Mathematical and numerical modeling of pollutant transport and dispersion phenomena in aquatic systems

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***Abstract* — The present paper deals with the pollution problem in aquatic systems. The importance of mathematical and numerical modeling for obtaining the pollutants concentration field in time and space is being discussed. A case study concerning the determination of the spatio-temporal evolution of pollutants on a sector of the Prut river in Ungheni is presented.**

***Keywords* — mathematical modeling, numerical modeling, aquatic systems, pollutant transport, concentration field.**

I. INTRODUCTION

Aquatic systems are an essential factor for the existence of life. Nowadays, there is a continuing deterioration of water quality in most regions of the world, which is increasingly influenced by pollution with different chemical, physical, biological substances.

In order to rehabilitate and maintain water quality in line with the requirements of the Water Framework Directive, water specialists need effective tools [1].

The problem of aquatic systems pollution requires rapid action in order to prevent a decrease in water quality. Choosing the methods for controlling water pollution and determining the quality degree is an important step in improving water quality.

An effective method of controlling and predicting water pollution is the use of information systems, consisting of two main components: mathematical models and software packages that generate numerical models [2].

Based on the above, the problem regarding the study of the mathematical and numerical modeling of the aquatic systems in order to determine the spatio-temporal evolution of the pollutants has been formulated.

II. RESEARCH ON MODELING THE SPATIO-TEMPORAL EVOLUTION OF POLLUTANTS

In the list of current issues solved by mathematical modeling, ecological problems play a distinct role. The problem of water quality is a difficult one because water is a physical, biochemical and ecological complex system. An effective solution for analyzing and solving different problems in aquatic systems is the methods based on the mathematical modeling of these systems. The use of mathematical modeling helps to predict the behavior of aquatic systems, as well as to determine the results of actions of different processes on aquatic systems [2].

Mathematical modeling of the environment began in the 1900s with Streeter and Phelps' works on dissolved oxygen. The modeling of environmental systems is a complex and difficult problem. Solving this problem, different mathematical models are used (Fig. 1).

Mathematical models regarding water systems are used for solving problems of waste water treatment, industrial pollution, agrarian pollution, protection of drinking water sources, etc. Models are used to disperse and transport pollutants, processes control and analysis, and so on [3].

A methodology for assessing the environmental status of small rivers has been developed in the paper [4]. The methodology was applied to the Oreto river in Italy. A mathematical model developed by Thomann and Mueller in 1987 and Chapra in 1997 was used, which is based on the advection-dispersion equation for a one-dimensional flow:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=D_L\frac{\partial^2 C}{\partial t^2}-f(C), \qquad (1)$$

where C – concentration of a generic pollutant, t – time, x – longitudinal displacement, u – velocity, D_L – diffusion coefficient, *f(C)* – a generic term for reactions involving the pollutant *C*.

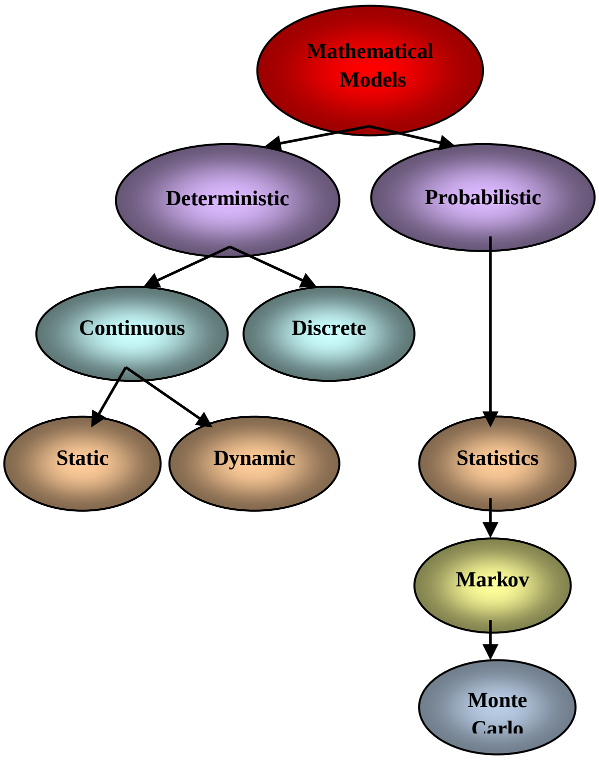

Fig. 1. Mathematical models used for the environment modeling.

In order to generate a large number of parameters for the given model, the Monte Carlo method was applied. Simulations were performed for each parameter set for comparison with the measured data (BOD, DO, NH4, and NO3). The effectiveness of this approach has been assessed with the reference to the interpretation of field data [4].

Surface water quality depends directly on groundwater status. The numerical simulation of the dispersion and transport of pollutants through permeable environments and the dispersion and transport of pollutants into rivers was carried out. This relation was performed by considering the numerical results obtained after studying the water movement and the transport of pollutants through permeable environments as limiting conditions for the transport of pollutants in the river Târnava Mică from Romania. The mathematical modeling of river water quality was achieved using the convection-diffusion equation:

$$\frac{\partial c}{\partial t}+v_x\frac{\partial c}{\partial x}+v_y\frac{\partial c}{\partial y}+v_z\frac{\partial c}{\partial z}=\frac{\partial}{\partial x}\left(D_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial c}{\partial z}\right)+ +S(x,y,z,t)\pm S_{internă}, \quad (2)$$

where C is pollutant concentration; D_x, D_y, D_z – diffusion coefficients in x, y and z directions; v_x, v_y, v_z – the velocity in x, y, şi z directions; t – time; $S(x,y,z,t)$ – external sources, space and time functions; $S_{internă}$ – internal sources whose evolution is influenced by C [5].

The modeling of pollutant transport in rivers is proposed in the paper [6]. The obtained mathematical models are based on the unidimensional shape of the advection-dispersion equation in the longitudinal direction:

$$\frac{\partial c}{\partial t}=-\frac{\partial(cV_x)}{\partial x}+\frac{\partial}{\partial x}\left(D_x\frac{\partial c}{\partial x}\right)+S_s\pm S_t, \quad (3)$$

where c is pollutant concentration; V_x – the convective velocity of water; D_x - the longitudinal dispersion coefficient; S_s – pollutant source; S_t – the changes that the pollutant suffers.

A deterministic mathematical model has been developed to determine the dispersion of pollutants in some sectors of the Prut River [7, 8].

To determine the dispersion of petroleum products, the two-dimensional form of the advection-dispersion equation applied to turbulent flow was used [9]:

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

where *h* – is water depth (m); *c* – pollutant concentration (mg/L); *t* – time (s); *u* - velocity in *x* (m/s) direction; *v* – velocity in *y* (m/s) direction; D_x- the turbulent diffusion coefficient in *x* (m^2/s) direction; D_y- the turbulent diffusion coefficient in *y* (m^2/s) direction; *k* - decay constant (s^{-1}); σ - local pollutant source term (the measure of the concentration/s), *R(c)* - precipitation/evaporation (concentration unit x m/s).

The local variation of the concentration is represented by the 1st term of the equation, the 2nd is an advection term in the *x* direction; the 3rd - advection term in the *y* direction. The phenomenon of dispersion in the *x* direction is represented by the 4th term, and in the *y* direction– by the 5th term; the 6th term represents the local source of the pollutant; the 7th models the exponential degradation of the pollutant; the 8th takes into account the effect of precipitation / evaporation.

Turbulent diffusion coefficients: D_x in *x* direction and D_y in *y* direction can be measured experimentally, but because the cross section of the flow is seldom of an uniform depth, this measurement is often complicated. Often, these coefficients are determined by empirical formulas:

$$D_x = 5{,}93hu_*, \quad (5)$$

where *h* is water depth; u_* – friction velocity:

$$u_* = \sqrt{\tau_0/\rho} \quad (6)$$

Here, τ_0 is average tangential effort to the wall, and ρ – water density. The D_y coefficient is determined as follows:

$$D_y = \alpha h u_*, \quad (7)$$

where α is a coefficient (after Fischer, 1979, α = 0,6; after Elder, 1959, α = 0,2) [10].

To effectively solve the problem of determining the spatio-temporal evolution of pollutants, mathematical models are transformed into numerical models using various numerical simulation systems. Most of these systems include several advanced modules, such as the physical model, the mathematical model, the hydrodynamic model, the geographic information system (GIS), the numerical models of pollutant transport and dispersion processes, the analysis of the obtained numerical models, management modules, the data export from the system in different formats.

Among the most representative systems in the field are the following: SMS (Surface-Water Modeling System), WMS (Watershed Modeling System), GMS (Groundwater Modeling System), developed by Aquaveo in the USA; ANSYS CFX (Computational Fluid Dynamics Software), developed by ANSYS in Canonsburg, Pennsylvania, USA; WASP (Water Quality Analysis Simulation Program), QUAL2E, AQUATOX - US Environmental Protection Agency; AGNPS (Agricultural Non-Point Source Pollution Model) - Agricultural Research Center and the US Natural Resources Center; GWLF (Generalized Watershed Loading Function) - MapTech Company in Blacksburg, Virginia, USA; MONERIS (Modeling Nutrient Emissions in River Systems) – Institute of Ecology of Sweet Water and Fisheries, Berlin, Germany; WQRRS (Water Quality for River Reservoir Systems) - US Army Hydrological Engineering Center.

Here is a brief description of the listed systems.

WMS was developed in the early 1990s at Brigham Young, USA, and represents a simulation graphical system for hydrographic basins in two-dimensional space. It can be used to model both, the quantity and water quality [8]. It has been implemented in Russia [11], Turkey [12], Iran [13] and other countries.

The GMS system allows 3D models to be created and provides solutions for hydrological and hydraulic modeling of groundwater and subsoil water. It contains a set of models that allows the determination of particle transport in time and space, simulation of complex biodegradation problems involving multiple substrates, including a multicomponent model for three-dimensional transport in saturated porous media [14].

SMS is an efficient surface water modeling system that includes a wide range of numerical models for applications that enable numerical models of river hydrodynamics, floods in rural and urban areas, wave modeling, tracking dynamics and physical properties of water particles, determination and analysis of pollutant dispersion. Two modules are used for determining the pollutant dispersion in river-type systems: RMA2 and RMA4. The RMA2 program is a two-dimensional model in a horizontal plane, omitting the accelerations in the vertical direction. It is used to solve dynamic and static problems, for example, the calculation of water levels and the distribution of speeds around islands, the flow of river areas with wetlands, hydrodynamic levels and hydrodynamic spectra of rivers, lakes, delta, estuaries, etc. [15]. RMA4 is an SMS module that is used to numerically simulate advection-diffusion processes at a mean depth in an aquatic system. This module can be applied to the analysis of the evolution of any conservative pollutant suspended or dissolved in water, as well as to the analysis of physical migration processes and the mixture of non-conservative substances in rivers, lakes and estuaries. Depending on the input data, this module uses the hydrodynamics resulting from RMA2 and calculates the evolution of the concentration field. Case studies with the application of this system are presented in the papers [16, 17, 18].

ANSYS CFX is a CFD fluid simulation software that has been in use for more than 20 years. It has a modern graphical interface and supports a wide range of physical models. It includes numerous models for solving turbulence issues. It allows the simulation of three-dimensional scenarios. The finite element method is used for the discretization of the field of study. A solution obtained can be used in another modeling. It is used by the largest companies in the world [19]. The results of the application of ANSYS CFX for the Argeş and Dâmboviţa rivers in Romania in order to obtain the numerical model of the dispersion of the pollutants are presented in the paper [20].

The WASP system allows simulation of dispersion and transport scenarios of different types of pollutants in uni-, bi- and three-dimensional systems. It can be connected to hydrodynamic and sediment transport models. It was used in the US to evaluate the phosphate load of Lake Okeechobee in the state of Florida, the eutrophication of the Coosa River, the pollution of the James River Estuary in Virginia, the heavy metals pollution of the Deep River from North Carolina, etc. [21].

QUAL2E is a one-dimensional water quality model. It has been developed for a steady stream and stable pollutant loading conditions. It simulates point and diffuse pollution, nutrient cycles, algae production [22]. It was used in Spain [23], Chile [24] and other parts of the world.

AQUATOX is a simulation model, which contains models of classic and dynamic ecosystems. It simulates the transport of different types of pollutants, such as nutrients and organic substances, as well as their effects on the ecosystem, including fish, invertebrates and aquatic plants. It is a valuable tool for ecologists, biologists, water quality modelers, who are involved in environmental risk assessment for aquatic ecosystems [25].

AGNPS is a prediction system for pollutant loads of river basins from diffuse agricultural sources. It consists of 3 components: hydrology, which allows the prediction of maximum flow; soil erosion - includes soil erosion and sedimentation, and, nutrient pollution - analyzes nitrogen, phosphorus and chemical oxygen demand. This system is applied on different continents to model river basins, to determine water quality, assess water storage systems, control nutrient levels, and so on [26].

GWLF is a simulation model that allows predicting the monthly load of hydrographic basins with nutrients (including nitrogen and phosphorus) and sediments. The model considers the river basin as a single unit and calculates the load from all the land near the basin. The model is based on the hypothesis that the relationship between erosion and sediment transport varies monthly. It is a continuous simulation model, which uses the daily meteorological data [27].

A case study on the application of GWLF in the US is presented in the paper [28].

MONERIS is a system used to calculate nitrogen and phosphorus basin loadings from point and diffuse sources. It has been developed and applied to the German river basins to determine their pollution with nutrients from point and diffuse sources. The model is based on flow and water quality data as well as on a geographic information system (GIS). It is an appropriate tool for modeling nutrient emissions in surface water, as confirmed by many international applications [29, 30].

The WQRRS system has been developed for the purpose of assessing the surface water quality according to the inlet / outlet flow. It allows to create one-dimensional and two-dimensional patterns. It is able to analyze 18 different water quality parameters: physical, chemical and biological with regard to lakes, rivers and river systems. It consists of 3 separate modules: reservoir, lacquer and flow quality. The first 2 modules can be executed, analyzed and interpreted independently. All three modules can be integrated into a system to perform a water quality analysis in an aquatic ecosystem [31].

III. Case Study: Determination of Spatio-Temporal Evolution of Pollutants on a Sector of the River Prut

The Prut River is an important source of water supply for both, the Republic of Moldova and Romania. Prut pollution has a negative impact on human health as well as on flora and fauna throughout the Black Sea basin.

A study was carried out on the water quality on a sector of the river Prut from Ungheni for the period 2011-2017. Based on the analysis of the samples taken by the Environmental Quality Monitoring Division of the State Hydrometeorological Service of the Republic of Moldova, it was found that the most frequently encountered pollutant in the studied sector is petroleum products (Fig.2), therefore the numerical modeling was done for mentioned pollutant [32].

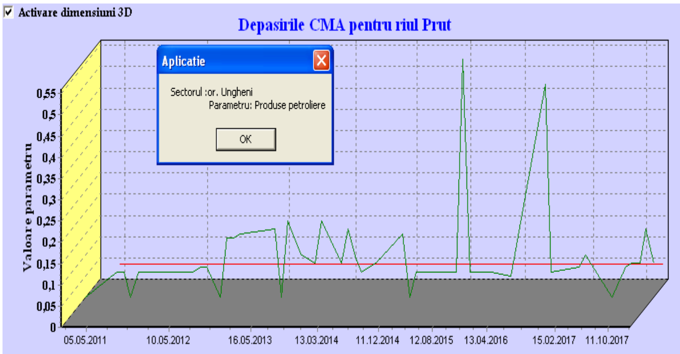

Fig. 2. Exceeding the CMA for petroleum products.

In order to obtain the concentration field of the pollutant in time and space, the SMS system was chosen.

A sector of the river Prut in Ungheni, 750 m in length, has been studied, which has been discretized directly in the SMS system in finite elements. Three specific areas were determined: the left bank, the right bank and the middle of the river (Fig. 3).

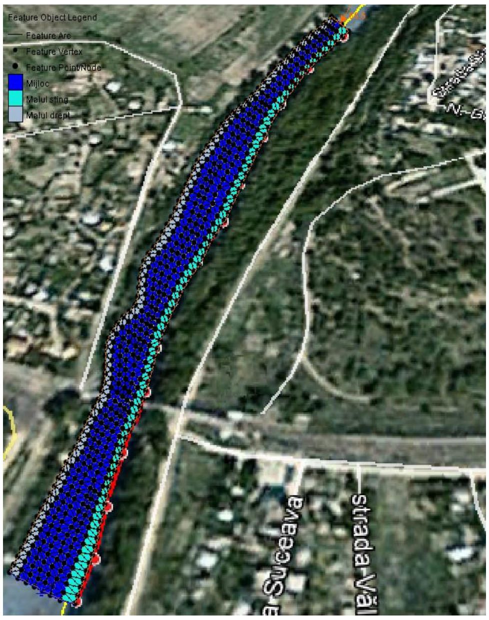

Fig.3. Computing network.

The hydrodynamics of the modeled sector was obtained through an SMS module under the name RMA2. The obtained results were taken over by the RMA4 module, with which the evolution of the pollutant concentration field was determined.

The mathematical modeling of pollutant transport and dispersion processes was accomplished using the fundamental advection-dispersion equation (13).

The simulations were performed in dynamic mode for 12 hours in the 0.5 hour step. The situations were simulated where the confluence zone of pollutant with the water is a sector of the left bank. The following conditions were set at the limit: upstream - flow $Q = 66.5$ m^3 / s, downstream - level $h = 0.83$ m.

Some of the results are shown in Figures 4 - 6. From Fig. 4 we can see the graphical representation of the concentration after 2 hours from the moment of the pollutant confluence with water.

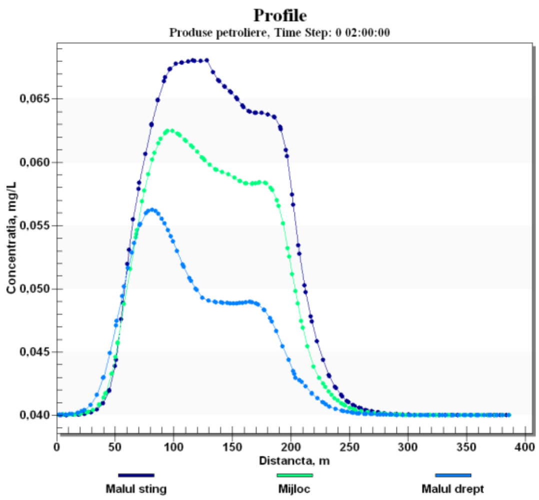

Fig. 4. Graphical representation of the concentration after 2 hours.

It can be noticed that after two hours from the moment of confluence with the water, the pollutant scattered and reached to the right bank

The pollutant dispersion in the confluence zone is shown in Fig. 5.

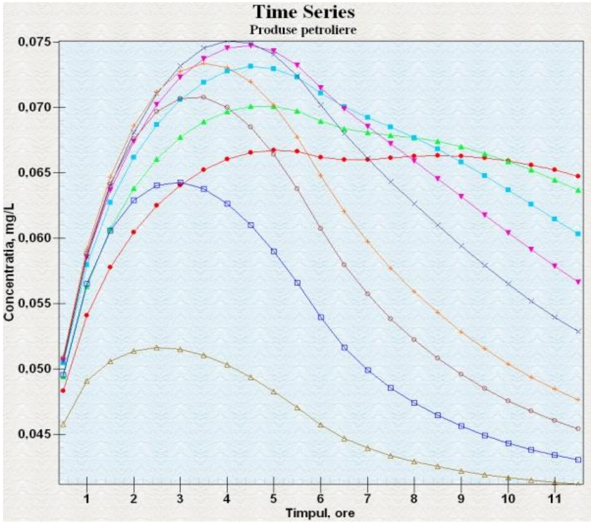

Fig. 5. Graphical representation of concentration in the confluence area.

The spatio-temporal evolution of the pollutant after 5 hours from the moment of confluence with water is shown in Fig. 6.

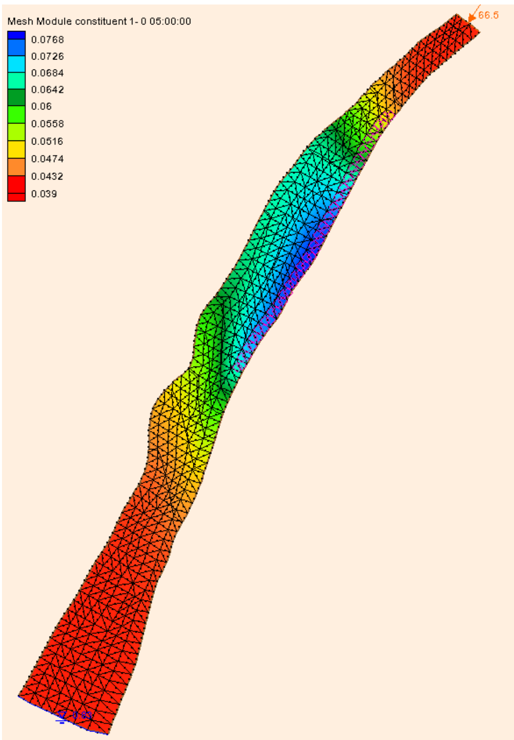

Fig. 6. Concentration field after 5 hours.

After 5 hours, the transport and dispersion of the pollutant were observed downstream of the confluence area.

The obtained data, using numerical models, were compared with measured data. The result of the comparison is shown in Fig. 7.

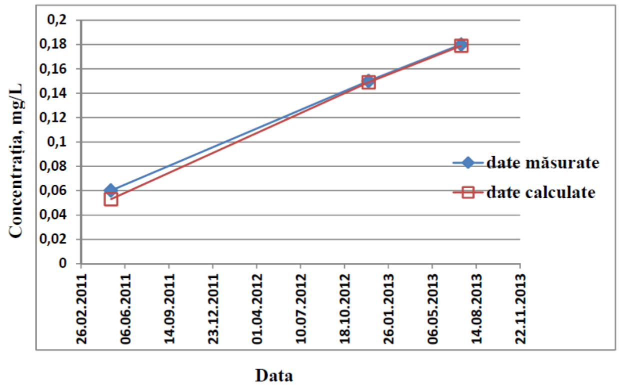

Fig. 7. The comparison of the measured data with calculated data.

A good correlation between measured data and calculated data is noticed.

Based on numerical simulations, it was established:

- during the first 2 hours from the time of confluence with water, the pollutant with the concentration of 0.075 mg / L taken over by the water stream has spread to the major part of the sector, reaching the right bank of 0.053 mg / L and 90 m downstream of the confluence area of 0.046 mg / L;

- in the next 5 hours the transport and dispersion processes of the pollutant downstream of the confluence area were observed, over a 240 m distance with decreasing concentration;

- after 10 hours, the pollutant spread over 270 m downstream of the confluence area;

- at the sampling point the concentration ranges from 0.04 to 0.06 mg / L;

- after 12 hours, the concentration was substantially reduced throughout the studied sector.

CONCLUSION

Based on the study, mathematical and numerical modeling has been found to be a powerful and useful tool for controlling and preventing pollution in aquatic systems.

The type of the mathematical model can be chosen depending on the flow regime and the studied processes.

An important stage in determining the spatio-temporal evolution of pollutants is the transposition of mathematical models into numerical models. Numerous simulation systems are used for this purpose.

The simulation results can be used to monitor water pollution and water quality of the aquatic systems, as well as the prediction and prevention of exceptional situations.

A case study on the determination of the spatio-temporal evolution of the pollutant on a sector of the Prut river in Ungheni is presented. Numerical simulations were performed using SMS. It has been demonstrated that this system is efficient and convenient to simulate real processes in aquatic ecosystems.

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