Supplementary material for

Assessment of surface water quality in the Podu Iloaiei Dam Lake (north-eastern Romania): Potential implications for aquaculture activities in the area

Cornelia Amarandei [1,2], Alina-Giorgiana Negru [2], Laurentiu-Valentin Soroaga [1,2], Simona-Maria Cucu-Man [1], Romeo-Iulian Olariu [1,2], and Cecilia Arsene [1,2,*]

[1]"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, Department of Chemistry, 11 Carol I, 700506 Iasi, Romania

[2]"Alexandru Ioan Cuza" University of Iasi, Integrated Centre of Environmental Science Studies in the North Eastern Region, 11 Carol I, 700506 Iasi, Romania

*Correspondence to: carsene@uaic.ro; Phone number: +40-232-201354; Fax: +40-232-201313; Postal address: Cecilia Arsene, "Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, Department of Chemistry, 11 Carol I, 700506 Iasi, Romania

Table S1. Classification of waters in the quality classes in order to establish the ecological status of water bodies (extracted from Order no. 161/2006).

Chemical and physico-chemical elements and quality standards in water

No.	Indicator of quality	U/M	Class of quality				
			I	II	III	IV	V
Thermal regime and acidification							
1	Temperature	°C	It is not standardized				
2	pH		6.5 – 8.5				
Nutrients							
1	Ammonium (N-NH$_4^+$)	mg N/L	0.4	0.8	1.2	3.2	> 3.2
2	Nitrite (N-NO$_2^-$)	mg N/L	0.01	0.03	0.06	0.3	> 0.3
3	Nitrate (N-NO$_3^-$)	mg N/L	1	3	5.6	11.2	> 11.2
4	Soluble orthophosphates (P-PO$_4^{3-}$)	mg P/L	0.1	0.2	0.4	0.9	> 0.9
Salinity							
1	Conductivity	μS/cm					
2	Chlorides (Cl$^-$)	mg/L	25	50	250	300	> 300
3	Sulphates (SO$_4^{2-}$)	mg/L	60	120	250	300	> 300
4	Calcium (Ca^{2+})	mg/L	50	100	200	300	> 300
5	Magnesium (Mg^{2+})	mg/L	12	50	100	200	> 200
6	Sodium (Na$^+$)	mg/L	12	50	100	200	> 200
Specific toxic pollutants of natural origin							
1	Total Chromium (Cr^{3+} + Cr^{6+})	μg/L	25	50	100	250	> 250
2	Zinc (Zn^{2+})	μg/L	100	200	500	1000	> 1000
3	Barium (Ba^{2+})	mg/L	0.05	0.1	0.5	1	> 1
4	Lead (Pb)	μg/L	5	10	25	50	> 50
5	Cadmium (Cd)	μg/L	0.5	1	2	5	> 5
6	Total Manganese (Mn^{2+} + Mn^{7+})	mg/L	0.05	0.1	0.3	1	> 1
7	Nickel (Ni)	μg/L	10	25	50	100	> 100

For the limits of detection (LoD) and limits of quantification (LoQ) estimation, the standard deviation 3 times and 10 times, respectively, of ten measurements corresponding to the standard with the lowest concentration have been used to perform the calibration curves, relative to the method sensitivity for each ionic species.

Table S2. Limits of detection (LoD) and limits of quantification (LoQ) for ion chromatography determined water-soluble ions in the water and sediment samples.
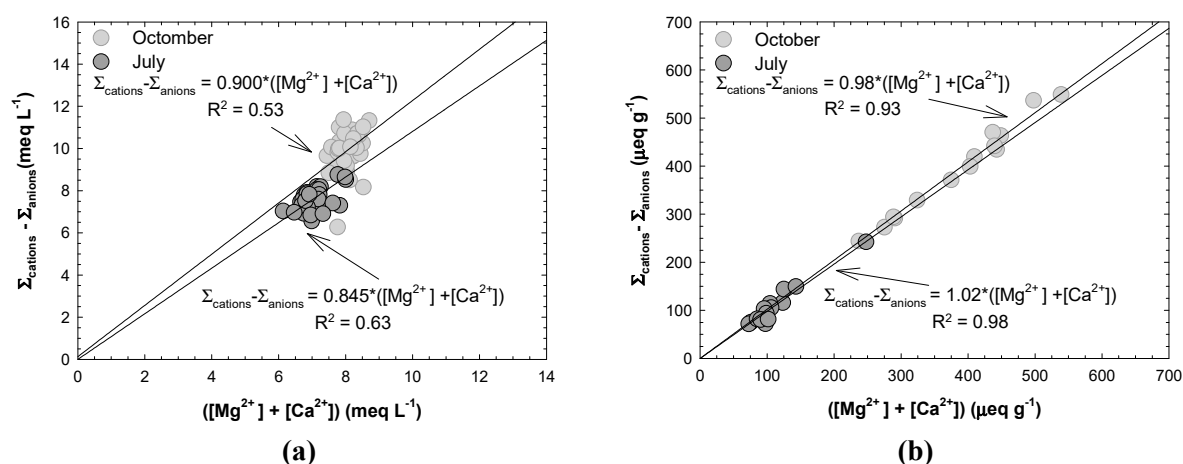
Anions	LoD ($\mu g\ L^{-1}$)	LoQ ($\mu g\ L^{-1}$)	Cations	LoD ($\mu g\ L^{-1}$)	LoQ ($\mu g\ L^{-1}$)
F^-	7.3	24.3	Li^+	0.4	1.5
Cl^-	31.0	103	Na^+	13.6	45.4
NO_2^-	20.0	66.6	NH_4^+	15.7	52.5
Br^-	14.7	48.9	K^+	44.4	148
NO_3^-	21.2	70.6	Mg^{2+}	18.7	62.4
PO_4^{3-}	17.8	59.3	Ca^{2+}	48.5	161
SO_4^{2-}	23.7	78.9			
$H_3C_2O_2^-$	106	356			
HCO_2^-	39.2	130			
$C_2O_4^{2-}$	56.3	188			

Table S3. Limits of detection (LoD) and limits of quantification (LoQ) for inductively coupled plasma mass spectrometry determined elements in the water and sediment samples.

| Element	LoD ($\mu g\ L^{-1}$)	LoQ ($\mu g\ L^{-1}$)	Element	LoD ($\mu g\ L^{-1}$)	LoQ ($\mu g\ L^{-1}$)
^{9}Be	1.86	6.20	^{85}Rb	0.62	2.07
^{11}B	71.7	239	^{88}Sr	0.02	0.05
^{24}Mg	0.72	2.41	^{95}Mo	1.87	6.23
^{27}Al	0.38	1.26	^{101}Ru	0.10	0.34
^{47}Ti	1.93	6.45	^{105}Pd	0.08	0.26
^{51}V	0.41	1.36	^{107}Ag	0.04	0.12
^{52}Cr	0.42	1.41	^{112}Cd	0.05	0.16
^{55}Mn	0.53	1.75	^{114}Cd	0.03	0.11
^{56}Fe	9.14	30.48	^{118}Sn	0.17	0.57
^{59}Co	0.19	0.62	^{121}Sb	0.14	0.47
^{60}Ni	1.70	5.65	^{125}Te	0.33	1.10
^{63}Cu	18.6	62.1	^{135}Ba	0.14	0.47
^{66}Zn	0.94	3.14	^{193}Ir	0.08	0.27
^{69}Ga	0.15	0.49	^{205}Tl	0.03	0.09
^{72}Ge	0.87	2.92	^{208}Pb	0.15	0.51
^{75}As	2.42	8.06	^{209}Bi	0.10	0.33
^{78}Se	3.81	12.71	^{238}U	0.005	0.016

Figure S1. Linear regression between ($\Sigma_{cations}$ - $\Sigma_{identified\ anions}$) and ($[Mg^{2+}]$ + $[Ca^{2+}]$) for water **(a)** and

sediment **(b)** samples in both sampling sessions.
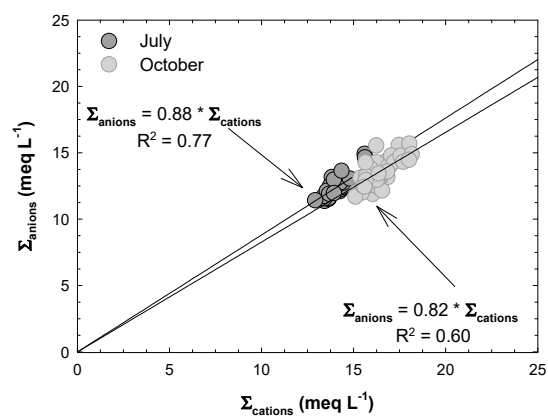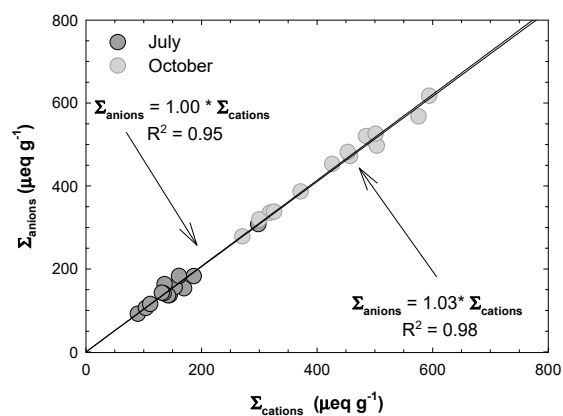
Figure S2. Linear regression for the ionic balance evaluation of water (**a**) and sediment (**b**) samples (including the HCO_3^- estimation).

Table S4. Pearson's correlation coefficient of chemical species, pH and conductivity (S) determined in water samples collected from Podu Iloaiei Dam Lake.

	Al	Cr	Mn	Ni	Zn	Ge	Sr	Ag	Sb	Ba	Pb	Cl⁻	SO₄²⁻	Na⁺	NH₄⁺	K⁺	Mg²⁺	Ca²⁺	pH	S
Al	1	0.10	0.12	-0.21	0.32	0.60	-0.15	-0.20	-0.15	0.13	0.39	-0.04	-0.09	0.06	-0.04	-0.14	0.03	0.03	-0.08	0.07
Cr		1	0.38	-0.28	0.33	-0.59	-0.26	-0.23	0.65	0.72	-0.25	0.23	-0.63	0.49	0.51	0.10	0.56	0.35	-0.56	0.55
Mn			1	-0.25	0.48	0.22	0.02	0.57	0.30	0.37	0.13	0.49	-0.44	0.44	0.68	0.39	-0.04	0.50	-0.46	0.40
Ni				1	-0.05	0.68	0.00	0.11	0.32	0.01	-0.16	0.04	-0.23	0.20	0.07	-0.07	0.13	0.02	-0.21	0.18
Zn					1	-0.05	-0.06	-0.05	0.93	-0.04	-0.04	0.00	-0.20	0.06	0.42	0.00	-0.08	0.14	-0.21	0.18
Ge						1	0.48	0.00	-0.11	0.54	-0.21	0.39	0.21	0.36	0.07	-0.01	0.39	0.45	-0.19	0.15
Sr							1	0.05	-0.02	0.08	-0.14	0.57	0.38	0.44	0.00	0.07	0.65	0.80	-0.09	0.09
Ag								1	0.49	0.30	0.24	0.13	-0.27	0.26	0.23	0.07	0.24	0.11	-0.30	0.29
Sb									1	0.16	0.22	-0.01	-0.40	0.24	0.63	0.50	0.18	0.05	-0.41	0.38
Ba										1	0.15	0.45	-0.34	0.43	0.33	0.41	0.30	0.15	-0.41	0.43
Pb											1	0.03	-0.01	0.10	0.08	0.30	0.07	0.08	-0.02	0.04
Cl⁻												1	-0.12	0.76	0.55	0.62	0.63	0.71	-0.49	0.49
SO₄²⁻													1	-0.54	-0.59	-0.18	-0.29	0.04	0.82	-0.76
Na⁺														1	0.65	0.47	0.86	0.70	-0.84	0.83
NH₄⁺															1	0.62	0.28	0.36	-0.66	0.64
K⁺																1	0.17	0.23	-0.26	0.24
Mg²⁺																	1	0.74	-0.67	0.68
Ca²⁺																		1	-0.42	0.43
pH																			1	-0.90
S																				1

Values highlighted with light grey colour present 0.001 < p-value < 0.05
Values highlighted with dark grey colour present p-value < 0.001

Table S5. Pearson's correlation coefficient of chemical species quantified in sediment samples collected from Podu Iloaiei Dam Lake.

	Al	Ti	Cr	Mn	Ni	Zn	Ge	Sr	Ag	Sb	Ba	Pb	Cl⁻	SO₄²⁻	C₂O₄²⁻	Na⁺	NH₄⁺	K⁺	Mg²⁺	Ca²⁺
Al	1	-0.30	-0.14	0.38	0.27	0.30	-0.28	0.27	0.34	-0.21	0.39	0.77	-0.25	-0.13	0.05	0.11	-0.17	0.18	0.24	0.29
Ti		1	-0.37	-0.30	-0.30	-0.33	0.06	-0.20	-0.43	0.60	-0.06	-0.20	-0.04	-0.20	-0.27	-0.27	0.01	-0.23	-0.22	-0.27
Cr			1	-0.27	-0.32	-0.25	-0.11	-0.19	-0.23	-0.37	-0.18	-0.12	-0.03	-0.01	0.23	-0.23	-0.04	-0.27	-0.18	-0.16

	Mn	Ni	Zn	Ge	Sr	Ag	Sb	Ba	Pb	Cl$^-$	SO$_4^{2-}$	C$_2$O$_4^{2-}$	Na$^+$	NH$_4^+$	K$^+$	Mg^{2+}	Ca^{2+}
Mn	1	0.22	0.83	-0.08	0.50	0.29	0.21	0.72	-0.10	-0.59	-0.19	-0.07	0.14	-0.13	0.35	0.47	0.46
Ni		1	0.09	0.19	0.26	0.58	0.10	0.33	0.11	-0.02	0.17	0.13	0.35	0.07	0.33	0.32	0.30
Zn			1	-0.25	0.63	0.66	0.09	0.60	-0.12	-0.33	-0.09	-0.05	0.39	0.15	0.40	0.51	0.53
Ge				1	-0.43	0.25	0.25	-0.18	0.04	-0.02	-0.23	-0.43	-0.43	-0.12	-0.39	-0.40	-0.43
Sr					1	0.27	0.02	0.59	-0.24	-0.27	0.20	0.33	0.53	-0.04	0.85	0.97	0.94
Ag						1	-0.33	0.43	-0.06	-0.09	0.45	-0.25	0.29	-0.23	0.51	0.37	0.24
Sb							1	-0.07	-0.09	0.14	-0.20	0.16	0.10	0.11	0.08	0.01	0.06
Ba								1	-0.08	-0.68	-0.18	-0.10	0.17	-0.06	0.42	0.55	0.51
Pb									1	0.16	-0.22	-0.11	-0.14	-0.09	-0.27	-0.29	-0.17
Cl$^-$										1	0.40	0.53	0.42	0.35	-0.01	-0.26	-0.22
SO$_4^{2-}$											1	0.37	0.54	0.05	0.53	0.33	0.23
C$_2$O$_4^{2-}$												1	0.79	0.64	0.47	0.39	0.47
Na$^+$													1	0.52	0.72	0.55	0.53
NH$_4^+$														1	0.03	-0.09	-0.06
K$^+$															1	0.92	0.86
Mg^{2+}																1	0.96
Ca^{2+}																	1

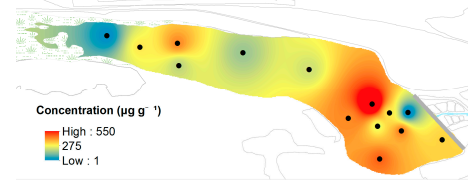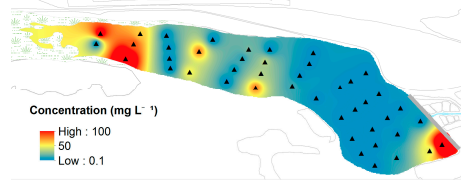Values highlighted with light grey colour present $0.001 <$ p-value < 0.05

Values highlighted with dark grey colour present p-value < 0.001

Figure S3. Spatial distribution of K$^+$, NO$_2^-$, H$_3$C$_2$O$_2^-$, and HCO$_2^-$ in water and sediment of Podu Iloaiei Dam Lake.
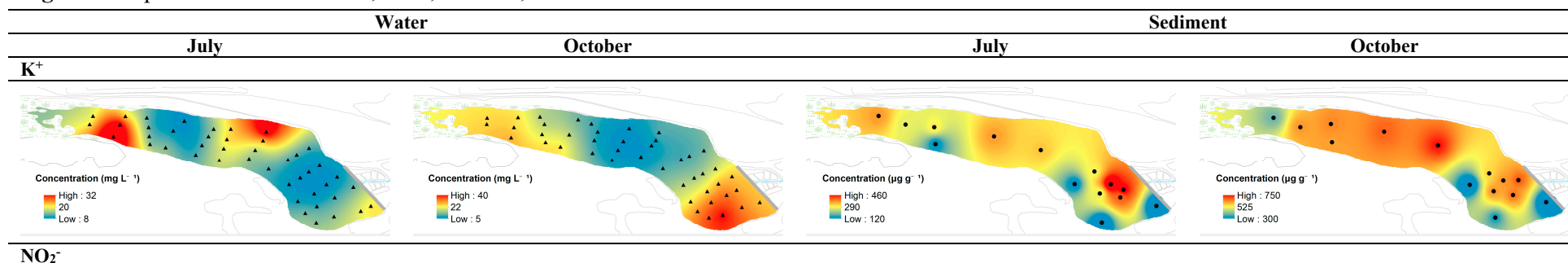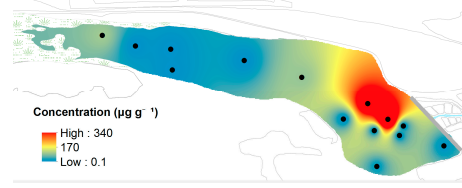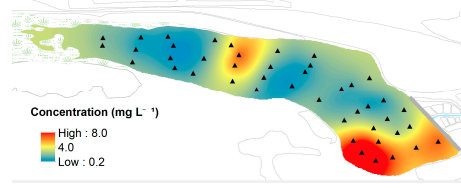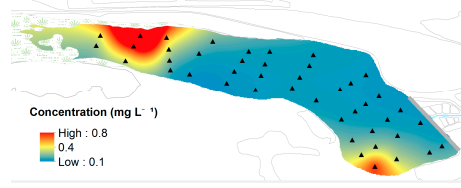
H₃C₂O₂⁻
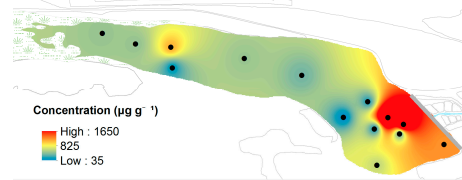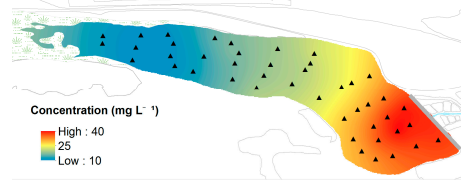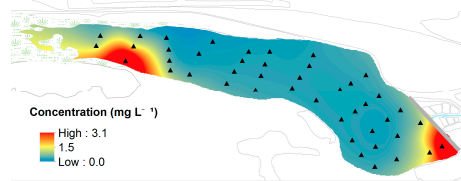

HCO₂⁻
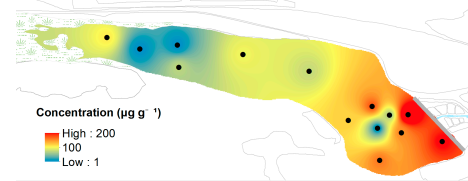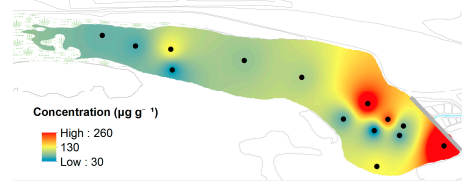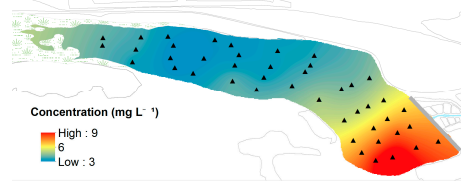
Figure S4. Spatial distribution of water-soluble Al, Ge, Ag, and Sb in water and sediment of Podu Iloaiei Dam Lake.