Numerical Modelling of Pollutant Dispersion in the Lower Danube River

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This paper presents the numerical modeling results of the pollutant dispersion in the Danube riverbed, using experimental data recorded monthly on the Borcea - Bala - Old Danube sector, for a 2 years period. The water samples were collected from the left bank, center and right bank of the river, and the follwing indicators were analyzed: lead, nickel, chromium, cadmium and copper. Heavy metals were determined by atomic absorption spectrophotometry with graphite furnace (GFAAS). Numerical modeling was performed using Delft3D software, taking into account a reference situation (a scenario regarding the pollutant dispersion for known concentrations) and a scenario that simulates an accidental pollution (where the concentrations of pollutants were increased by 50 % compared to the values corresponding to Class V of water quality according to M.O. 161-2006). In order to properly assess the pollutant dispersion, the construction of the numerical model was developed taking into account a number of complex hydraulic works (bottom sill, dredging operations on the Danube in the area of confluence and downstream, on the whole width of the fairway). The results of numerical modeling generated the pollutant dispersion maps and the dispersion coefficients (indicating the transport of substances). Higher levels of the monitored indicators were observed on Borcea, caused by water coming from different sources of pollution (industry, agriculture, etc.) and discharged at a low flow, limiting the dilution.

Keywords: pollutants, dispersion, modelling, Danube River

The role of water and its necessity are paramount for human life, plants and animals, as well as for industrial, commercial and agriculture activities within urban settlements and rural areas [1, 2], its pollution becoming one of the main environmental concerns [3].

River pollution consists in water quality change considering the intake of contaminants from the outside, altering the previous qualities [4, 5]. This condition is a consequence of both the economic development and the increase of population's living standards, which is the direct effect of the increased volume of used water, and therefore of the quantities of wastewater discharged [6].

Most environmental problems encountered in surface waters are caused by the discharge of pollutants [7, 8]. Discharging wastewater into watercourses, lakes, seas, oceans may be punctiform - concentrated under the form of a jet at shore or inside the water body, or distributed along the riverbanks – in the case of outflows from the mountainsides that carries along the fertilizers, pesticides etc. used in agriculture [9-11]. Heavy metals in aquatic environments appear from numerous anthropogenic sources, typically from urban effluent wastewater treatment plants, from industrial processes for manufacturing, mining and from agriculture [12]. The heavy metals are considered harmful to organisms when their concentrations exceed the legally allowed limits for water [13].

The existing concentrations at the entry point of a given section differs, from a quantitative point of view, from the ones found at some point in the receiver, which are affected by the dilution and dispersion phenomena operating in the affected area, and by the reactions occuring among pollutants [14, 15].

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The assessment of the dispersion coefficient can identify complex phenomena controlling the transport of the substance in the water bodies [16].

Therefore, the water quality models are very useful in describing the ecological state of the river and to anticipate the change of its status, following pollution or the changes that appear along its course [17, 18].

In order to determine the pollutant dispersion, hydrodynamic mathematical modeling was performed, using Delft3D numerical simulation program [19]. For the calibration and subsequent numerical modeling the experimentally determined concentrations of lead (Pb), nickel (Ni), chromium (Cr), cadmium (Cd) and copper (Cu) were used as input values.

Experimental part

The computing domain used for the development of the mathematical model represents the Danube sector between Calarasi and Braila towns (km 355 - km 330 on the Old Danube, km 76 - km 66 on Borcea Branch and the whole section of Bala Branch) (fig. 1) and has been defined by building a computing grid equal to MxN = 1047x626 cells. This computing grid was developed in order to meet the orthogonal and aspect ratio conditions required by the program. The bathymetric model of the concerned Danube sector was built by interpolating a series of complex data, resulted from multibeam and singlebeam bathymetric measurements, ADCP transects and topographic measurements.

The obtained numerical model was calibrated step-by-step, based on field measurements of the water flow, water level and velocity, examining if the simulated values are close to the measured ones. The main parameters of calibration were viscosity and roughness.

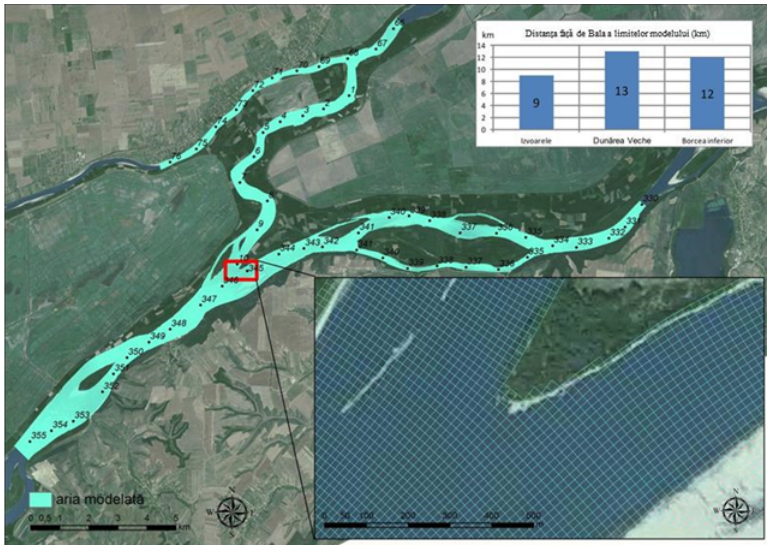


Fig. 1. The hydrological modeled area

Indicators (µg/L)	Current situation			
	Borcea upstream	Borcea downstream	Old Danube upstream	Old Danube downstream
Pb	1.301	1.150	0.937	1.230
Ni	3.288	1.647	1.647	1.627
Cd	0.021	0.030	0.027	0.027
Cu	2.554	3.717	3.687	3.573
Cr	1.136	0.640	1.313	0.653

Table 1
CONCENTRATIONS OF POLLUTANTS USED AS INPUT IN THE SIMULATED SCENARIOS

After the calibration process, the two scenarios were run at a water flow rate of 5830 m^3/s, value which was also used in the validation of the model.

The water samples were collected from the left bank, center and right bank of the lower section of the Danube River (Borcea - Bala - Old Danube), for a two years period and the results of this in situ monitoring are presented in table 1.

During the sampling campaigns, each water sample was directly collected from the river into a 5 liters polyethylene container, being directly transported to the laboratory for analysis, then stored at 4 ^{0}C. After their transport and conservation, the samples were treated and then the concentration of heavy metals (Pb, Ni, Cd, Cu, Cr) was determined using Atomic Absorption Spectrometry (Solaar M5, Thermo). All the reagents used had high purity grade and the solutions for calibration, samples and rinsing were prepared using ultrapure water and Suprapur® nitric acid (65 %, v/v) purchased from Merck, Germany. Certified stock standard solutions of metals were purchased from Fluka and all solutions were prepared with deionized water using the MicroPure ST system. All stages of sample preparation and analysis were carried out in a clean environment without element contamination.

The quality of the results was ensured by first testing a reference material for water (TM - 28.3).

Besides the reference scenario, where field measurements were used, another scenario simulated an accidental release on the Borcea Branch of the Danube River of a pollution source. The input data considered for this scenario were the pollutant values characteristic of the Class V of water quality (as proposed by M.O. 161/ 2006 [20]) increased by 50 % .

Results and discussions

In order to assess the dispersion of pollutants in the Borcea - Bala - Old Danube area, the scenarios were run in 2D, thus leading to a better understanding of the control and evaluation methods of the water quality. The results were analyzed in terms of pollutant distribution and dispersion coeficient.

Figure 2 shows the distribution of one of the analyzed heavy metals (Pb) on the entire analyzed region for the reference scenario, emphasizing the higher values on the Borcea Branch. One possible explanation for this behavior is that this branch of the Danube is characterized by an excessive load of water from various sources of pollution (industry, agriculture, etc.), collected in a small flow of water, therefore limiting the diluting.

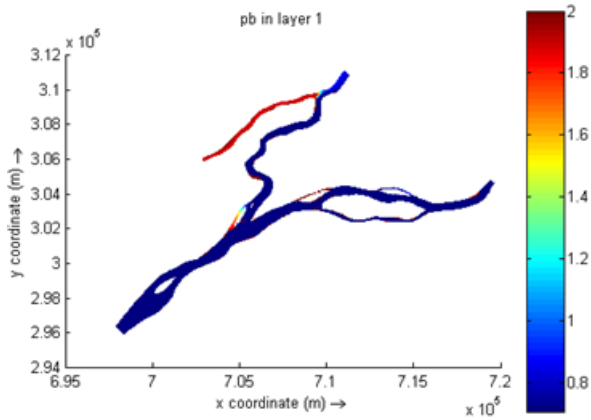


Fig. 2. Pb distribution in the studied area (Old Danube - Bala - Borcea)

Because only the Borcea Branch has a higher concentration of pollutants, the subsequent analysis of the dispersion phenomenon was focused on this area. Thus, the distribution of Pb on Borcea Branch can be seen in figure 3, resulted from the numerical simulation of an accidental pollution.

Analyzing the results of the two scenarios, it can be seen that, regardless of the value of the pollutant concentration in the Borcea Branch a narrow belt of pollutant dispersion is formed at the confluence between Bala - Borcea, due to

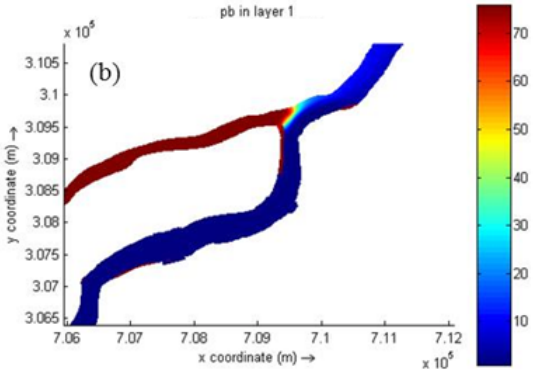


Fig. 3. Pb distribution on the Borcea Branch in the case of an accidental pollution

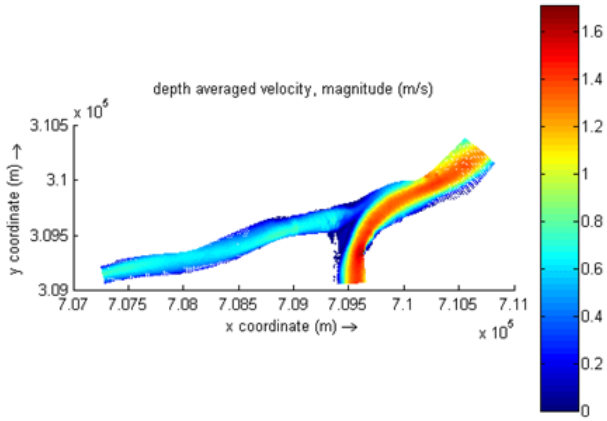


Fig. 4. Water velocities distribution at the Borcea - Bala confluence

the difference of water flow and water velocity between the two branches (fig. 4).

A similar behavior can be observed in the case of Ni (fig. 5) and Cr (fig. 6) indicators.

The numerical simulations results for the reference scenario showed that the Cd indicator presents concentration values relatively smaller on the Borcea Branch compared to the values recorded on the Bala Branch (fig. 7), due to the results obtained in laboratory tests (indicating higher values of Cd on the Borcea Branch), as shown in table 1. This behavior is an indicator of the sensitivity of the developed model, given that a variation of 0.006μg/L influences the nature of the dispersion. For the scenario of an accidental pollution, numerical simulations of Cd showed higher concentrations on the Borcea Branch (due to the low flow on this branch).

Copper presents a similar behavior as cadmium, both for the reference scenario and for the accidental pollution (fig. 8).

For the comparative analysis of the reference situation and the accidental pollution (where the input values were considered to be 50 % higher than the Class V of water quality values established by the M.O. 161/2006), the dispersion coefficient has been calculated using the numerical simulation software (Delft3D).

From figure 9 it can be seen that in the initial area of the model (entrance) the value of the dispersion coefficient remains constant throughout the run (24 h) on the Borcea Branch, both in the case of the reference situation and in the event of an accidental pollution, the difference between them being due to the higher concentrations values of the analyzed indicator.

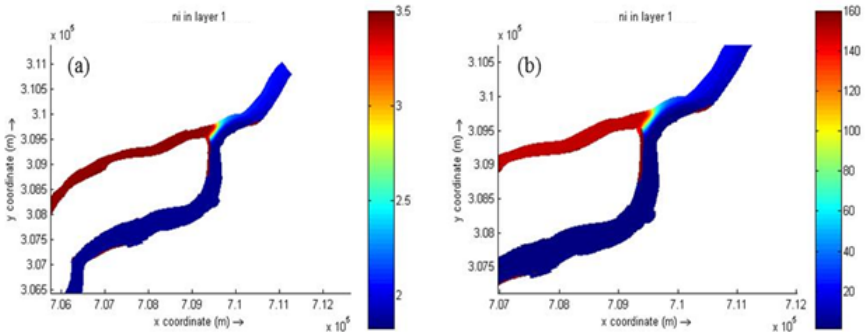


Fig. 5. Ni distribution on Borcea Branch: a) reference situation; b) accidental pollution

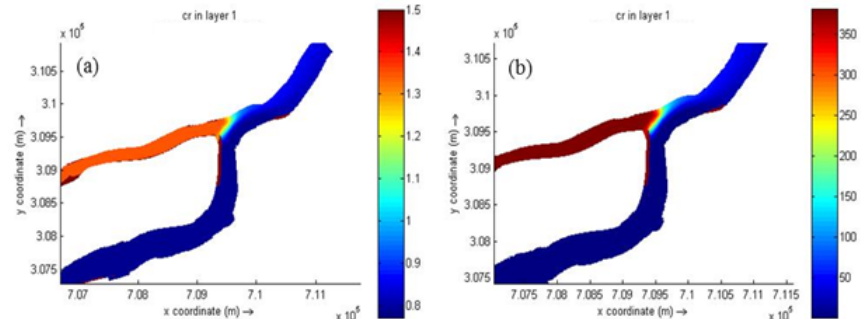


Fig. 6. Cr distribution on Borcea Branch: a) reference situation; b) accidental pollution

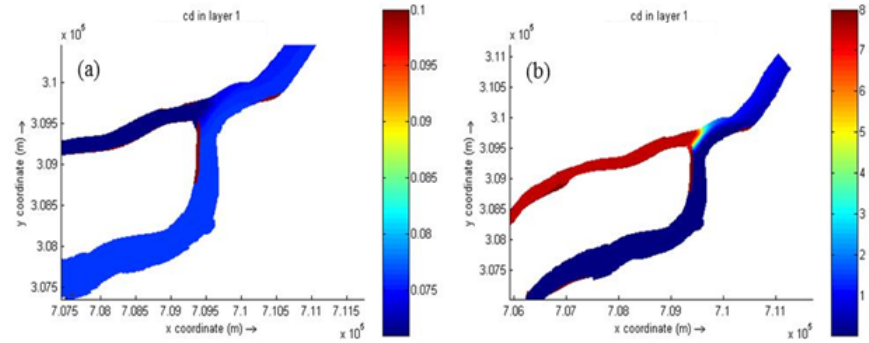


Fig. 7. Cd distribution on Borcea Branch: a) reference situation; b) accidental pollution

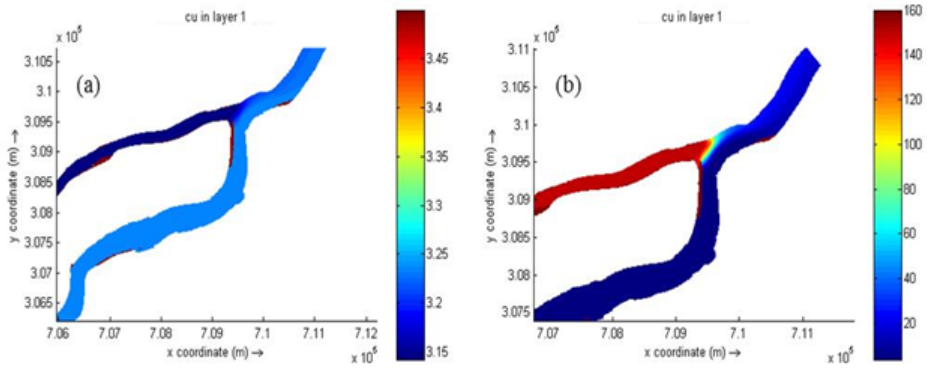


Fig. 8. Cu distribution on Borcea Branch: a) reference situation; b) accidental pollution

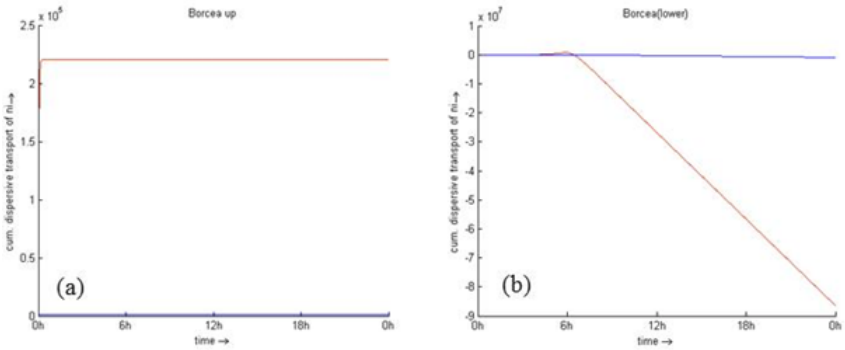
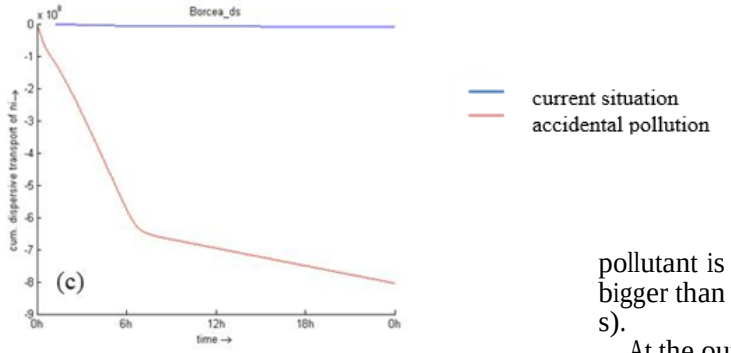


Fig. 9. The dispersion coefficient for Ni on Borcea Branch: a) input; b) confluence; c) output



However, after approximately 6 h of running, the model shows a sudden decrease of the dispersion coefficient at the Borcea-Bala confluence, which could be explained by an increase in the dispersion of this pollutant in water. One explanation for this behavior may be that in this area, the pollutant is dispersed in a water flow of about 10 times bigger than the initial flow of the Borcea Branch (371 m^3/s).

At the output of the considered models, the dispersion coefficient continues to fall rapidly during the first 6 h of running, with a subsequent reduction of this rate after this period of time. A similar trend is also recorded for the Cr indicator (fig.10).

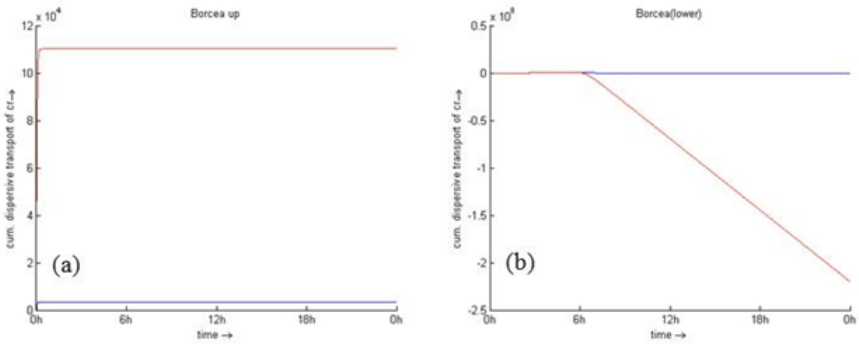
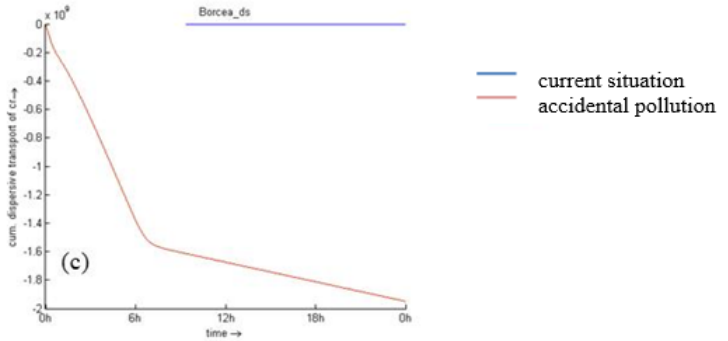


Fig. 10. The dispersion coefficient for Cr on Borcea Branch: a) input; b) confluence; c) output



The concentration trend of the pollutant has a high dispersion tendency along the Bala branch. However, the dispersion is slower at the entry point of the model (on the Borcea Branch) due to higher concentrations of the pollutants. Along the flow direction, at the observation points Borcea upper, Borcea lower and Borcea ds, the dispersion coefficient values indicate a high mixing rate, so that at the output of the model the dispersion tendency is total (fig. 10).

Conclusions

Using the mathematical model developed on the studied area (Old Danube-Bala-Borcea) two scenarios type 2D were numerically simulated, one representing the situation in the field (reference scenario) and the second simulating an accidental pollution.

The results of mathematical modeling revealed high concentrations of Pb, Ni and Cr indicators on the Borcea Branch. This behavior was caused by water from different sources of pollution (industry, agriculture, etc.) discharged in a low flow, the dilution being thus limited throughout the Borcea Branch.

It was noted that at the confluence between the Borcea and Bala branches a reduced interface of dilution (dispersion area) appears in the case of the analyzed pollutants, which may be explained by the higher water velocities on the Bala Branch compared to Borcea Branch. This behavior was confirmed by the results of the dispersion coefficient (for all analyzed indicators) calculated by the mathematical model, which indicated that at the confluence with the Bala Branch it (dispersion coefficient) presents a rapid decline shortly after the start of the simulation, meaning that the dispersion of pollutants in the water is enhanced.

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