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MATHEMATICAL MODELING OF POLLUTANT TRANSPORT AND DISPERSION PROCESSES IN THE DNIESTER RIVER

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Abstract. This paper approaches the issue of water quality in river-type aquatic systems. It is discussed the importance of applying the mathematical and numerical models in order to assess the water quality and to predict different water pollution scenarios. It is presented an analysis of the field regarding the mathematical modeling of the spatio-temporal evolution of pollutants in river-type aquatic systems. As well, it is examined the water quality and are discussed the environmental issues regarding the pollution of the Dniester River. In the paper it is presented an analysis of the water samples taken from the Dniester River by the State Hydrometeorological Service, highlighting the pollutants that have exceeded the maximum permissible concentration on some sectors of the river. It is analyzed, as well as, the domain of mathematical models use for the calculation of the pollutant concentration area in the Dniester River and is proposed the development of the mathematical model based on the Navier-Stokes system of equations for the determination of hydrodynamic processes. In this paper it is also proposed a methodology for determining the spatio-temporal evolution of pollutants based on mathematical modeling using the fundamental equation of advection-dispersion.

Keywords: *advection-dispersion equation, aquatic systems, mathematical modeling, mathematical modeling, Navier-Stokes equations, pollutants, the Dniester river.*

1. Introduction

The issue of water protection and monitoring is actual as well as for national and international plan. The water quality in the country often does not correspond to national and international standards [1, 2]. The national legislative framework is continuously harmonized with the most important Council of Europe directives in the field of water resources [3, 4]. In most cases, water from rivers is used for human needs. The most important source of water supply for the population of the Republic of Moldova is the Dniester River, therefore its pollution poses a major risk to human health [5].

The use of mathematical and numerical modeling and then their implementation has become an important tool in the analysis of ecological systems by offering the possibility of exploring hypotheses that can not be easily tested in the field or during the laboratory experiments. The essence of the modeling method consists in replacing the real studied process by a more accessible model to be studied [6].

The urgency of research to determine the pollution degree of the aquatic environment and to establish the means to combat the pollution is significant. So, the elaboration and development of mathematical models for determining the spatio-temporal evolution of pollutants in river-type aquatic systems is the basis of the proposed research.

An effective tool in determining the spatio-temporal evolution of pollutants is the application of information systems. Choosing the right mathematical model and simulation program will significantly help to correctly assess water quality and prevent exceptional situations. Currently there are and are constantly developing the software techniques that are used for mathematical and numerical modeling of aquatic systems [7].

2. Problem statement

2.1 Mathematical modeling of processes in the river-type aquatic systems

Mathematical modeling is an isomorphic representation of reality, which, offering an intuitive and yet rigorous image, in the sense of logical structure, of the studied phenomenon, facilitates the discovery of connections and legalities that are impossible or very difficult to find in other ways. Mathematical modeling of pollutant transport processes is one of the possibilities to model certain pollutant transport processes that are actually either expensive to perform or are not economically viable.

There is no universal procedure that can be applied for the mathematical modeling of aquatic systems. In order to use a specific model, it is necessary to formulate the conditions that must meet them. So, the first step is to formulate the purpose of the mathematical model that is necessary to be obtained. The first water quality control model was created in 1925 in the USA. The model in question was one-dimensional that checked the oxygen balance by simple linear equations. The level of simulation of the calculations can be adapted to specific needs, ie according to the type of aquatic system, pollution sources, environmental parameters. The simulation is based on the differential solution of the mass (volume) equilibrium as it is shown in formula (1). The simplified differential equation has the form:

$$\frac{\partial}{\partial t}(Ac) = \frac{\partial}{\partial x}\left(-U_x Ac + E_x A\frac{\partial c}{\partial x \partial t}\right) + A(S_l + S_b) + AS_k \tag{1}$$

where:
c - component concentration of water quality;
t - simulation time;
U_x - longitudinal advection speed;
E_x - dispersion coefficient during water flow;
S_i - direct and diffuse external contamination load;
S_b - load changed between portions of the watercourse due to longitudinal dispersion;
S_k - load of contamination caused by kinetic transformation.

Most flow problems are solved using the continuity equation and the Navier-Stokes equations [8].

The equation of continuity of conservation of mass or transport is:

$$\frac{\partial \rho}{\partial t} + + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial y} = 0 \tag{2}$$

Navier Stokes Equation is:

$$\frac{d\vec{V}}{dt} = \vec{f} - \frac{1}{\rho} grad(p) + \nu \Delta \vec{V} \tag{3}$$

Continuity equation for two-dimensional flow:

$$\frac{\partial \rho}{\partial t} + + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0 \tag{4}$$

Using the equation (2), (3), and (4) can be deducted the Navier-Stokes equations for two-dimensional flows (5):

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = f_x - \frac{1}{\rho}\frac{\partial p}{\partial x} + v\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = f_x - \frac{1}{\rho}\frac{\partial p}{\partial y} + v\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) \tag{5}$$

Mathematical models based on the study of quality allow monitoring the quality of aquatic resources and their improvement from an ecological and chemical point of view. The key element in water quality protection is the development of the model for a specific period of time using the analysis of the pollution process (of certain pollutants), knowledge of emission data, flows and other mandatory coefficients to achieve the mathematical model as close as possible to real situations. Given that flow rates and concentrations vary visibly over a year, the following equations (6), (7), (8) can be used to determine average annual concentrations and annual immissions (annual loads) from point sources [9]:

$$Annual\ loads(t/year) = \bar{C}x(mg/l) * Q_{year}(m^3/s) * 31{,}5 \tag{6}$$

$$\bar{C}x = \frac{\sum_{i=1}^{n} C_{xi}Q_i}{\sum_{i=1}^{n} Q_i} \tag{7}$$

$$Q_{year} = \frac{1}{days(year)} * \sum_{i=1}^{days(year)} Q_i \tag{8}$$

where:

Q_{year} - average annual flow;

Q_i - average daily flow;

C_{xi} - instantaneous concentration of the chemical indicator *x;*

$\bar{C}x$ - the average annual concentration of the indicator *x*;

n - number of analyzes per year;

31,5 – transformation constant.

To assess the environmental impact of Damodar River water pollution in Jharkhand (India), have been developed mathematical models that play a major role in predicting the level of pollution in the considered regions. When developing different mathematical models, several important factors are taken into account in the evolution of water contamination with pollutants.

An important factor in the qualitative assessment of water is the calculation of the contaminants' transport. The formula (9) for a single chemical element is:

$$\frac{\partial}{\partial t}\left(C + \frac{\rho\beta}{\in}\right) = \nabla.\left(D.\nabla C\right)\left(x,t\right) - V.\nabla C - \Lambda^{\omega} C^{\omega} - \frac{S_s}{\in}\frac{Q}{vol} \tag{9}$$

While the description of the contaminant's transport requires the solution of the equation for the transport of saturated water (10) and the convection-dispersion-reaction equation for the transport of the contaminant through porous media [10], according the equation (11):

$$R_f \frac{\partial_{sc}}{\in} = \nabla.\left(D.\nabla C\right) - V.\nabla C - \Lambda - \frac{S_s}{\in}\frac{Q}{vol} \tag{10}$$

$$R_f = 1 + \frac{\rho \beta K_\omega}{\in} \tag{11}$$

For monitoring the water quality of the river Una (Brazil) was used the QUAL-UFMG model, which is widely used in Brazil to simulate scenarios and predict water quality. It is a one-dimensional model and among the basic parameters that were used to assess the quality of aquatic resources were the dissolved oxygen and biochemical oxygen consumption. To model of dissolved oxygen and the biochemical oxygen consumption in watercourses, the equation below (12) is used to calculate the weighted average of the concentrations with the aggregate element flows. It is observed that the C_0 value is obtained by a weighted average of the flows, dissolved oxygen and biochemical oxygen consumption [11].

$$C_0 = \frac{Q_r \times C_r + Q_r \times C_e}{Q_r + Q_e} \tag{12}$$

where:
C_0 - (dissolved oxygen or biochemical oxygen consumption) is the concentration of the mixture;
C_r - is the concentration in the river upstream of the mixing point;
C_e - is the concentration in the flow channel upstream of the mixing point;
Q_r and Q_e - are the flows of the river and the flow channel.

Mathematical models for the transport of pollutants in semi-infinite aquifers are based on the advection-dispersion equation and its variants.

The advection-diffusion mechanism can be described by a series of mathematical equations. These equations use the advection-scattering equation that incorporates scattering and velocity that are time-dependent and space-time-dependent source and flow, expressed by a single function [12]. The representation of the advection-diffusion mechanism of the concentration of pollutants flowing in one direction can be described by equation (13):

$$\frac{\partial C}{\partial t} = -\frac{\partial (uC)}{\partial x} + D_{mx} \frac{\partial^2 C}{\partial x^2} \tag{13}$$

where:
C - oxygen consumption concentration;
u - flow velocity;
D_{mx} - one-way diffusion coefficient.

The problem of mathematical modeling of water pollution is very complex. because the objective function is not explicitly defined in terms of direct control. Therefore, it is necessary to solve constraint-governing equations that are also complex, because we couple the model that describes the dissolution of pollutants with the Navier-Stokes equations. To overcome these difficulties we can use the Gelfand triplet and the theory of differential solutions to transform partial differential equations into ordinary differential equations [13]. There are many processes that influence water quality. They can be divided into transport processes that similarly affect all water quality parameters and transformation processes.

Taken into consideration the fact that the rivers are much longer than large in width and the pollutants at the discharge are rapidly dispersed in the riverbed, so a one-dimensional approach would often be justified.

In this case only the longitudinal variations of the constituent concentrations are solved in the form of mean values of the cross section. The general conservation of mass equation is averaged over the cross-section of the flow, for constituents subjected to a single first-order decay process [14] accoring the equation (14):

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + \frac{\partial}{\partial x}\left[(D_x + D_L)\frac{\partial C}{\partial x}\right] + KC + \Sigma I \quad (14)$$

where:
$\mathcal{X}$ - is the longitudional lenagth of the river L;
D_L - is the longitudinal coefficient of dispersion, $L^2/_T$.

The dispersion in natural currents is mainly due to variations in lateral velocity, and the following formula (15) can be used to estimate the coefficient:

$$D_L = 0.011\frac{u^2 B^2}{Hu^*} \quad (15)$$

where:
D_L - is the longitudinal coefficient of dispersion, $L^2/_T$;

u - average cross section velocity $L/_T$;
B - flow width, L;
H - flow depth, L;
u^*= shear velocity;
$L/_T = \sqrt{gHs}$;
g - acceleration due to gravity;
$L^2/_T$ and s - downhill flow, $L/_L$.

But the concentration of pollutant in the river is governed by an equation of diffusion of equilibrium advection in a horizontal dimension as in the ecuation below (16):

$$D\frac{d^2C}{dx^2} - u\frac{dC}{dx} - kC = 0 \quad (16)$$

where:
D, u and k are the dispersion coefficients, the river velocity and the decomposition rate of the pollutants.
If the constant source of the pollutant is $Q\ at\ x = 0$, then the solution of the given equation can be written as in formulas (17) and (18):

$$C_1(x \geq 0) = A\ exp(-m_1 x) \quad (17)$$

$$C_2(x \leq 0) = B\ \exp(m_2 x) \quad (18)$$

where A and B are constants, and as it is shown in the formula (19) m_1 and m_2 are:

$$m_{1,2} = \frac{u}{2D}\left[1 \pm \sqrt{1 + 4kv/D^2}\right] \quad (19)$$

A and B can be obtained if the following conditions:

$$C_1(0) = C_2(0) \quad (20)$$

$$\int_{-\infty}^{\infty} C(x)dx = Q \quad (21)$$

From the first condition it comes $A = B$, and from the second condition: $A = \frac{kQ}{u\sqrt{1+4ku/D^2}}$

So, according to the formulas (20) and (21) the solution of the equation of defusion of advection in the state of horizontal equilibrium it is obtained the formulas (22) and (23):

$$C_1(x \geq 0) = \frac{kQ}{u\sqrt{1+4ku/D^2}} exp\left[-\frac{ux}{2D}\left[\sqrt{1+4kv/D^2}\right]\right] \tag{22}$$

$$C_1(x \leq 0) = \frac{kQ}{u\sqrt{1+4ku/D^2}} exp\left[\frac{ux}{2D}\left[\sqrt{1-4kv/D^2}\right]\right] \tag{23}$$

Thus, the constant dispersion can be determined for given values of the source, velocity, diffusion coefficient and the first condition is $A = B$, and the second condition is the decomposition rate. If the source $Q(t)$ is time dependent then the equation (16) can be written as follows in the equation below (24):

$$D\frac{d^2C}{dx^2} - u\frac{dC}{dx} - kC = \frac{\partial C}{\partial t} \tag{24}$$

The following conditions are indicated in the formulas (25) and are required to solve it:

$$\begin{gathered} C(x,0) = C_0 \\ C(0,t) = C_s \\ C(\pm\infty, t) = 0 \end{gathered} \tag{25}$$

The analytical solution of the distribution of the pollutant concentration is given by the equation:

$$C(x,t) = C_0 + \frac{(C_S - C_0)}{2}\left[erfc\left(\frac{x-ut}{\sqrt{4D}}\right) + exp\left(-\frac{ux}{D}\right) erfc\left(\frac{x+ut}{\sqrt{4D}}\right)\right] \tag{26}$$

2.2 The current state of water quality in the Dniester river

The Dniester River is a very important drinking water artery for both the Republic of Moldova and Ukraine, and the fact that it flows into the Black Sea shows that the pollution of the Dniester can have a negative impact both locally and internationally. The problem of developing mathematical models for determining the transport processes of pollutants in the Dniester River is stringent for both national and international significance.

At present there are many environmental problems in the aquatic system of the Dniester River, in particular:

a) pollution with organic substances from untreated wastewater discharges,

b) nutrient pollution;

c) pollution with priority substances, which include organic micro-pollutants, heavy metals, along with pesticides, which cause problems even in low concentrations;

d) hydromorphological alterations, which include the change of the natural course of the river, the disconnection of wetlands, the change of the hydrological regime of the river, the deterioration of the aquatic biological diversity, all having a considerable impact on the aquatic environment;

e) groundwater pollution as a result of irresponsible management, non-compliance with the requirements, which is manifested by the lack of reconditioning works of protection areas and the abandonment of unsealed artesian wells and their direct exposure to pollution risk. The mentioned problems strongly affect both the aquatic flora and fauna, as well as the state of the waters as a whole.

The quality of water resources and aquatic biological resources of the Dniester River are largely affected by the activity of the Dniester Hydropower Complex, which has a negative impact throughout the Dniester River downstream of the Hydroelectric Power Plant (HEPP) by reducing water flow by almost 2/3, by changing the thermal regime of the water in the cross-border part of the Dniester river, below HEPP-2 (Naslavcea dam); the structural state of the river, marked by the grassing of the riverbed, which is an indicator of its gradual transformation into a swamp; worsening living conditions for pollution-sensitive macroinvertebrates, which is an indicator of worsening river water quality; extinction of precious fish species, etc [15].

According to the results of the water quality assessment, it was found that water from the Dniester can be attributed to quality class III, while all tributaries are highly polluted and have quality class V. This indicates that only water from the Dniester river can be used in food, in irrigation and recreation purposes, and the water from the tributaries of the Dniester river can be used only for purposes of transport and generation of electricity, except for the Raut river. The current monitoring system for surface water pollution sources, which operates at the branch level, covers only sources from the activities of primary water users due to insufficient wastewater treatment or their discharge from untreated sewage systems. As a result of the fact that the surface water monitoring network and programs do not provide sufficient information for effective water quality monitoring and are practically not an adequate support for a rightful management of water resources, is strictly necessary the implementation of information technologies [16].

Table 1 presents the obtained results from the analysis of water samples taken from the Dniester River in several localities in 2018. Pollution with petroleum products, nitrites and CBO_5 is observed, which contributes to reducing the amount of dissolved oxygen in water and have negative effects on aquatic systems [17].

Table 1

Exceedances of the maximum allowable concentration (MAC) on the Dniester River sectors (2018)

Locality	**Date**	**Pollutants that have exceeded MAC**	**Maximum allowable concentration (MAC), mg/l**	**The registered value**	
				mg/l	**exceedance MAC**
village Sanatauca	06.11.2018	Petroleum products	0,05	0,07	1,4
Town Vadul lui Voda		Petroleum products	0,05	0,06	1,2
village Cremenciuc	22.11.2018	Ammonium ions	0,39	0,48	1,23
		Petroleum products	0,05	0,26	5,2
village Palanca		nitriți	0,02	0,029	1,45
		Petroleum products	0,05	0,15	3,0
Town Naslavcea	03.10.2018	Petroleum products	0,05	0,10	2,0

Continuation Table 1

village Olanesti	16.10.2018	Petroleum products	0,05	0,07	1,4
Town Naslavcea	06.09.2018	nitriți	0,02	0,048	2,4
		Petroleum products	0,05	0,08	1,6
village Olanesti	18.09.2018	CBO_5	3,0	3,18	
		Petroleum products	0,05	0,17	3,4
village Vasilcau	1.08.2018	Petroleum products	0,05	0,07	1,4
village Cremenciug	21.08.2018	CBO_5	3,0	3,04	
		Petroleum products	0,05	0,12	2,4
village Palanca		CBO_5	3,0	3,12	
		Petroleum products	0,05	0,10	2,0
Village Olanesti	17.07.2018	nitriți	0,02	0,040	2,0
		Petroleum products	0,05	0,07	1,4
Town Naslavcea	06.06.2018	Petroleum products	0,05	0,07	1,4
village Olanesti	19.06.2018	nitrites	0,02	0,042	2,1
		Petroleum products	0,05	0,08	1,6
Town Naslavcea	04.04.2018	Petroleum products	0,05	0,14	2,8
village Olanesti	20.04.2018	Petroleum products	0,05	0,09	1,8
Town Vadul lui Voda	06.02.2018	Petroleum products	0,05	0,13	2,6
village Olanesti	25.01.2018	CBO_5	3,0	3,50	
		Petroleum products	0,05	0,06	1,2
Town Naslavcea	10.01.2018	Petroleum products	0,05	0,12	2,4

According to the data in Table 1, it was noted that the largest increases of the maximum allowable concentration are for petroleum products. This can be seen in figure 1 which shows the increase of the maximum admissible concentration during 2018 in several localities.

Currently there are few attempts concerning the mathematical modeling of pollutant transport and dispersal processes in the Dniester River.

Based on the above, it is formulated the problem of elaborating the methodology for the development of mathematical models regarding the determination of the processes of transport and dispersion of pollutants in the Dniester River.

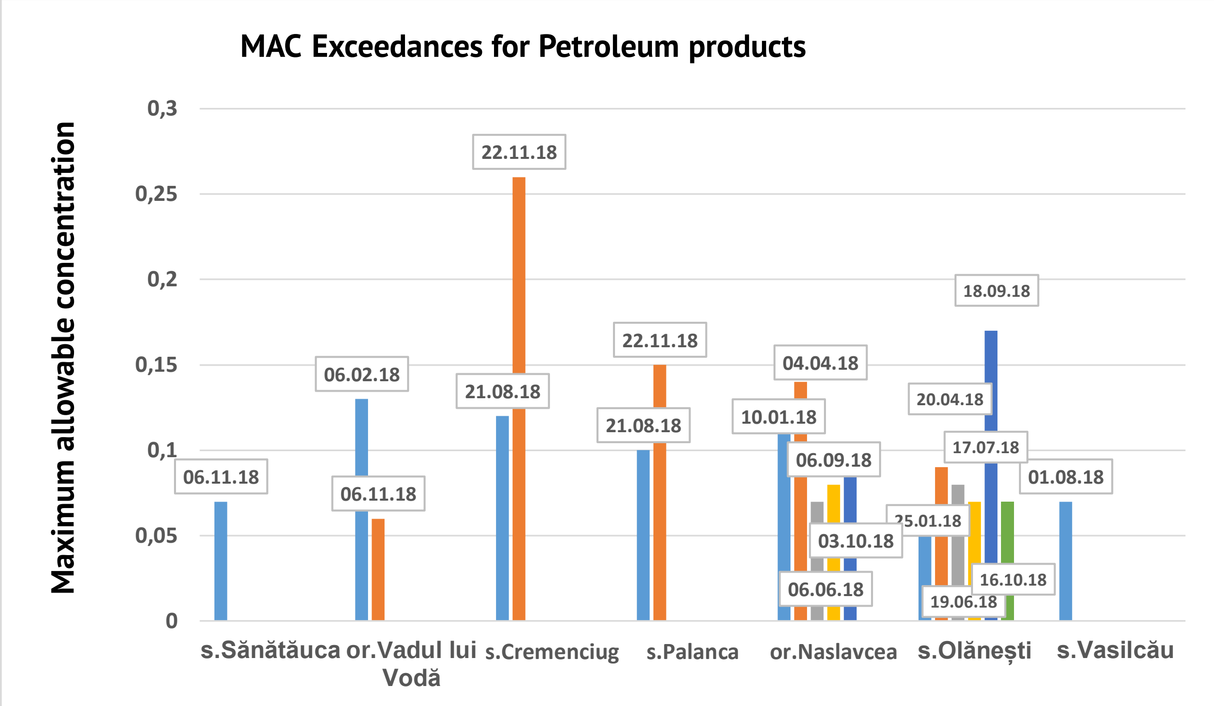

Figure 1. MAC Exceedances for Petroleum products.

3. Problem solutions

For a correct evaluation of the water quality, an important factor is the choice of the mathematical model and of the simulation program that should be appropriate to the studied aquatic system. Based on the analysis of the bibliographic sources, it was found that currently no mathematical models are developed on the processes of transport and dispersion of pollutants for the Dniester River. At the same time, the analysis shows the frequency of use of the Navier-Stokes equation system and the advection-dispersion equation for the mathematical modeling of river-type systems in order to determine different hydrodynamic processes, including transport and dispersion of pollutants.

In order to model different processes in river type systems, it is necessary first of all to know the sizes characteristic of the hydrodynamics of the studied aquatic systems. In river systems the flow is a turbulent one. The mathematical model for turbulent hydrodynamics is described by the Navier-Stokes equation system, composed of the Navier-Stokes equations (27) and the continuity equation (28):

$$\frac{\partial \mathrm{v}}{\partial t} + \mathrm{v}\nabla\mathrm{v} = f - \frac{1}{\rho}\nabla p + \nu\Delta\mathrm{v}, \tag{27}$$

$$\frac{\partial \rho}{\partial t} + \nabla(\rho\mathrm{v}) = 0 \tag{28}$$

where:

∇ - is the Hamilton operator;

Δ – the Laplace operator;

t – time;

ν – viscosity coefficient;

ρ – density;

p – pressure;

v – fluid velocity;

f – external forces (per unit volume) acting on the fluid.

The left side of the Navier-Stokes equations represents the unit inertia forces, and the right side - the mass forces, the pressure forces and, respectively, the viscous friction forces. The Navier-Stokes equations represent a system of differential equations with second order partial derivatives, inhomogeneous and nonlinear. The main source of turbulence is considered the term inertia $v\nabla v$, which represents the nonlinearity of the system. Solving these equations is possible only for simplified cases. At present, only the existence of weak solutions is demonstrated.

The movement and scattering of the pollutant occur due to the process called dispersion. The mechanism of dispersion is complex and can be explained by the simultaneous action of the phenomenon of molecular diffusion of the pollutant and the phenomenon of convection-advection. Molecular diffusion is the movement of molecules of a fluid from one region to another. This shift can only occur when there is a concentration gradient between the two regions. The displacement of molecules is performed in the direction of decreasing the concentration. The phenomenon of dispersion is described with the help of the fundamental advection-dispersion equation [18]:

$$\frac{\partial C}{\partial t} + \frac{\partial (u_i C)}{\partial x_i} = D\frac{\partial^2 C}{\partial x_i^2} \tag{29}$$

where:
C - the pollutant concentration;
u_i – transverse flow rate, which depends on the flow rate in the directions x, y and z;
D – diffusion coefficient;
t – time;
x – direction.

In order to obtain detailed and highly accurate information about the simulated system, further the mathematical models that are using computational fluid dynamics (CFD) are transformed into numerical models.

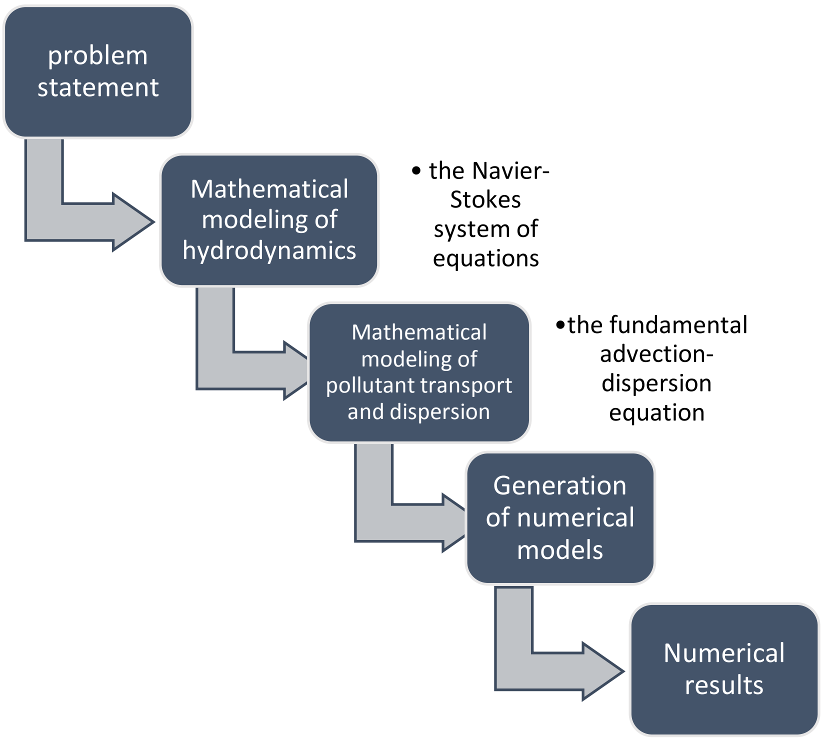

Figure 2. Research methodology.

In order to solve the problem of determining the processes of transport and dispersion of pollutants in the Dniester River, including the development of the scenarios for predicting water pollution, it is proposed to develop mathematical models based on specific parameters for the Dniester River, with subsequent application in various scenarios for predicting the water pollution. The research will be performed according to the methodology, presented in figure 2:

Conclusions

It was performed an analysis of the bibliographic sources regarding the mathematical modeling of the river type aquatic systems, which shows the importance of the approached topic. The analysis of aquatic systems with the help of mathematical models is an important research tool that can be used to solve problems where field research is not possible for economic or technical reasons.

Based on the analysis of bibliographic sources on the Dniester River, it was found that there are different works on the ecological and chemical state of the river, but there are no works related to the mathematical modeling of the processes of transport and dispersion of pollutants.

It was made an analysis of water samples taken from the Dniester River for the period of 2018. It was found that most of the exceedances were recorded for Petroleum products and nitrites. It is proposed a methodology for defining the transport and dispersion processes of pollutants for the Dniester River, which includes the determining of the hydrodynamics of the Dniester River based on the development of the mathematical model composed of the Navier-Stokes system of equations and defining the spatio-temporal evolution of pollutants on the basis of the fundamental advection-dispersion equation.

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