urla W.W.T.P. discharge channel's negative effect has been observed in this factor's data.

Four main factors that were affecting the study area were identified as lithogenic factor (50.6%) anthropogenic factor caused by untreated domestic waste (13.2%), anthropogenic factor caused by marine traffic/port activities (9.3%) and anthropogenic factor caused by small-scale industrial activities (with 6.9% of the total variance). The main source of metals in the study area were determined as maritime traffic/harbor activities (Cu and Zn), untreated domestic waste discharges (TOC and S) and discharges of other wastes caused by urbanization. Assessment of contamination ranking calculated based on preindustrial local metal concentrations observed as Hg>As>Ni>Cd>Cu>Cr >Pb>Zn in the Gülbahçe Bay, while the contamination ranking based on preindustrial global metal concentrations was determined as As>Pb>Cr>Ni>Zn>Hg>Cu>Cd.

The main metal element that poses the most significant risk for benthic organisms was determined as Ni in the study area. All environmental indices showed non to moderate pollution existing in Gülbahçe Bay. It has been observed that most prominent feature of the distribution of elemental concentrations and assessment of pollution indices maps were that the pollutants carried inwards to Gülbahçe Bay from Izmir Central Bay with inflows, following the sediment transport directions, and pollutants' tendency to accumulate inside the fine sediment deposition zones have been very high.

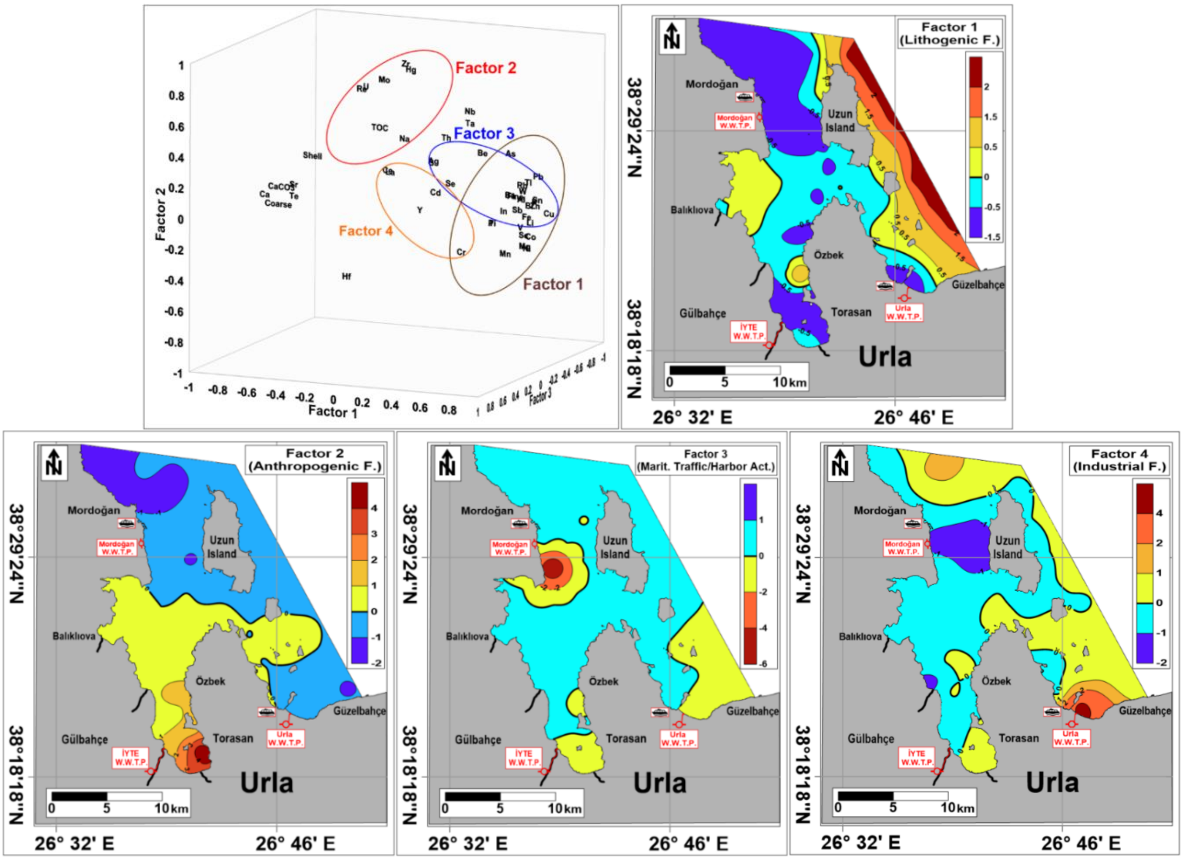

Fig. 5. The spatial distribution of factors affecting the study area.

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) Appendix A. Supplementary Data

Table S1. The equations and calculation parameters used for environmental pollution indexes.

Index	Equations	Explanation	References
Normalized Total Organic Content (TOC_N)	$TOC_{\boldsymbol{N}} = TOC_{(mg/g)} + 18(1 - GS_{Fine})$	$TOC_{(mg/g)}$: Total organic carbon content of the sample as mg/g GS_{Fine}: the proportion (%) fine fraction (<63 µm) of the sample	Molvær et al., 1997; Carroll et al., 2003
Contamination Factor (C_f)	$C_f^i = \bar{C}_{0-1}^i / C_n^i$	C_f^i: Contamination factor of element in the location $\bar{C}_{0-1}^i$: Mean content of the substance in question in the location (at least 5 samples should be used) C_n^i:The standard preindustrial reference of substance	Håkanson, 1980
Contamination Degree (C_{deg})	$C_{deg} = \sum_{i=1}^{n} C_f^i$	C_{deg}: Contamination degree	Håkanson, 1980
Modified Contamination Degree (mC_d)	$mC_d = \frac{1}{n} \times \sum_{i=1}^{n} C_f^i$	mC_d: Modified contamination degree	Abrahim and Parker, 2008
Pollution Load Index (PLI)	$PLI = \left(\prod_{i=1}^{n} C_f^i \right)^{1/n}$	PLI: Pollution Load Index	Tomlinson et al., 1980
Nemerow Poll. Index (PI_{Nem})	$PI_{Nem} = \sqrt{\frac{(Cf_{mean})^2 + (Cf_{max})^2}{2}}$	PI_{Nem}: Nemerow Pollution Index	Nemerow, 1991; Jie-Liang et al., 2007
Enrichment Factor (EF)	$EF = \frac{C_{S.Me}^i / C_{S.Ref(Al)}^i}{C_{B.Me}^i / C_{B.Ref(Al)}^i}$	$C_{S.Me}^i$: The content of the element in sample $C_{S.Ref(Al)}^i$: The content of the reference element (Al) in sample $C_{B.Me}^i$: The standard preindustrial reference of metal $C_{B.Ref(Al)}^i$: The standard preindustrial reference of reference metal (Al)	Zoller et al., 1974; Idris, 2008; Qingjie et al., 2008; Kowalska et al., 2018
Modified Pollution Index (MPI)	$MPI = \sqrt{\frac{(EF_{mean})^2 + (EF_{max})^2}{2}}$	MPI: Modified Pollution Index	Brady et al.,2015
Geoaccumulation Index (Igeo)	$I_{geo} = \log_2 \left(\frac{C_{S.Me}^i}{1.5 \times C_{B.Me}^i} \right)$	Igeo: Geoaccumulation Index $C_{S.Me}^i$: The content of the element in sample $C_{B.Me}^i$: The standard preindustrial reference of metal	Muller, 1969, Loska et al., 2003; Ji et al., 2008; Zhang et al., 2009
The Risk Quotient Based on TEL (QTEL)	$\boldsymbol{Q_{TEL}} = \sum_{i=1}^{n} \frac{C_{S.Me}^i}{TEL_i}$	QTEL: The Risk Quotient Based on TEL $C_{S.Me}^i$: The content of the element in sample TEL_i: Referenced sediment quality TEL value in question	Zhang et al., 2017b
The Risk Quotient Based on PEL (QPEL)	$\boldsymbol{Q_{PEL}} = \sum_{i=1}^{n} \frac{C_{S.Me}^i}{PEL_i}$	QPEL: The Risk Quotient Based on PEL $C_{S.Me}^i$: The content of the element in sample PEL_i: Referenced sediment quality PEL value in question	Zhang et al., 2017b
Toxic Risk Index (TRI)	$TRI_i = \sqrt{\frac{\left(\frac{C_i}{TEL_i}\right)^2 + \left(\frac{C_i}{PEL_i}\right)^2}{2}}$ $TRI = \sum_{i=1}^{n} TRI_i$	$C_{S.Me}^i$: The content of the element in sample TEL_i: Referenced sediment quality TEL value in question PEL_i: Referenced sediment quality PEL value in question TRI_i: The toxic risk value of per metal in question TRI: Toxic Risk Index (The total of TRI_i for per sample)	Zhang et al., 2017b

Table S2. The grades and categorizations for environmental pollution indexes.

Index	Value Grades	Categorization	References
Normalized Total Organic Content (TOC_N)	$TOC_N < 20$ $20 \leq TOC_N < 27$ $27 \leq TOC_N < 34$ $34 \leq TOC_N \leq 41$ $41 < TOC_N$	Excellent, Good, Intermediate, Poor, Very Poor.	Molvær et al., 1997; Carroll et al., 2003
Contamination Factor (C_f)	$C_f < 1$ $1 \leq C_f < 3$ $3 \leq C_f < 6$ $6 \leq C_f$	Low Contamination Factor, Moderate Contamination Factor, Considerable Contamination Factor, Very High Contamination Factor.	Håkanson, 1980
Contamination Degree (C_{deg})	$C_{deg} < 8$ $8 \leq C_{deg} < 16$ $16 \leq C_{deg} < 32$ $32 \leq C_{deg}$	Low Degree of Contamination, Moderate Degree of Contamination, Considerable Degree of Cont., Very High Degree of Contamination.	Håkanson, 1980
Modified Contamination Degree (mC_d)	mCd < 1.5 1.5 ≤ mCd < 2 2 ≤ mCd < 4 4 ≤ mCd < 8 8 ≤ mCd < 16 16 ≤ mCd < 32 32 ≤ mCd	Nil to Very Low Degree of Cont., Low Degree of Contamination, Moderate Degree of Contamination, High Degree of Contamination, Very High Degree of Contamination, Extremely High Degree of Cont., Ultra High Degree of Contamination.	Abrahim and Parker, 2008
Pollution Load Index (PLI)	PLI < 1 PLI > 1	Unpolluted Polluted	Tomlinson et al., 1980
Nemerow Poll. Index (PI_{Nem})	$PI_{Nem} \leq 0.07$ $0.7 < PI_{Nem} \leq 1$ $1 < PI_{Nem} \leq 2$ $2 < PI_{Nem} \leq 3$ $3 < PI_{Nem}$	Safety Domain, Precaution Domain, Slightly Polluted Domain, Moderately Polluted Domain, Seriously Polluted Domain.	Nemerow, 1991; Jie-Liang et al., 2007
Enrichment Factor (EF)	EF < 2 2 ≤ EF < 5 5 ≤ EF < 20 20 ≤ EF < 40 40 ≤ EF	Deficiency to Minimal Mineral E., Moderate Enrichment, Significant Enrichment, Very High Enrichment, Extremely High Enrichment.	Zoller et al., 1974; Idris, 2008; Qingjie et al., 2008; Kowalska et al., 2018
Modified Pollution Index (MPI)	MPI < 1 1 ≤ MPI < 2 2 ≤ MPI < 3 3 ≤ MPI < 5 5 ≤ MPI < 10 10 ≤ MPI	Unpolluted, Slightly Polluted, Moderately Polluted, Moderately Heavily Polluted, Heavily Polluted, Extremely Polluted.	Brady et al.,2015
Geoaccumulation Index (Igeo)	Igeo < 0 0 ≤ Igeo < 1 1 ≤ Igeo < 2 2 ≤ Igeo < 3 3 ≤ Igeo < 4 4 ≤ Igeo < 5 5 ≤ Igeo	Uncontaminated, Uncontaminated to Moderately Cont., Moderately Contaminated, Moderately to Strongly Contaminated, Strongly Contaminated, Strongly to Extremely Contaminated, Extremely High Contaminated.	Muller, 1969, Loska et al., 2003; Ji et al., 2008; Zhang et al., 2009
QTEL and QPEL	QTEL < 1 QPEL ≤ 1 ≤ QTEL 1 < QPEL	Sediment is nontoxic - toxicity < 10%) Sediment is uncertain - 10% ≤ toxicity ≤ 30%) Sediment is toxic - 30% < toxicity	Zhang et al., 2017b
Toxic Risk Index (TRI)	TRI ≤ 5 5 < TRI ≤ 10 10 < TRI ≤ 15 15 < TRI ≤ 20 20 < TRI	No Toxic Risk, Low Toxic Risk, Moderate Toxic Risk, Considerable Toxic Risk, Very High Toxic Risk.	Zhang et al., 2017b

Table S3. Factor loadings of and eigenvalue scores of environmental variables calculated according to Varimax normalized principal components analysis.

Factor Loadings (Varimax normalized) Extraction: Principal components (Marked loadings are >0.7000)				
Variable (ppm)	**Factor 1**	**Factor 2**	**Factor 3**	**Factor 4**
Coarse%	-0.844	-0.103	-0.056	0.006
Fine%	0.844	0.103	0.056	-0.006
Shell%	-0.543	0.261	0.096	-0.387
CaCO3%	-0.707	0.066	0.213	-0.535
TOC%	-0.146	0.448	-0.061	-0.690
Ag	-0.146	0.080	-0.920	-0.002
Al_%	0.927	0.106	0.150	0.286
As	0.729	0.339	-0.131	0.051
Ba	0.870	0.138	0.198	0.156
Be	0.624	0.369	0.073	0.371
Bi	0.916	0.038	0.000	0.012
Ca_%	-0.832	0.005	0.191	-0.439
Cd	-0.135	-0.126	-0.928	-0.135
Ce	-0.016	0.212	0.112	0.901
Co	0.929	-0.161	0.005	0.248
Cr	0.464	-0.293	0.039	0.753
Cu	0.913	-0.071	-0.322	0.073
Fe_%	0.928	-0.022	0.067	0.325
Hg	0.162	0.889	0.154	0.091
Hf	-0.316	-0.509	0.069	-0.147
In	0.738	-0.013	-0.006	0.004
K_%	0.964	0.069	0.026	0.150
La	0.001	0.201	0.108	0.902
Li	0.962	-0.053	0.092	0.182
Mg_%	0.899	-0.221	0.030	-0.095
Mn	0.713	-0.305	-0.088	0.485
Mo	-0.158	0.741	-0.157	-0.007
Na_%	-0.010	0.373	-0.141	-0.242
Nb	0.586	0.657	0.189	0.355
Ni	0.888	-0.247	-0.030	0.260
P_%	0.276	-0.281	-0.866	0.169
Pb	0.917	0.203	-0.139	0.027
Rb	0.925	0.195	0.132	0.144
Re	-0.245	0.703	0.002	-0.146
S_%	-0.168	0.063	-0.936	-0.176
Sb	0.828	0.001	-0.012	-0.123
Sc	0.911	-0.140	0.076	0.318
Se	0.200	0.055	-0.392	0.024
Sn	0.927	0.057	-0.107	0.196
Sr	-0.658	0.071	0.128	-0.582
Ta	0.607	0.590	0.237	0.381
Te	-0.617	0.016	0.219	-0.488
Th	0.500	0.510	0.366	0.476
Ti_%	0.738	-0.059	0.174	0.562
Tl	0.907	0.188	-0.005	0.048
U	-0.134	0.760	0.188	-0.227
V	0.876	-0.098	0.048	0.350
W	0.900	0.142	0.065	0.303
Y	0.421	0.076	0.602	0.263
Zn	0.644	-0.113	-0.724	0.122
Zr	0.115	0.917	0.131	0.094
Eigenvalue	25.83	6.72	4.74	3.50
Total Eigen.%	**50.64**	**13.18**	**9.30**	**6.86**
Cumulative	25.83	32.55	37.29	40.79
Total Cumul.%	**50.64**	**63.82**	**73.12**	**79.98**