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ORIGINAL RESEARCH PAPER

COMPUTATIONAL SOLUTIONS FOR DETERMINING THE SPATIAL-TEMPORAL EVOLUTION OF POLLUTANTS ON THE PRUT RIVER SECTOR IN GIURGIULEȘTI LOCALITY

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Abstract: This work represents a research in the field of modeling the spatial-temporal evolution of pollutants. The Navier-Stokes equations were applied for the mathematical formulation of the spatial-temporal evolution of pollutants in river ecosystems, which are fundamental in fluid mechanics and describe the motion of fluids under different conditions. The SMS (Surface-water Modeling System) environment was used to determine the spatial-temporal evolution of pollutants, which is a software developed for modeling and simulation of surface water flows. An important evolution was the use of the application of 2/3D hydrodynamic models that simulate water flow in one plane, taking into account two spatial dimensions (longitude and latitude). The pollutant behavior simulation approach will contribute to the assessment and forecasting of potential natural catastrophes of riverine aquatic ecosystems. This research aims to explore the computational methods and technologies and comes up with some solutions that can be used to analyze the distribution and evolution of pollutants on the Prut river sector in Giurgiulești locality. A comparative analysis of several commercial Software (ANSYS Fluent, COMSOL Multiphysics, STAR-CCM+) and Open-Source Software (OpenFOAM, SU2, Gerris) was carried out, and the advantages of each software in the process of numerical simulation of the spatial-temporal evolution of pollutants were found.

Keywords: *computational solutions, ecosystems, modeling, pollution, river, spatial-temporal evolution*

INTRODUCTION

The aquatic river systems are essential for life on Earth. They provide many important resources for life, such as fresh water, food, habitat for numerous species and vital ecosystem services for society. However, rivers around the world are under increasing pressure from human activities, resulting in widespread pollution that threatens the health of ecosystems and human populations. River pollution is a complex global problem with multiple causes and devastating effects [1 – 3].

The most widespread types of pollution of riverine aquatic ecosystems can be mentioned: **Chemical Pollution** manifested by the presence of pesticides and herbicides, heavy metals and nutrients; **Biological Pollution** manifested by the presence of organic wastes and pathogenic microorganisms; **Physical Pollution** manifested by the presence of solid wastes and sediments [2, 3].

The most prevalent cause and sources of pollution globally are: agricultural activities, industrialization, urbanization and infrastructure development and deforestation [1 – 3].

The impact of pollution on ecosystems and human health is a global problem and manifests itself in: effects on biodiversity, effects on human health and economic effects [3].

At the same time, humankind is looking for solutions and strategies to reduce the pollution of riverine aquatic ecosystems found in: regulations and legislation; treatment technologies; reforestation and soil conservation; education and awareness programs and International cooperation [1, 3].

The pollution of riverine aquatic ecosystems is therefore a major global challenge that requires a coordinated and sustainable response from governments, communities and industry. Computational, technological and legislative solutions are essential to protect these vital ecosystems, thus ensuring public health and biodiversity conservation for future generations. It is imperative that society at a global level act in concert to prevent and remediate river pollution, thereby contributing to a healthier and more balanced environment [1 – 9].

The problem of pollution of the aquatic ecosystem of the Prut River, especially in the area of Giurgiulești, faces significant challenges due to agricultural, industrial and urban activities in the region. Determination of the spatial-temporal evolution of pollutants in this sector is essential for the adoption of effective environmental protection and remediation measures [4 – 9].

In this context, computational solutions play an important role, providing powerful tools for monitoring, modeling and prediction of the evolution of pollutants in the aquatic environment. This research aims to explore computational methods and technologies and comes up with some solutions that can be used to analyze the distribution and evolution of pollutants in the Prut River sector of Giurgiulești locality.

The importance of monitoring pollutants in the Prut River is determined by the fact that it is an important transboundary watercourse, being the natural border between Romania and the Republic of Moldova. The locality of Giurgiulesti is located in the extreme south of the Republic of Moldova, at the confluence of Prut and Danube, making this region ecologically and economically strategic. The Danube Delta is one of the most important and valuable natural areas in Europe and even in the world, recognized for its extraordinary biodiversity, picturesque landscapes and ecological importance. Located in the eastern part of Romania, where the Danube River flows into the Black Sea, the Danube Delta is the second largest and best preserved delta in Europe. The Danube Delta is home to over 5500 species of plants and animals, including rare and protected species. These include over 300 species of birds (including pelicans, cormorants, and egrets) and around 45 species of freshwater fish (such as sturgeons). It is an important site for bird migration, serving as breeding, feeding and resting habitat for many migratory species. In 1991, the Danube Delta was listed as a UNESCO World Heritage Site because of its exceptional ecological value and biodiversity. It is also recognized as a Biosphere Reserve, underlining its international importance for nature conservation [5, 6, 9].

Although the Danube Delta is a protected area, it faces threats such as pollution, climate change and unsustainable development. Proper management and protection of this unique region is essential to ensure the long-term conservation of biodiversity and natural resources. The application of computational solutions to determine the spatial-temporal evolution of rainfall on the Prut River sector in Giurgiulesti locality will allow to assess and forecast potential natural catastrophes of this ecosystem (Figure 1) [9].

Figure 1. *Drainage area of the Prut River into the Danube River*

MODELING THE SPATIAL-TEMPORAL EVOLUTION OF POLLUTANTS IN RIVER-TYPE ECOSYSTEMS

Numerical modeling is an important approach for determining the spatial-temporal evolution of pollutants in river ecosystems. It involves the use of mathematical algorithms and numerical methods to simulate pollutant transport and dispersion processes [10 – 15].

There are several modeling methods that can be used to analyze the dynamics of the pollution process in space and time in river-type ecosystems, of which can be mentioned: **Hydrodynamic models**, which simulate the flow of water and its interaction with pollutants, taking into account factors such as current velocity, water depth and bed morphology; **Transport and dispersion models**, which follow the movement and dispersion of pollutants in water, including advection, diffusion and chemical degradation processes; **Reaction models**, which simulate chemical and biological reactions that can transform pollutants into other substances.

Hydrodynamic models are important tools in the study of water movement in aquatic river ecosystems. These models are used to simulate the hydrodynamic behavior of water in various contexts such as rivers, lakes, estuaries, seas and oceans. They allow the user to better understand the physical processes that govern water flow and to make predictions about how these systems will evolve under the influence of natural and anthropogenic factors.

Hydrodynamic models are oriented towards the application of a set of fundamental equations that describe fluid motion and are very effective in water resource management, flood simulation, environmental impact assessment, and pollutant dispersion modeling. The most important equations used in the simulation process are:

Navier-Stokes equations are partial differential equations describing the conservation of mass (continuity) and momentum (motion) in a fluid. They are applied to model flow in environments where there is a viscosity and external force such as gravity and friction;

The continuity equation describes the conservation of mass in a fluid volume, ensuring that what goes into a volume must equal what comes out plus what accumulates in that volume;

Shallow water equations (Small Water) are simplifications of the Navier-Stokes equations, applicable in cases where the wavelength of water movement is much greater than the water depth. They are commonly used in river and coastal modeling.

In order to simulate the spatial-temporal evolution of pollutants on the Prut River sector in Giurgiulești locality, 2/3D hydrodynamic models are applied, which simulate the water flow in a plane, taking into account two spatial dimensions (longitude and latitude). These are sufficient to simulate the water movement in rivers and estuaries, deltas and flood zones, where the lateral flow distribution is significant.

MATHEMATICAL FORMULATION OF THE SPATIAL-TEMPORAL EVOLUTION OF POLLUTANTS IN RIVER-TYPE ECOSYSTEMS

For the mathematical formulation of the spatial-temporal evolution of pollutants in river ecosystems, the Navier-Stokes equations are applied, which are fundamental in fluid mechanics and describe the motion of fluids under different conditions. There is a set of partial differential equations derived from the laws of conservation of mass (equation 1), momentum (equation 2) and energy [16 – 18].

Continuity equation (conservation of mass)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \mathrm{v} \right) = 0 \tag{1}$$

where: ρ is the fluid density in the simulation area [kg·m^{-3}]; v is the fluid velocity in the simulation area [m·s^{-1}]; t is time [s].

Momentum equation (fluid dynamics)

$$\rho\left(\frac{\partial \mathrm{v}}{\partial t}+\mathrm{v}\cdot\nabla\mathrm{v}\right)=-\nabla p+\mu\nabla^2\mathrm{v}+\mathrm{f} \tag{2}$$

where: v is the fluid velocity in the simulation area [$m\cdot s^{-1}$]; p is the fluid pressure in the simulation area [$N\cdot m^{-2}$]; μ is the dynamic viscosity [$N\cdot m^{-2}$]; f are the external forces that influence the fluid flow process in that area.

Physical interpretation of the Navier-Stokes equations

$\rho\left(\frac{\partial \mathrm{v}}{\partial t}\right)$ - the acceleration term [$kg\cdot(m^{-2}\cdot s^{-2})$], which represents the change in momentum per unit volume over time;

$\rho(\mathrm{v}\cdot\nabla\mathrm{v})$ - the convection term [$kg\cdot(m^{-2}\cdot s^{-2})$] representing the momentum changes due to fluid motion through a velocity field;

$-\nabla p$ - pressure gradients [$kg\cdot(m^{-2}\cdot s^{-2})$], which represent the forces exerted on the fluid due to pressure differences;

$\mu\nabla^2\mathrm{v}$ - viscous diffusion [$kg\cdot(m^{-2}\cdot s^{-2})$], which is responsible for the dissipation of kinetic energy from the fluid due to viscosity;

f - external forces which include any other forces acting on the fluid flow process (gravity, river banks, obstacles, etc.).

Although the Navier-Stokes equations are mathematically well-defined, they have no analytical solution for real problems. For this reason, numerical solutions, using methods such as finite differences, finite elements or finite volumes, are frequently used. These methods allow the simulation of fluid behavior under complex conditions, but require considerable computational resources.

ENVIRONMENTS FOR NUMERICAL SIMULATION OF THE SPATIAL - TEMPORAL EVOLUTION OF POLLUTANTS IN RIVER-TYPE ECOSYSTEMS

There are a variety of methods and environments available for solving the Navier-Stokes equations for the numerical simulation of the spatial-temporal evolution of pollutants in river ecosystems. It should be considered that solving the Navier-Stokes equations, due to their complexity, requires the use of advanced computational environments. These can be software applications, numerical computational libraries, or dedicated platforms for fluid simulation. Whether they are commercial software, open-source packages or numerical libraries, modern solutions allow successfully tackling complex fluid problems and solving them efficiently. The choice of an environment depends on the specific requirements of the project (domain size, boundary conditions, or desired accuracy), the available resources and the user's level of expertise.

Commercial software

ANSYS Fluent – is one of the most popular commercial Computational Fluid Dynamics (CFD) software. Fluent is used for simulations of fluid flow, heat transfer and related processes, providing a wide range of solutions for complex industrial problems [19];

COMSOL Multiphysics – is software that provides an integrated environment for simulating fluid phenomena and coupling with other physical phenomena such as heat transfer or chemical reactions [20];

STAR-CCM+ - software developed by Siemens, are used for fluid simulation, but also for other multidisciplinary applications, and are prized for its ability to handle large and complex simulations [21].

Open-Source Software

OpenFOAM – is the most widely used open-source CFD package. OpenFOAM allows customization of simulations and can be used for a wide range of applications, including solving Navier-Stokes equations [22];

SU2 – originally developed for aerodynamics, it is now a complete CFD simulation package supporting a wide range of applications, including solving Navier-Stokes equations [23];

Gerris – is open-source software specialized in multiphase flow simulation. It is optimized for complex problems such as the interaction of fluids with solid surfaces.

In the present work to determine the spatial-temporal evolution of pollutants on the Prut river sector in Giurgiulesti, **SMS (Surface-water Modeling System)** was used, which is a software developed for modeling and simulation of surface water flows [24]. SMS is used in environmental engineering and hydrology to create two- and three-dimensional models of water flow in various environments, including rivers, lakes, estuaries and coastal zones. This system provides efficient solutions for analyzing water hydrodynamic behavior, sediment transport, pollutant dispersion, and other water-related processes.

Features and advantages of SMS

2D and 3D hydrodynamic modeling - which allows the simulation of water flow in two or three dimensions, providing a detailed picture of water behavior as a function of watershed geometry, boundary conditions and hydrological parameters;

Integration with various simulation engines - SMS supports several simulation engines, such as TUFLOW, ADCIRC, STWAVE, RMA2 and RMA4, which can be used to perform detailed calculations of water flow, wave propagation, and other dynamic processes;

Preprocessing and post-processing tools - SMS includes powerful tools for preprocessing data (creating computational networks, defining initial and boundary conditions) and post-processing results (visualizing data, graphical analysis, and generating reports);

Advanced visualization - SMS provides advanced capabilities for visualizing simulation results, including water flow animations, vector plots, and representations of velocity and depth distributions.

Multiple applications - SMS can be used in a wide range of applications, including hydraulic infrastructure design and management, water quality management, environmental impact assessment, flood risk management, and aquatic restoration studies.

RESULTS OF THE SIMULATION OF THE SPATIAL-TEMPORAL EVOLUTION OF POLLUTANTS ON THE PRUT RIVER SECTOR IN GIURGIULEȘTI LOCALITY

From the analysis of the monthly bulletins on the quality of the environment on the territory of the Republic of Moldova [4 – 9, 25 – 28] for the period of 2019 – 2023, it was noticed that on the sector of the Prut river in the Giurgiulesti town (see Table 1) the most frequently encountered pollutants were: dissolved O_2, CCOCr (chemical oxygen consumption determined using potassium dichromate method), total phosphorus and mineral phosphorus. The highest exceedances of the MAC (maximum admissible concentration) among the mentioned pollutants were recorded for mineral phosphorus. From these considerations, a scenario with exceedances of the MAC for mineral phosphorus was chosen for the numerical modeling. The modeling was done using the SMS system.

Table 1. *The frequency of exceeding the MAC of pollutants on the river Prut sector from the Giurgiulești locality, period 2019-2023*

Year of monitoring	Magnesium ion	The hardness	Suspended substances	Mineral phosphorus	Total phosphorus	CCOCr	Ammonium nitrogen	Dissolved O_2	Petroleum products	Nitrate nitrogen	Nitrite nitrogen	$Na^+ + K^+$	orthophosphate	Total iron
2019	5	1	4	2	1	1	1	2	-	-	1	1	-	-
2020	-	-	-	5	3	3	3	-	1	-	1	-	-	-
2021	-	-	-	-	2	5	1	1	-	-	1	-	3	1
2022	-	1	1	3	3	3	2	5	1	1	1	-	2	4
2023	-	-	-	3	2	2	1	4	2	-	2	-	-	-

It was selected for the simulation a sector with a length of 1.02 km (Figure 2). There were identified three specific areas and their properties: left bank, right bank, middle of the river (Figure 3).

Figure 2. *The sector selected for simulation*

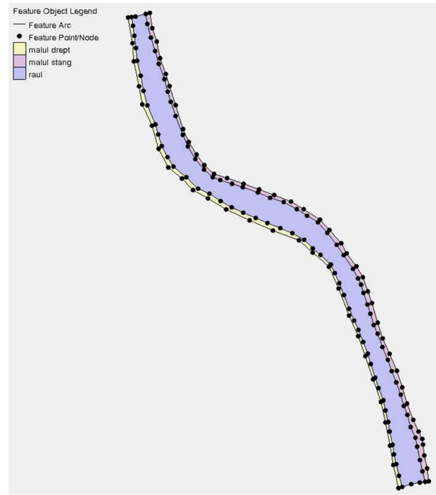

Figure 3. *2D representation of geometry*

In order to carry out the simulation process in the SMS environment the selected sector was discretized into finite elements. The computational network is denser in the areas of particular interest, at the river bends, the discretization step is smaller and the number of finite elements is higher (Figure 4). The simulations were carried out in dynamic regime for 12 hours with step 0.5 hour. The situation was simulated when the zone of confluence of the pollutant with water is a portion of the left bank of the studied sector, sample concentration 0.186 $mg \cdot L^{-1}$ and boundary conditions: upstream - flow Q = 260 $m^3 \cdot s^{-1}$, downstream - level h = 1.96 m.

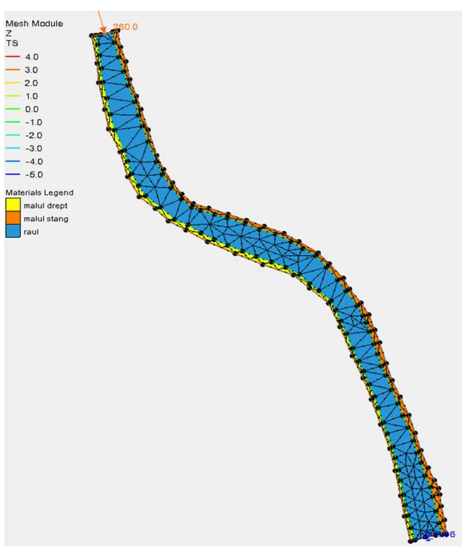

Figure 4. *Calculation network*

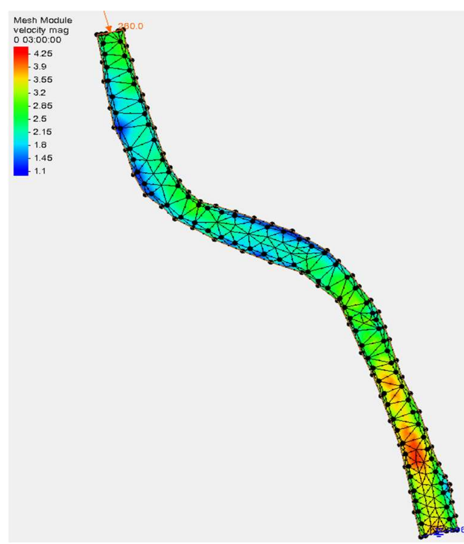

Figure 5. *Field of resultant velocities*

The following results have been obtained as a result of the RMA2 program:

- The resulting velocity field (Figure 5);
- Field of local velocities in the x direction (Figure 6);
- Field of local velocities in the y direction (Figure 7);

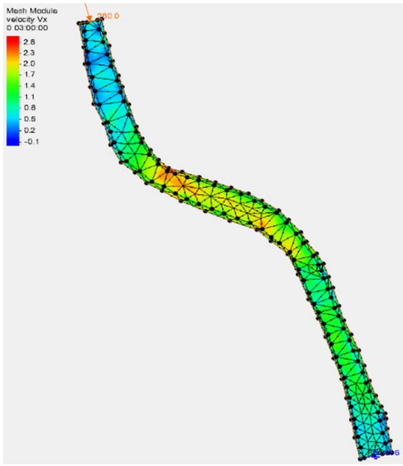

Figure 6. *Local velocity field in the x direction*

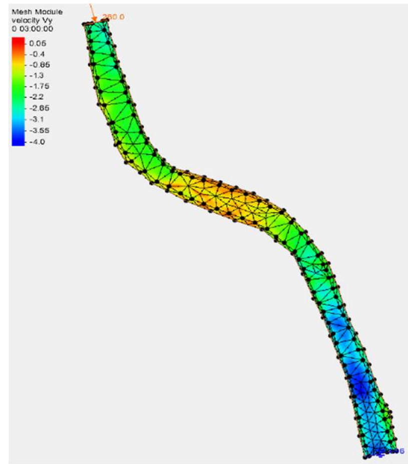

Figure 7. *Local velocity field in the y direction*

It was found that in the x-direction the water particles move with a higher velocity compared to the y-direction, with a maximum velocity of 2.6 $m \cdot s^{-1}$ in the x-axis and 0.05 $m \cdot s^{-1}$ in the y-axis. The results regarding the water depth are presented in Figure 8.

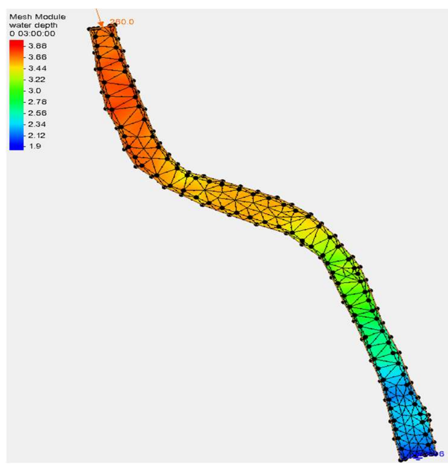

***Figure 8**. Water depth on the simulated section*

The data obtained as a result of RMA2 were used as input data for RMA4. The results obtained using RMA4. Some of the obtained results with the help of the RMA4 program are presented in Figures 9 and 10:

- The field of concentrations obtained over 30 minutes after the moment of confluence of the pollutant with the water (Figure 9). It is noticed that the pollutant concentration value is still high in the confluence area, including in the middle of the river and on the right bank.
- The field of concentrations obtained over one hour after the moment of confluence of the pollutant with the water (Figure 10). It is noticed a decrease in the concentration value.

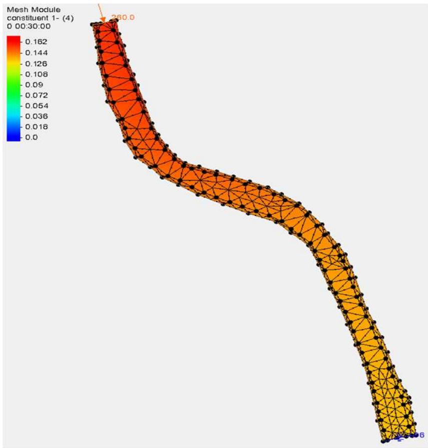

Figure 9. *Concentration field after 30 min*

Figure 10. *Concentration field after one hour*

The field of concentrations obtained after 2 hours from the moment of confluence of the pollutant with the water is presented in Figure 11. It is noticed that the value of the concentration of the pollutant decreases throughout the studied river sector.
The field of concentrations obtained after 10 hours from the moment of confluence of the pollutant with the water is presented in Figure 12. It was found out that the value of the concentration of the pollutant is significantly reduced throughout the studied river sector.

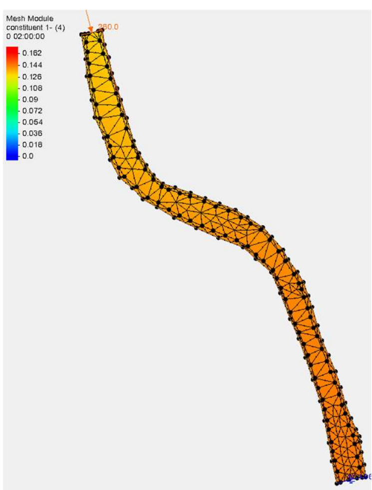

Figure 11. *Concentration field after 2 hours*

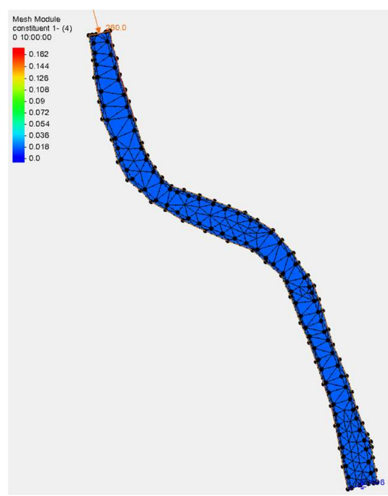

Figure 12. *Concentration field after 10 hours*

The temporal evolution of pollutant concentration on the left bank is presented in Figure 13.

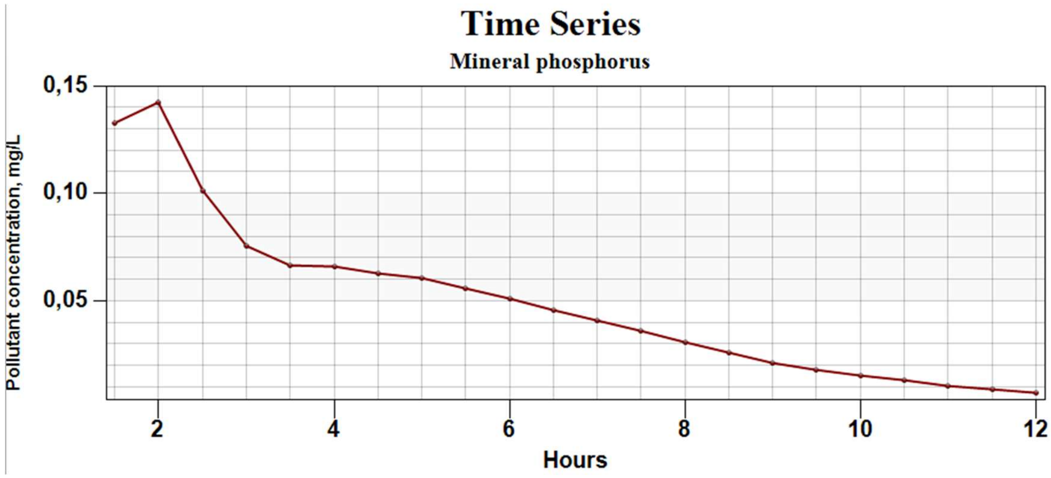

Figure 13. *Temporal evolution of pollutant concentration at the left bank*

It was found that the pollutant concentration value decreases significantly after more than 9 hours of the confluence with water and reaches a lower value than the MAC (maximum admissible concentration).

CONCLUSIONS

It was carried out a study on water quality on the Prut river sector in Giurgiulești, highlighting the most frequently encountered pollutants: dissolved O2, CCOCr, total Phosphorus and mineral Phosphorus. It was found that the highest exceedances of the MAC among the mentioned pollutants were recorded for mineral Phosphorus.

It was carried out an analysis of software products for the numerical simulation of the spatial-temporal evolution of pollutants, highlighting their advantages.

With the help of the SMS environment, the modeling for the mentioned sector regarding the transport and dispersion of Mineral Phosphorus was carried out.

Following the application of the RMA2 program, the following results were obtained: the field of resultant velocities, the field of local velocities in the x direction, the field of local velocities in the y direction. Thus it was concluded that in the **x** direction the water particles move with a higher speed compared to the movement in the **y** direction.

The data obtained as a result of the application of the RMA2 program were used as input data for the RMA4 program in order to obtain the spatial-temporal evolution of the simulated pollutant. It was found that after 10 hours from the moment of confluence with the water, the value of the concentration of the pollutant is significantly reduced throughout the studied river sector.

The obtained results allow the development of prediction scenarios regarding the transport and dispersion of pollutants in river-type aquatic systems.

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