Use of Finite Element Method (FEM) to determine spatio-temporal evolution of pollutants in river-type systems

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Abstract: - This paper addresses the problem of water quality and water pollution in river-type systems. A bibliographic study on determination of spatial-temporal evolution of pollutants on Computational Fluid Dynamics (CFD) basis, particularly using Finite Element Method (FEM), was done. A case study on the determination of the concentration field of pollutants in 4 sectors of the Prut River is presented.

Key-Words: - water quality, modeling, Computational Fluid Dynamics (CFD) simulation, Finite Element Method (FEM), river, transport and dispersion of pollutants.

1 Introduction

Water constitutes an essential factor for the existence of life on Earth. It is permanently in a hydrological process, which allows to modify its physical, chemical and biological properties [1].

Water quality is a primordial problem for the sustainable development of the country. Currently there is an ongoing degradation of water quality in the majority of regions around the globe. To stop this process it is necessary that specialists from various fields initiate studies and take complex actions.

According to Water Framework Directive 2000/60/EC (amended by Directive 2008/32 / EC), water quality can be: very good, good, moderate, weak and poor [2].

As a result of human activities, water quality has dramatically decreased. Quality evaluation of several water bodies from Europe, according to the Water Framework Directive, shows a satisfactory or unsatisfactory ecological status. For rehabilitation and maintaining aquatic systems in a very good state [2], their thorough analysis is needed

In the most cases, for human necessities, such as water supply, irrigation, energy generation, etc., water from rivers is used. Due to erosion and sedimentation processes, river shape is in permanent change and influences water quality parameters [3].

Water quality is more often influenced by the pollution with various chemical, physical and biological substances. In the specialty literature, it is mentioned that there are various analytical methods for determination of water quality, according to the parameters and national standards established in the field. Usually, these methods include: selection of parameters, adjustments of measurement units to the same scale, establishing the weight of each parameter and calculation of water quality index [4].

Lately, methods for controlling water pollution more efficient than analytical methods are implemented. Their effectiveness consists in application of informational systems consisting of 2 components: mathematical modeling of the studied river sector and water quality evaluation using numerical models obtained [5, 6, 7].

Numerical modeling is performed by CFD techniques, with the help of which equations with spatial derivatives are transformed into systems of algebraic equations, whose solutions represent an aproximation of state quantities in the defined nodes of the computational field [8, 9, 10, 11].

A powerful tool in solving water quality problems is the Finite Element Method (FEM), which is a CFD approximation numerical computation technique that has the purpose to reduce the differential equations systems that describe a real physical process with an infinite number of degrees of freedom to an algebraic system of equations with a finite number of degrees of freedom. It consists in meshing the field of study to finite elements and their analysis. A finite element is considered a standalone device that interacts with other elements only at nodes. To be possible for the finite element to be used in the calculation process, it must be designed in every detail: geometrically, physically, mathematically etc. [8, 9, 10, 11].

2 Problem Formulation

Of the total volume of water covering the Earth, surface waters bring a considerable contribution to the sustainable development of the society. To be used, water must be of a high quality. An important problem in the surface waters field is their pollution by various substances. Water specialists need efficient tools to rehabilitate and maintain them in a very good state, according to Water Framework Directive [2].

According to the examined bibliographic sources, the problem of water quality is actual for the majority of places on Earth. The problem of modeling water quality based on CFD simulation methods is formulated in the papers [12, 13, 6, 14, 15, 16, 17, 18, 19, 26].

The problem of water quality is also very actual for the Republic of Moldova. Water quality in the country, in most cases, is not consistent with national and international standards [20, 21, 26, 27].

Management of water resources in the Republic of Moldova is unbalanced, which doesn't allow an adequate protection of water resources. In 2009 the percentage of water samples that were not consistent with the quality standard was 70,8% and in 2010 - 67,8% [22, 26].

An important source of water supply for the Republic of Moldova, as well as for Romania, is the Prut river, therefore its pollution presents a risk to human health.

In this paper a study on water quality in the Prut river for the 2008-2013 period was conducted. Investigated sectors, indications for the major pollutants, as well as geographic coordinates of the sampling points of the State Hydrometeorogical Service of the Republic of Moldova [28] are presented in the table 1.

Table 1. Investigated sectors

Nr.	Sector name	Geographical coordinates of the sampling points	Major pollutants
1.	s. Criva	48°15′ 42,6″ N 26°37′ 51,9″ E	petroleum products, phenols, nitrites
2.	or. Ungheni	47°12′00,6″ N 27°47′12,7″ E	petroleum products, phenols
3.	or. Leova	46°29′35,3″ N 28°13′47,9″ E	petroleum products, phenols, nitrites
4.	s.Giurgiuleşti	45°28′17,16″ N 28°11′52,20″ E	petroleum products, nitrites, phenols

The table shows that the most frequent pollutant found in all the studied sectors are petroleum products. The maximum value of the concentration of this pollutant for the samples taken during the 2011-2013 period are presented in the figure 1.

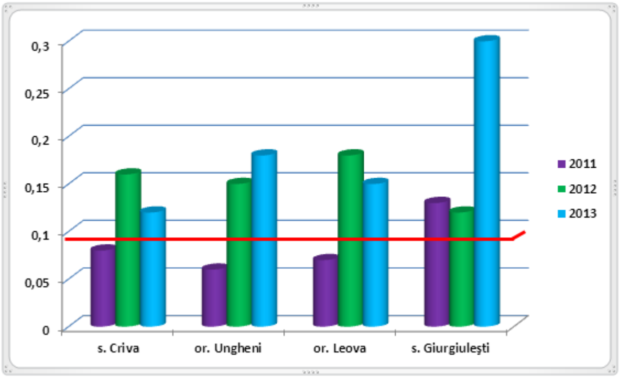

Fig. 1. Maximum concentration of petroleum products.

In the figure 1 it can be observed that the concentration of petroleum products exceeded the Maximum Admisible Value (MAC) of 0,05 mg/L for all of the scenarios presented.

Proceeding from the above, the problem of determining pollutant dispersion in river-type system was formulated with the purpose to estimate water quality parameters.

3 Problem Solution

Rivers are complex aquatic systems. Water flow in rivers is a turbulent flow that can be described using Navier-Stokes partial differential equations [19].

To solve Navier-Stokes equations, CFD numerical simulation methods are used [19, 8, 9, 10].

The problem of determining transport and dispersion processes of pollutants in river-type systems by using CFD, particularly Finite Elements Method, was solved in the papers [14, 15, 16, 17, 18, 6, 7, 19].

In this paper, a deterministic mathematical model was developed to determine the dispersion of petroleum products in the studied sectors of Prut river. Hydrodynamics was modeled using Navier-Stokes system of equations in the Reynolds form (1) and (2), together with the continuity equation (3):

$$h\frac{\partial u}{\partial t}+hu\frac{\partial u}{\partial x}+hv\frac{\partial u}{\partial y}-\frac{h}{\rho}\left(E_{xx}\frac{\partial^2 u}{\partial x^2}+E_{xy}\frac{\partial^2 u}{\partial y^2}\right)+gh\left(\frac{\partial H}{\partial x}+\frac{\partial h}{\partial x}\right)+$$
$$+\frac{gun^2}{\left(h^{1/6}\right)^2}\times\left(u^2+v^2\right)^{1/2}-\varsigma V_a^2\sin\psi+2h\omega v\sin\phi=0 \tag{1}$$

$$h\frac{\partial v}{\partial t}+hu\frac{\partial v}{\partial x}+hv\frac{\partial v}{\partial y}-\frac{h}{\rho}\left(E_{yx}\frac{\partial^2 v}{\partial x^2}+E_{yy}\frac{\partial^2 v}{\partial y^2}\right)+gh\left(\frac{\partial H}{\partial y}+\frac{\partial h}{\partial y}\right)+$$
$$+\frac{gvn^2}{\left(h^{1/6}\right)^2}\times\left(u^2+v^2\right)^{1/2}-\varsigma V_a^2\sin\omega+2h\omega v\sin\phi=0 \tag{2}$$

$$\frac{\partial h}{\partial t}+h\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)+u\frac{\partial h}{\partial x}+v\frac{\partial h}{\partial y}=0 \tag{3}$$

where: h - water depth (m); u - local velocity in the x direction (m/s); v - speed local in the y direction (m/s); t - time (s); ρ - density of water (kg/m^3); E - coefficient of turbulent viscosity (Pa.s or kg/m/s); g - acceleration of gravity (m/s^2); H - geodetic share of the riverbed (m); n - manning's roughness coefficient; ζ - empirical coefficient concerning the friction with the air; V_a - wind speed (m/s); ψ - wind direction; ω - angular velocity of the Earth rotation (rad/s); φ - latitude of the place [24].

To determine the dispersion of petroleum products, two-dimensional form of the fundamental equation of advection-dispersion applied to the turbulent flow was used [5, 23]:

$$h\left(\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}-\frac{\partial}{\partial x}D_x\frac{\partial c}{\partial x}-\frac{\partial}{\partial y}D_y\frac{\partial c}{\partial y}-\sigma+kc+\frac{R(c)}{h}\right)=0 \tag{4}$$

where h - is the water depth (m); c - concentration of pollutant (mg/l); t - time (s); u - velocity in x direction (m/); v - velocity in y direction (m/s);

D_x - turbulent diffusion coefficient in the x direction (m^2/s); D_y - turbulent diffusion coefficient in y direction (m^2/s); k - decay constant (s^{-1}); σ - term local source of pollutant (concentration unit/s); $R(c)$ - precipitation / evaporation (concentration unit × m/s) [25].

Numerical solving of the flow equations was done using the SMS (Surface Water Modeling System), particularly the modules RMA2 and RMA4, that can solve problems of water flow and pollutant transport in river-type systems.

RMA2 software builds the mathematical model of the water movement, which determines the field of local vertical averaged velocities u and v, the resultant average velocity, and the water depth.

RMA4 module helps to determine the evolution of the concentration field of pollutants.

To solve the above mentioned system of equations, the Finite Element Method with the Galerkin method of weighted residues is used. Interpolation functions are of the second degree for velocities and of the first degree for depths. Derivatives in relation to time are replaced by the approximations of nonlinear finite differences. It is assumed that variables vary in each time frame in the form [24]:

$$f(t)=f(0)+at+bt^c \tag{5}$$
$$t_0\le t<t_0+\Delta t$$

where a, b and c are constants.

In the process of meshing the studied domain, two-dimensional triangle elements were used (three corners and three nodes in the middle).

Numerical stability of the RMA2 software was verified using the Froude number:

$$F_r=\frac{V}{\sqrt{gh}} \tag{6}$$

where V is the velocity of water particles; g – free-fall acceleration; h – depth.

Froude number is a dimensionless number that describes the flow. RMA2 can become numerically unstable if the Froude number is greater than 0,6.

Computational networks were built using the Finite Elements Method for each of the studied sectors of Prut rivers (figures 2 - 4):

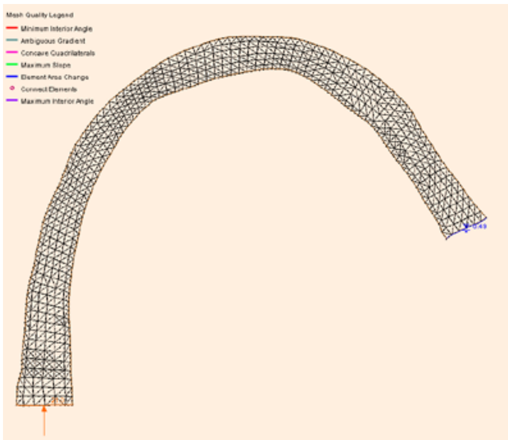

Fig. 2. Prut river, Criva sector.

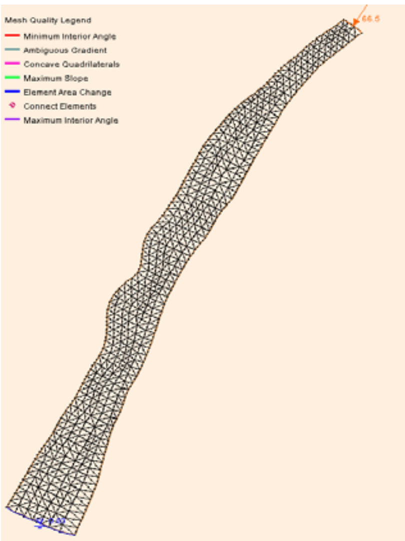

Fig. 3. Prut river, Ungheni sector.

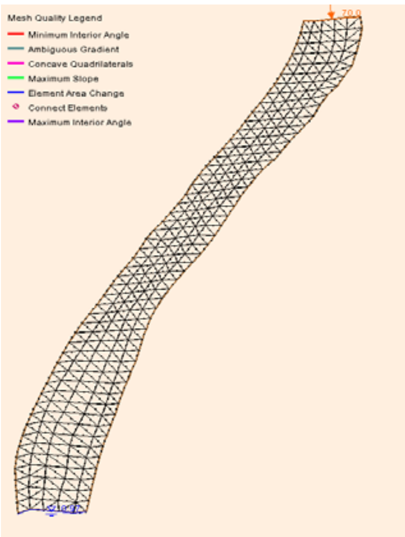

Fig. 4. Prut river, Leova sector.

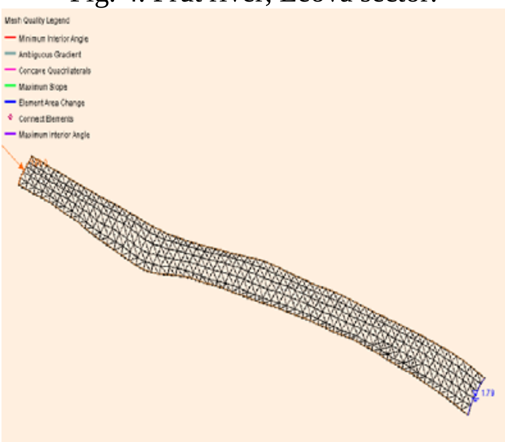

Fig. 5. Prut river, Giurgiulesti sector.

The evolution of the pollutant concentration fields in the studied sectors, in different time frames is presented in the figures 6 - 9:

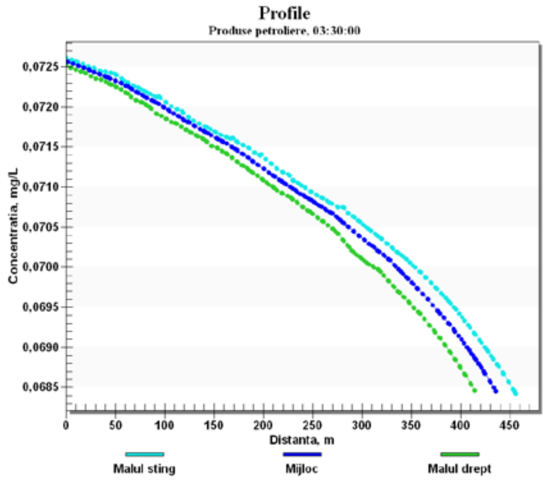

Fig. 6. Criva, concentration field after 3:30 hours.

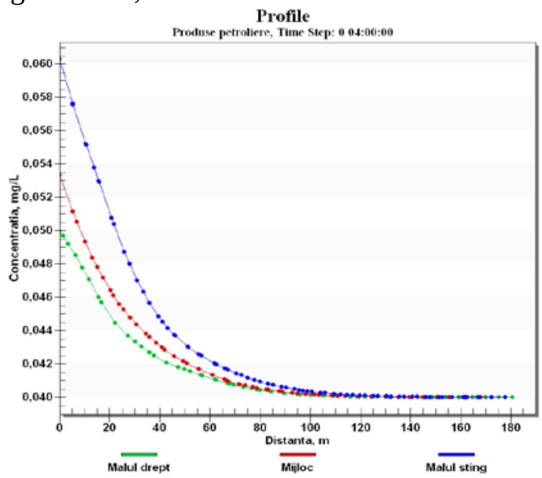

Fig. 7. Ungheni, concentration field after 4 hours.

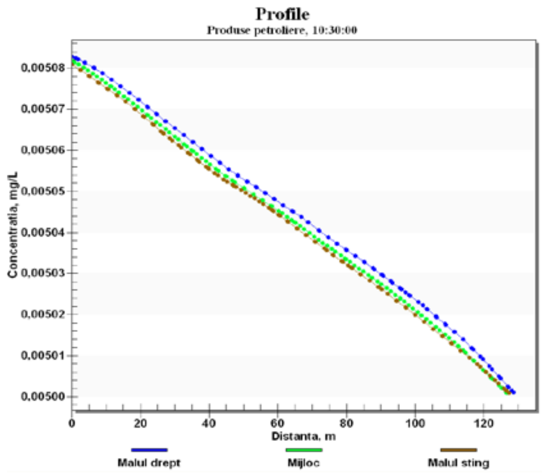

Fig. 8. Leova, concentration field after 10:30 hours.

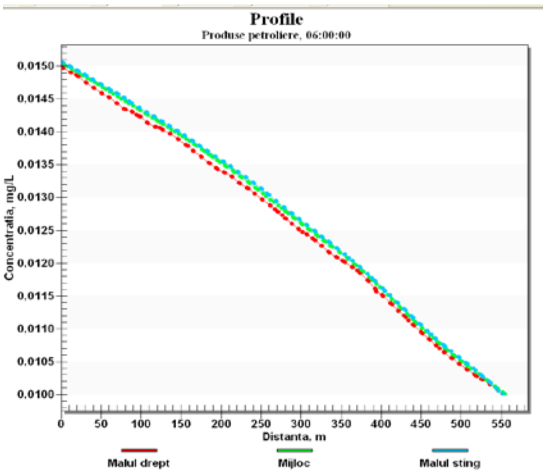

Fig. 9. Giurgiulesti, concentration field after 3:30 hours.

The maximum value of the Froude number (6) for each of the studied sector, according to the simulation, calibration and validation scenarios for the numerical models obtained using the RMA2 software are presented in the figure 10:

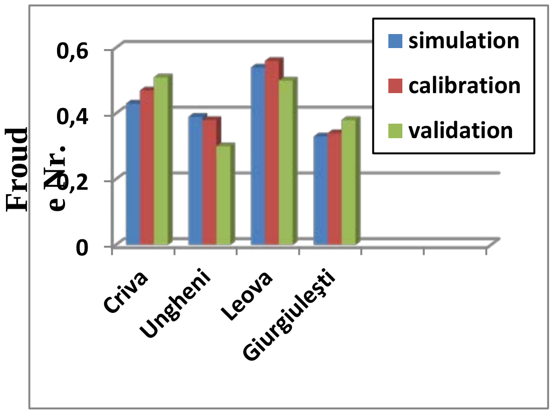

Fig. 10. Maximum value of the Froude number in the studied sectors.

It can be observed that the maximum value of the Froude number does not exceed the critical value of 0,6.

The models were calibrated on a data set collected in 2012. For calibration, the same computational network used in modeling, with the same dimensions and roughness, was used. Following the mentioned procedure and performing numerous numerical simulations, the coefficients *Dx* and *Dy* were optimized.

For the validation of models, the same computational network, used for calibration, under the same conditions, was applied. The models were validated fot a data set collected in 2013.

A good correlation between the measured data and the calculated data was noted by means of the numerical models.

Based on numerical simulation results, were determined: water depth variation, resultant velocity variation, field of velocities on *x* and *y* directions, field of concentrations in time and space.

A part of the results obtained from numerical simulations on hydrodynamics and dispersion of petroleum products, particularly minimum and maximum values of the examined parameters, are presented in the table 2.

Table 2. Results of the numerical simulations

Locality	Scenario	Resultant velocity, m/s		Water depth, m		Concentration in the confluence area, mg/L		Concentration in the sampling point, mg/L	
		min	max	min	max	min	max	min	max
Criva	11.05.2011	0,430	2,016	0,692	2,218	0,001	0,079	0,001	0,079
	07.11.2012	0,318	1,930	0,403	1,708	0,001	0,158	0,001	0,160
	14.05.2013	0,595	2,739	0,905	2,951	0,001	0,119	0,001	0,120
Ungheni	05.05.2011	0,533	1,851	0,845	4,182	0,042	0,054	0,046	0,059
	12.12.2012	0,303	1,649	0,271	2,482	0,140	0,148	0,145	0,150
	11.07.2013	0,443	2,339	0,406	3,518	0,161	0,179	0,164	0,180
Leova	25.05.2011	0,641	4,380	1,377	4,838	0,002	0,069	0,001	0,070
	26.10.2012	0,750	2,854	0,380	4,827	0,001	0,176	0,001	0,180
	21.05.2013	0,633	4,262	0,867	4,789	0,146	0,179	0,001	0,179
Giurgiulești	28.07.2011	0,792	1,999	1,783	3,787	0,00004	0,128	0,00004	0,129
	22.11.2012	0,854	2,127	1,953	4,079	0,020	0,118	0,020	0,119
	22.05.2013	0,939	2,403	2,092	4,475	0,001	0,318	0,001	0,319

Based on CFD numerical simulations for transport and dispersion of petroleum products, the concentration of the mentioned pollutant in time and space was estimated, as follows:

- for the sector of the Prut river from the Criva village, pollutant is taken by the mainstream of the river and in the first 3 hours from the moment of confluence with water the concentration of the pollutant was decreased insignificantly from 0,08 mg/L to 0,079 mg/L in the sampling point; after 5 hours it reached the value of 0,03 mg/L, and after 12 hours it was reduced substantially to 0,00081 mg/L. The value of concentration decreased significantly on the entire studied sector and didn't exceed CMA after 5 hours from the moment of confluence of petroleum products with water;

- for the sector of the Prut river from the Ungheni city, pollutant remains on the left bank in the first 2 hours from the moment of confluence with water. The initial concentration of pollutant of 0,06 mg/L in the sampling point reached the value of 0,051 mg/L after 3 hours, 0,047 mg/L - after 5 hours, and 0,046 mg/L - after 12 hours. The process of petroleum products dispersion is very slow.
- for the sector of the Prut river from the Leova locality, in the confluence area pollutant is taken up by the mainstream of the river. In the sampling point, the concentration of pollutant maintained the value of 0,07 mg/L during 1 hour 30 minutes after the moment of confluence with water; after 3 hours and 30 minutes became 0,04 mg/L, after 12 hours – 0,0008 mg/L. After 3 hours and 30 minutes the concentration of pollutant reaches a value less than MAC on the entire sector.
- for the sector of the Prut river from the Giurgiulesti locality, the pollutant is taken by the mainstream of the river and after 3 hours from the moment of confluence with water, in the sampling point, the concentration decreases from the value of 0,13 mg/L to 0,129 mg/L; after 5 hours and 30 minutes - to 0,031 mg/L, and after 12 hours - to 0,00004 mg/L. The concentration of petroleum products decreases significantly in the sampling point and on the entire studied sector after 5 hours and 30 minutes from the moment of confluence with water.

5 Conclusion

As a result of the bibliographic study, it was determined that Finite Element Method is a powerful tool for solving problems regarding water quality management and preventing the risk of water pollution.

Using the Finite Element Method, the dispersion of petroleum products in 4 sectors of the Prut river was determined.

Numerical simulations were performed based on real data from the field. The mesh was created with a sufficient number of finite elements, thus assuring an acceptable calculation error.

The numerical simulations demonstrated a good capacity of the mathematical model to faithfully reproduce real processes in river-type aquatic systems, confirmed by comparing real data, collected in situ, with data obtained through elaborated numerical models.

Based on the results of numerical simulations, it was proved that the obtained numerical models, calibrated and validated, can be directly used for any scenario of pollution in the studied sectors, in urgent and accidental situations.

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