Implementation of a far-field water quality model for the simulation of trace elements in an Eastern Mediterranean coastal embayment receiving high anthropogenic pressure.

SUPPLEMENTARY MATERIAL

Table S1. Sampling Stations network information.

Subarea name	Monitoring Stations[1]	Longitude (Decimal Degrees)	Latitude (Decimal Degrees)	Maximum depth (m)	Anthropogenic Pressure
Elefsis Gulf	S1	23.5545	38.0175	20	high
	S2	23.4530	38.0000	30	high
Inner Saronikos	S3	23.5833	37.9500	30	high
	S7	23.5908	37.9237	75	high
	S8	23.5333	37.8833	90	medium
	S11	23.6383	37.8772	75	medium
	S43	23.5872	37.8778	90	medium
Outer Saronikos	S16	23.7007	37.7872	85	low
	S18	23.5900	37.7680	70	low
Western Saronikos	S13	23.4550	37.8408	90	low

Table S2. Analytical table of processes activated in Delft3D-WAQ module for the simulation of ecosystem dynamics.

Main Processes selected			
Group	**Substance (variable)**	**Process**	**[proc_id]**
Oxygen-BOD	Dissolved Oxygen	Uptake of nutrients by growth of algae	[NutUpt_Alg]
		Denitrification in water column	[DenWat_NO3]
		Nitrification of ammonium	[Nitrif_NH4]
		Nett primary production and mortality green	[GroMrt_Gre]
		Nett primary production and mortality diatoms	[GroMrt_Dia]
		Limitation	[PPrLim]
	Ammonium (NH4)	Uptake of nutrients by growth of algae	[NutUpt_Alg]

Dissolved inorganic matter	Nitrate (NO3) Ortho-Phosphate (PO4) Dissolved Silica (Si)	Composition	[Compos]
		Nitrification of ammonium	[Nitrif_NH4]
		Release	[NutRel_Alg]
		Denitrification in water column	[DenWat_NO3]
		Atmospheric deposition NH4	[AtmDep_NH4]
		Atmospheric deposition NO3	[AtmDep_NO3]
		Atmospheric deposition PO4	[AtmDep_PO4]
Organic matter	Particulate Organic Carbon (POC) Dissolved Organic Carbon (DOC) Dissolved Organic Nitrogen (DON) Dissolved Organic Phosphorus (DOP)	Release	[NutRel_Alg]
		Sedimentation POC	[Sed_POC]
		Mineralization fast decomp. detritus POC	[DecFast]
		Mineralization DOC	[DecDOC]
Algae (phytoplankton)	Diatoms Algae (non-Diatoms)	Nett primary production and mortality	[GroMrt_Gre]
		Limitation	[PPrLim]
		Sedimentation	[SedGre]
Extra Processes selected			
		Process	**[proc_id]**
		Daylength function for green algae	[DL_Green]
		Nutrient limitation function for green algae	[NLGreen]
		Light efficiency function green algae	[Rad_Green]
		Temperature functions for green algae	[TF_Green]
		Daylength function for diatoms	[DL_Diat]
		Nutrient limitation function for diatoms	[DL_Diat]
		Light efficiency function diatoms	[Rad_Diat]
		Temperature functions for diatoms	[TF_Diat]
		Computation of phytoplankton - Dynamo	[Phy_dyn]
		dynamic calculation of the depth	[DynDepth]
		Extinction of visible light	[Extinc_VLG]
		Partitioning OMP in water column	[PartWK_OMP]
		Gas and liquid exchange coefficients	[TrCoef_OMP]
		Total of all sedimenting substances	[Sum_Sedim]

	Sum sedimentation of algae - Dynamo	[SedPhyDyn]
	Daylength calculation	[Daylength]
	Radiation at segment upper/lower boundary	[CalcRad]
	Extinction of visible light by algae	[ExtPhDVL]
	Horizontal flow velocity	[Veloc]
	Sedimentation IM1	[Sed_IM1
	Reflection calculation	[Reflection]

[1] According to Deltares (2020), D-Water quality processes library description, technical reference manual. v.5.01, Deltares [51].

Table S3. Table of processes values, activated in Delft3D-WAQ module for the simulation of ecosystem dynamics.

Input/Output parameters	[proc_id]	type	Value/Equation	Unit	source
Process: Uptake of nutrients by growth of algae [NutUpt_Alg]					
numerical maximum flux Greens	fcPPGreeN	PPrLim	[PPrLim]	$gN/m^3/d$	[1]
N:C ratio Greens	NCRatGreen	constant	0.16	gN/gC	[1]
P:C ratio Greens	PCRatGreen	constant	0.02	gP/gC	[1]
numerical maximum flux Diatoms	fcPPDiat	PPrLim	[PPrLim]	$gN/m^3/d$	[1]
N:C ratio Greens	NCRatGreen	constant	0.16	gN/gC	[1]
P:C ratio Greens	PCRatGreen	constant	0.02	gP/gC	[1]
Si:C ratio Diatoms	SCRatDiat	constant	0.49	gSi/gC	[1]
critical NH4 concentration	NH4KRIT	constant	0.01	$gN/m^3/d$	[1]
Process: Nitrification of ammonium [Nitrif_NH4]					
zeroth-order nitrification flux	Znit	constant	0	$gN/m^3/d$	[1]
MM-nitrification rate at 20°C	Rcnit20	constant	0.1	$gN/m^3/d$	[1]
temperature coefficient for nitrification	TcNit	constant	1.07	(-)	[1]
half saturation constant for ammonium co	KsAmNit	constant	0.5	gN/m^3	[1]
half saturation constant for DO	KsOxNit	constant	1	g/m^3	[1]
ambient water temperature	Temp	4D file	.tem	°C	[2]
critical temperature for nitrification	CTNit	constant	3	°C	[1]
zeroth-order nitrification rate at neg. D	Rc0NitOx	constant	0	$gN/m^3/d$	[1]
critical oxygen concentration for nitrif	COXNIT	constant	1	g/m^3	[1]

volumetric porosity	Poros	constant	1	(-)	[1]
first-order nitrification rate	RcNit	constant	0.1	(1/d)	[1]
optimum oxygen concentration for nitrification	OOXNIT	constant	5	gO_2/m^3	[1]
oxygen function level for oxygen bellow CO	CFLNIT	constant	0	(-)	[1]
curvate of DO function for nitrification	CurvNit	constant	0	(-)	[1]
Process: Net primary production and mortality green [GroMrt_Gre]					
salinity		4D file	.sal	g/kg	[2]
daylength limitation function for Greens	LimDLGreen	DL_Green	[DL_Green]	(-)	[1]
nutrient limitation function Greens <	LimNutGreen	NLGreen	[NLGreen]	(-)	[1]
radiation limitation function Greens	LimRadGree	Rad_Green	[Rad_Green]	(-)	[1]
temperature function growth Greens <0		TF_Green	[TF_Green]	(-)	[1]
temperature function mortality Greens	TFMrtGreen	TF_Green	[TF_Green]	(-)	[1]
maximum production rate Greens	PPMaxGreen	constant	1.8	1/d	[1]
maintenance respiration Greens st.tem		constant	0.045	(-)	[1]
growth respiration factor Greens	GRespGreen	constant	0.15	(-)	[1]
mortality rate constant Greens	Mort0Green	constant	0.35	1/d	[1]
mortality rate Greens at high salinity	MortSGreen	constant	0.35	1/d	[1]
lower salinity limit for mortality Greens	SalM1Green	constant	20	g/kg	defined by user
upper salinity limit for mortality Greens	SalM1Green	constant	45	g/kg	defined by user
Minimum level Greens in mortality	MinGreen	constant	0	gC/m^3	[1]
Process: Limitation (numerical) on primary production [PPrLim]					
net primary production of Greens	fPPGreen	GroMrt_Gre	[GroMrt_Gre]	$gC/m^2/d$	[1]
N:C ratio Greens	NCRatGreen	single value	0.16	gN/gC	[1]
P:C ratio Greens	PCRatGreen	single value	0.02	gP/gC	[1]
net primary production of Diatoms	fPPDiat	GroMrt_Dia	[GroMrt_Dia]	$gC/m^2/d$	[1]
N:C ratio Diatoms	NCRatDiat	single value	0.16	gN/gC	[1]
P:C ratio Diatoms	PCRatDiat	single value	0.02	gP/gC	[1]
Si:C ratio Diatoms	SCRatDiat	single value	0.49	gSi/gC	[1]
Process: Composition [Compos]					

inorganic matter	IM1	timeserries	.tim	gDM/m³	[3]
total carbon in phytoplankton	Phyt	Phy_dyn	[Phy_dyn]	gC/m³	[1]
total nitrogen in algae	AlgN	Phy_dyn	[Phy_dyn]	gN/m³	[1]
total phosphorus in algae	AlgP	Phy_dyn	[Phy_dyn]	gP/m³	[1]
total silica in algae	AlgSi	Phy_dyn	[Phy_dyn]	gSi/m³	[1]
total DM in algae	AlgDM	Phy_dyn	[Phy_dyn]	gDM/m³	[1]
DM:C ratio IM1	DMCFIM1	single value	1	gDM/gDM	[1]
DM:C ratio POC1	DmCfPOC1	single value	2.5	gDM/gC	[1]
Process: Release (nutrient/detritus) by of mortality algae [NutRel_Alg]					
mortality flux Greens	fMrtGreen	GroMrt_Gre	[GroMrt_Gre]	gC/m²/d	[1]
N:C ratio Greens	NCRatGreen	single value	0.16	gN/gC	[1]
P:C ratio Greens	PCRatGreen	single value	0.02	gP/gC	[1]
fraction autolysis Greens	FrAutGreen	single value	0.3	(-)	[1]
fraction to detritus by mortality Gre	FrDetGreen	single value	0.7	(-)	[1]
mortality flux Diatoms	fMrtDiat	GroMrt_Dia	[GroMrt_Dia]	gC/m²/d	[1]
N:C ratio Diatoms	NCRatDiat	single value	0.16	gN/gC	[1]
P:C ratio Diatoms	PCRatDiat	single value	0.02	gP/gC	[1]
Si:C ratio Diatoms	SCRatDiat	single value	0.49	gSi/gC	[1]
fraction autolysis Diatoms	FrAutDiat	single value	0.3	(-)	[1]
fraction to detritus by mortality Diatoms	FrDetDiat	single value	0.7	(-)	[1]
Process: Atmospheric deposition [AtmDep]					
Atmospheric deposition flux NH4	fAtmDep_NH4	single value	0.0016	gN/m²/d	[4]
Atmospheric deposition flux NO3	fAtmDep_NO3	single value	0.001	gN/m²/d	[4]
Atmospheric deposition flux PO4	fAtmDep_PO4	single value	0.00005	gP/m²/d	[4]
Process: Secchi depth for visible-light (370-680nm)					
total extinction coefficient visible light	ExtVl	Extinc_VLG	[Extinc_VLG]	1/m	[1]
Poole-Atkins constant	PAConstant	single value	1.7	(-)	[1]
Process: Sedimentation diatoms [SedDiat], Greens [SedGreen], POC [SedPOC], IM [SedIM]					
total bottom shear stress	Tau	4D file	.tau	N/m²	[2]
critical shear stress for sedimentation	TaucSDiat	single value	0.1	N/m²	[1]

depth of segment	Depth	DynDepth	[DynDepth]	m/d	[1]
minimum waterdepth for sedimentation/resuspension		single value	0.1	m	[1]
zeroth-order sedimentation flux diatoms	ZSedDiat	single value	0	$gC/m^2/d$	[1]
sedimentation velocity Diatoms	VSedDiat	single value	0.1	m/d	[1]
zeroth-order sedimentation flux Greens	ZSedGreen	single value	0	$gC/m^2/d$	[1]
sedimentation velocity Greens	VSedGreen	single value	0.1	m/d	[1]
zeroth-order sedimentation flux POC	ZSedPOC	single value	3	$gC/m^2/d$	[1]
sedimentation velocity POC	VSedPOC	single value	0.5	m/d	[1]
zeroth-order sedimentation flux IM	ZSedIM	single value	0	$gC/m^2/d$	[1]
sedimentation velocity IM	VSedIM	single value	10	m/d	[1]
Extra processes: Nutrient Limitation for Greens/Diatoms					
Ammonium preferency over Nitrate Greens/Diatoms	prefNH4	single value	1	-	[1]
Half-saturation value N Greens/Diatoms	KMDIN	single value	0.0028	gN/m^3	[5]
Half-saturation value P Greens/Diatoms	KMP	single value	0.00035	gP/m^3	[6]
Half-saturation value Si Diatoms	KMPDiat	single value	0.027	gSi/m^3	[1]
Extra processes: Temperature function for Greens/Diatoms					
Temperature coeff. for growth process	TcGro	single value	1.04	-	[1]
Temperature coeff. for respiration and mortality	TcDec	single value	1.07	-	[1]
Extra processes: Light efficiency function Diatoms					
Irradiation at the segment upper-boundary	Rad	CalcRad	CalcRad	W/m^2	[1]
Total radiation growth saturation Diatoms	RadSatDiat	single value	25	W/m^2	[1]
Extra processes: Radiation at segment upper and lower					
Irradiation at the water surface	RadSurf	timeserries	.tim	W/m^2	[7]

[1] According to Deltares (2020), D-Water Processes Library Tables, Technical Reference Manual. v.5.02, Deltares [52].
[2] Outcome of hydrodynamic simulations via Delft3D-FLOW module.
[3] According to Krasakopoulou & Karagiorgis (2005) [42].
[4] According to Beyn et al. (2014) [88].
[5] According to Mac Isaac and Dugdale (1969) [89] and Eppley et al. (1969) [90].
[6] According to Kolovoyiannis and Tsirtsis (2013) [91].
[7] Timeserries file with actual irradiation, data from ERA5 hourly data [39]

Table S4. Nutrient loads introduced in the modelling area as discharges.

Name of Discharge	Type	flow [m^3 s^{-1}]	NH_4 [gN m^{-3}]	NO_3 [gN m^{-3}]	PO_4 [gP m^{-3}]	POC [gC m^{-3}]	DOC [gC m^{-3}]	DON [gN m^{-3}]	DOP [gP m^{-3}]	pollution data reference
Kifisos	River	varying [1]	0.028	3.1	0.038	0.45	2.6	0.06	0.0168	[6,7]
Sarantapotamos	Stream	varying [2]	0.028	3.1	0.038	0.45	2.6	0.06	0.0168	[6,7]
ElefsisCWbasin	Stream	varying [2]	0.028	3.1	0.038	0.45	2.6	0.06	0.0168	[6,7]
Psittalia	WWTP	7.75 [3]	0.6	3.5	2.03	1.71	14.2	1.74	0.315	[3,8]
MEYAThriasiou	WWTP	0.07 [3]	38.5	10	5.11	26.5	151.6	1.74	0.315	[3,8]
Oil ref. Aspropyrgos	Oil Refinery	0.06 [4]	5	10	0	4	25	5	0	[9,10]
Oil ref. Elefsina	Oil Refinery	0.13 [4]	5	10	0	4	25	5	0	[9,10]
Oil ref. Corinthos	Oil Refinery	0.45 [5]	5	10	0	4	25	5	0	[9,10]

[1] discharge measurements obtained from the Hellenic Integrated Marine Inland Water Observing, Forecasting and offshore Technology System HIMIOFoTs [43]
[2] prediction data provided by the Swedish Meteorological and Hydrological Institute (SMHI, platform Hypeweb) [40]
[3] Special Secretariat for Water, WWTP monitoring database [44]
[4] according to the company's published data [45]
[5] according to the company's published data [47]
[6] according to Skoulikidis et al. 2021 [92], Reddy et al. 2021 [93], and Wetzel 2001 [94]
[7] according to monitoring values from the National Water Monitoring Network [49]
[8] according to Bali and Gueddari 2019 [95] and Yang et al. 2014 [96]
[9] according to emission levels permitted by Directive 2010/75/EU, national legislation [50] (Decision 17823/79, FEK 1132 B/21-12-79)
[10] according to Sperling, 2007 [46]

Table S5. Inorganic Matter (IM) average monthly concentration used in the simulations.

Time Period	Inorganic Matter (IM) concentration (g m^{-3})[1]
01/11/2009 – 30/11/2009	0.37
01/12/2009 – 31/12/2009	0.39
01/01/2010 – 31/01/2010	0.28
01/02/2010 – 28/02/2010	0.17
01/03/2010 – 31/03/2010	0.28
01/04/2010 – 30/04/2010	0.40
01/05/2010 – 31/05/2010	0.53
01/06/2010 – 30/06/2010	0.38

01/07/2010 – 31/07/2010	0.35
01/08/2010 – 31/08/2010	0.32
01/09/2010 – 30/09/2010	0.34
01/10/2010 – 31/10/2010	0.35

[1] according to Krasakopoulou and Karageorgis (2005) [42]

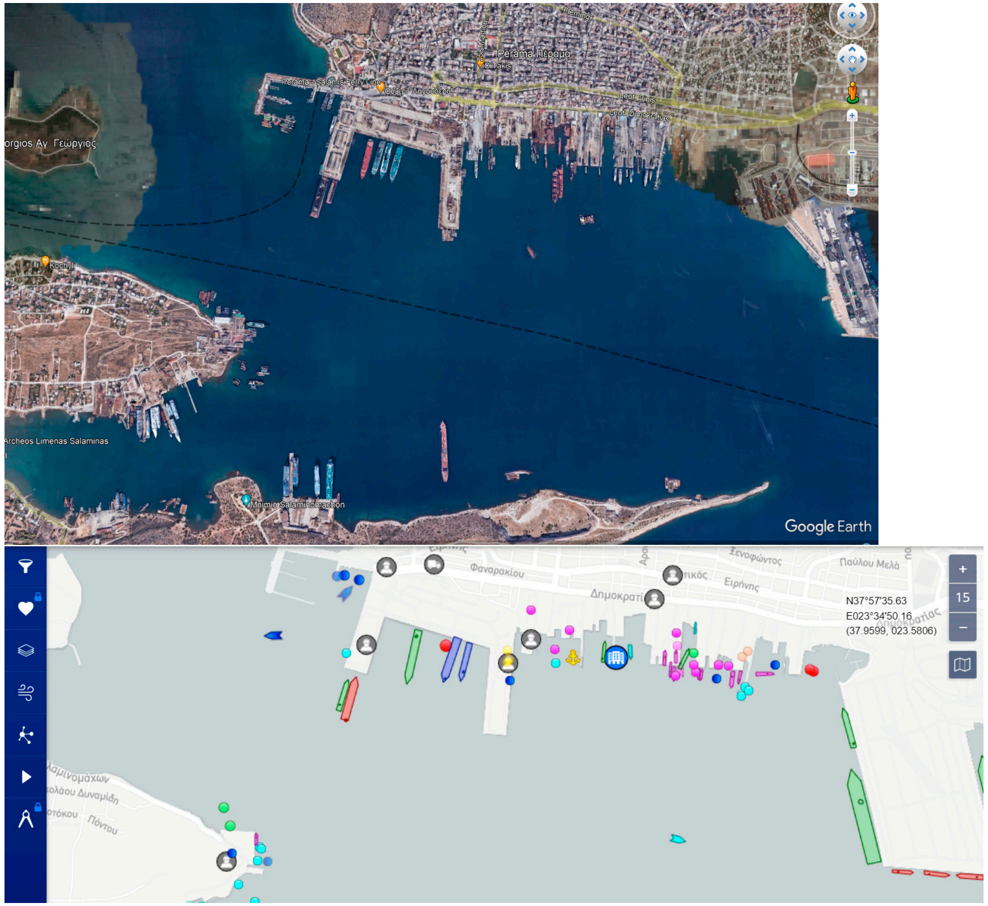

Figure S1. Perama small-scale industries ship repairing zone, a) google earth capture, and b) marine traffic capture.

Methodology for the estimation of pollution from the ship repairing zone - MAMPEC description of application.

The software MAMPEC v 3.1.0.5 was used to calculate discharges of Zn, Cu and Pb from ship restoration activities, occurring in the Perama industrial zone. To estimate an annual mass balance for trace elements discharges, statistical data from OLP (Piraeus Port Authority) was retrieved for the time period 2010-2011 [48]. The following data were considered to create an emission scenario, where the pollution occurred from maintenance activities. a) an average of 200 boats were maintained during the year 2010, with an average hull surface of 1255 m^2 (corresponding to average ship length of 80 m), b) the concentration of active ingredient in the antifouling paints used was 200 g L^{-1} for Zn and Cu and 25 g L^{-1} for Pb, c) the covering capacity of the paint was estimated to be 10 m^2 L^{-1} and that 3 layers of coating were applied per ship. The operation of the model lead to the following total daily average mass loads per pollutant: Cu, 39.7 kg d^{-1}; Zn, 39.7 kg d^{-1}; Pb, 5.16 kg d^{-1}. These mass loads were assumed to be discharged steadily throughout the modelling year as no data is available on the timeframe of operations of the shipyards. This point pollution source aims to summarize all pollution occurring in the area from shipping maintenance activities.

Table S6. Kd timeseries table – seasonal values, calculated according to monitoring data [21] and average SS concentrations [42].

Time period	SS[a]	Cadmium (Cd)			Lead (Pb)			Nickel (Ni)			Copper (Cu)			Zinc (Zn)		
		fp[b]	Log Kd[c]	Kd[d]	fp[b]	Log Kd[c]	Kd[d]	fp[b]	Log Kd[c]	Kd[d]	fp[b]	Log Kd[c]	Kd[d]	fp[b]	Log Kd[c]	Kd[d]
November, December 2009	0.3	10^{-5}	1.30	0.02	0.29	6.25	1768	0.10	5.62	413	0.25	6.33	2140	0.11	5.53	337
January, February, March 2010	0.6	10^{-5}	1.30	0.02	0.35	5.76	570	0.11	5.29	195	0.39	5.67	469	0.09	5.27	188
April, May, June 2010	0.5	10^{-5}	1.30	0.02	0.25	5.84	684	0.10	5.37	234	0.22	5.75	563	0.10	5.35	225
July, August, September, October 2010	0.5	10^{-5}	1.30	0.02	0.27	5.86	731	0.08	5.22	167	0.13	5.47	297	0.13	5.49	307

[a] average SS concentration (g m^{-3})

[b] fraction of trace element in the particulate phase

[c] kd in L/kg

[d] kd values, as implemented in the form of time series in the model (m^3/kgDM)

Table S7. Initial concentrations of trace elements used for the start-up of the model and concentrations at open boundaries.

Modelled variable	Initial Conditions (g m^{-3})	Boundary Conditions (g m^{-3}) Paraskevopoulou et al. 2014
Cadmium (Cd)	0.02 E-03	0.02 E-03
Lead (Pb)	0.2 E-03	0.2 E-03
Nickel (Ni)	1 E-03	0.32 E-03
Copper (Cu)	0.14 E-03	0.14 E-03
Zinc (Zn)	8 E-03	7 E-03

Hydrodynamic model performance – short discussion

The left panel of Figure S2 presents a comparison of the annual variability of Delft3D-FLOW simulated sea surface temperature (SST) with satellite-derived SST obtained from the Copernicus Marine Service ([97], L4 product, 1 km resolution). Both data series are averaged over the inner Saronikos gulf basin. The low RMSE (0.84 ^{o}C) and high correlation coefficient (r>0.99) underlines the good performance of the model in simulating ocean-atmosphere heat exchange and the adequacy of open boundary conditions used. On the right, the daily SST anomaly (monthly average subtracted) derived from the model and satellite data averaged over the model domain is presented. Both negative and positive SST anomalies were efficiently reproduced by the hydrodynamic model, as indicated by the high correlation (r=0.91) and small RMSE (0.33 ^{o}C).

Figures S3 and S4 present the simulated annual timeseries for temperature and salinity respectively along with the CTD field measurements at various depths of sampling station S16. Station S16 in this case acts as a representative of inner Saronikos Gulf. All timeseries indicate that the model performs quite well and reproduces the thermohaline annual variability of the basin, that is a major driver for circulation of water masses in the study area [25]. The quantitative metrics reported in the captions support this claim, as high and statistically significant correlation coefficients, and low simulation errors were calculated.

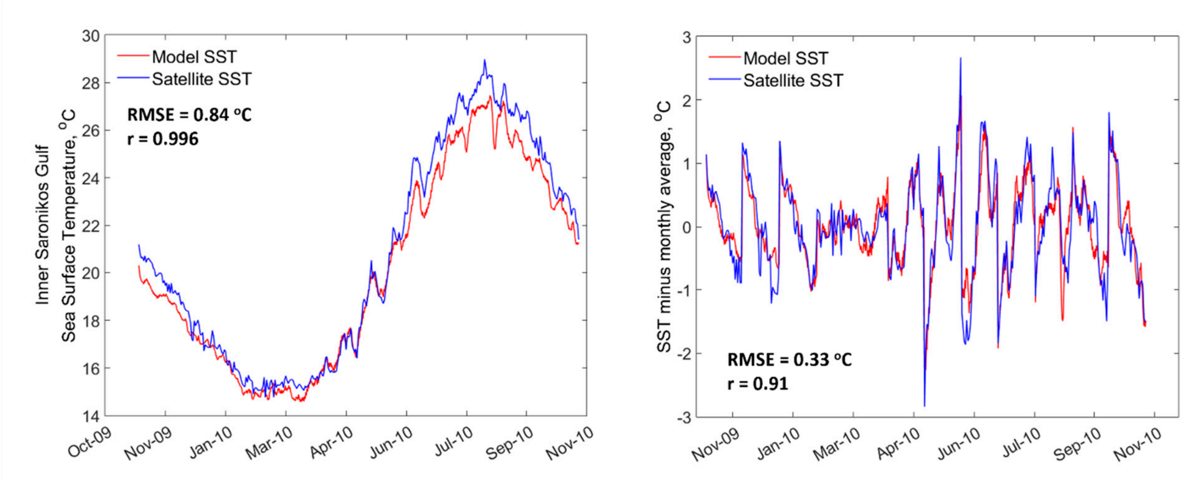

Figure S2. Comparison of Sea Surface Temperature (SST, °C, left) and SST anomaly (monthly average subtracted, right) derived from Delft3D-FLOW simulation (red line) and Copernicus satellite data (blue line), averaged over the inner Saronikos Gulf basin. The Root Mean Square Error (RMSE) and the correlation coefficient (r) in each case are reported.

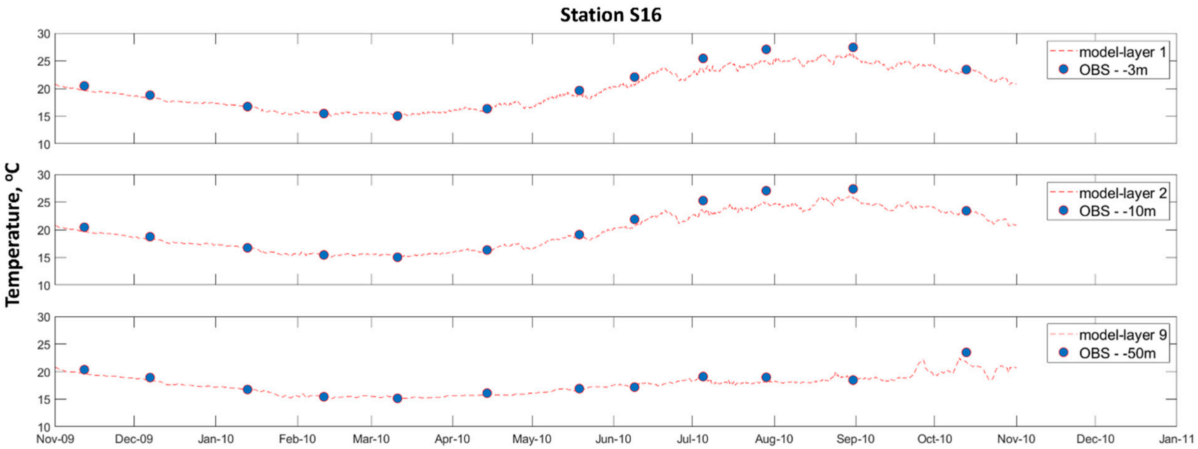

Figure S3. Simulated (line) and measured with CTD (dots) sea water temperature (°C) at various depths of station S16 (inner Saronikos Gulf) during the study period (November 2009 – October 2010). Simulation mean error = -0.44 °C, statistically significant correlation coefficient r = 0.93 (p-value<0.001).

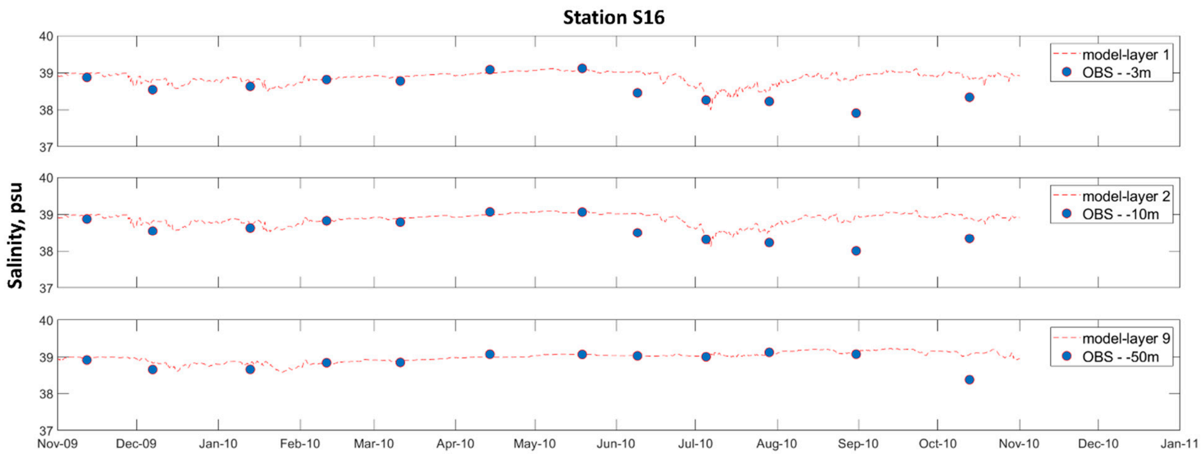

Figure S4. Simulated (line) and measured with CTD (dots) salinity (psu) at various depths of station S16 (inner Saronikos Gulf) during the study period (November 2009 – October 2010). Simulation mean error = 0.26 psu, statistically significant correlation coefficient r =0.61 (p-value<0.001).

Table S8. Statistical analysis of observed vs modelled concentrations of trace elements.

Modelled variable	MEAN-OBS ($g\ m^{-3}$)	STDEV-OBS ($g\ m^{-3}$)	MEAN-Model ($g\ m^{-3}$)	STDEV-Model ($g\ m^{-3}$)	BIAS ($g\ m^{-3}$)	MAE ($g\ m^{-3}$)	RMSE ($g\ m^{-3}$)	∣% bias∣	CF	Willmott Model Skill	R	N
Cadmium (Cd)	3.63×10^{-5}	3.76×10^{-5}	2.63×10^{-5}	1.45×10^{-5}	-9.92×10^{-6}	2.68×10^{-5}	4.18×10^{-5}	**27.36**	**0.71**	**0.68**	-0.04	87
Lead (Pb)	1.51×10^{-4}	7.33×10^{-5}	1.27×10^{-4}	8.70×10^{-5}	-2.38×10^{-5}	7.21×10^{-5}	1.08×10^{-4}	**15.76**	**0.98**	**0.87**	0.14	87
Nickel (Ni)	4.55×10^{-4}	1.49×10^{-4}	3.73×10^{-4}	2.51×10^{-4}	-8.20×10^{-5}	1.60×10^{-4}	1.98×10^{-4}	**18.04**	**1.07**	**0.95**	0.70	87
Copper (Cu)	3.35×10^{-4}	3.40×10^{-4}	2.92×10^{-4}	4.83×10^{-4}	-4.26×10^{-5}	2.09×10^{-4}	3.82×10^{-4}	**12.71**	**0.61**	**0.84**	0.62	87
Zinc (Zn)	6.11×10^{-3}	2.92×10^{-3}	5.65×10^{-3}	1.63×10^{-3}	-4.63×10^{-4}	2.62×10^{-3}	3.16×10^{-3}	**7.58**	**0.90**	**0.93**	0.14	87

Table S9. Predicted mass of heavy metals reaching the top sediment layer after 365 days of simulation (in mg m^{-2} $year^{-1}$).

Modelled variable	S1[1]	S7[1]
Cd	4.5 E-04	7.5 E-04
Pb	61	214
Ni	114	152
Cu	389	293
Zn	742	2796

[1] The predicted sedimentation rate for DM (Dry Matter) is 0.41 kg m^{-2} $year^{-1}$ at S1 station and 1.28 kg m^{-2} $year^{-1}$ at S7.

Table S10. Measured concentrations of heavy metals in the top sediment layer (in mg kg^{-1}), year 2010, as reported by Karageorgis et al. 2020 [62].

Trace Element	S1	S1W	S1E	S7	S7W	S7N
Pb	163	123	52	128	46	190
Ni	99	76	63	88	29	86
Cu	167	85	37	118	21	115
Zn	445.8	384.2	167.2	301	75	376

Prifti et al. (2022) [63] reported sedimentation rates of 0.11cm/y for S1 and 0.62cm/y for S7, which could be transformed to 0.825 kg m^{-2} $year^{-1}$ at S1 station and 4.65 kg m^{-2} $year^{-1}$ at S7, with the use of HELCOM guidelines for the conversion of sediment volume to dry weight. According to HELCOM [98] and Cato (1977) [99], 1 m^3 of sediment corresponds to 0.75tns dry weight (for unknown type of sediment). Based on this information, the concentrations of Table S10 are transformed to mass fluxes, to be comparable with the output of the model (Table S9).

Table S11. Mass fluxes of trace elements (in mg m^{-2} $year^{-1}$), based on measured concentrations [62] (Table S10) and reported sedimentation rates [63].

Trace Element	S1	S1W	S1E	S7	S7W	S7N
Pb	134	102	43	595	214	884
Ni	81	62	52	408	133	402
Cu	138	70	30	548	99	536
Zn	368	317	138	1397	351	1747

References related only to SM file. References 1-87 can be found in the reference list of the main article.

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