Journal of Engineering Science *Vol. XXXIII, no. 1 (2026), pp. 120 - 132*
Fascicle *Architecture, Civil and Environmental Engineering* *ISSN 2587-3474*
Topic *Environmental Engineering* *eISSN 2587-3482*

https://doi.org/10.52326/jes.utm.2026.33(1).08
UDC 532.5:556.53:004.94

NUMERICAL MODELING OF HYDRODYNAMICS OF RIVER-TYPE AQUATIC SYSTEMS

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Received: 01. 22. 2026
Accepted: 03. 02. 2026

Abstract. The prediction and monitoring of pollutants in riverine ecosystems are essential for environmental protection and public health. This study proposes a methodology for the numerical modeling of hydrodynamics in aquatic systems using ANSYS Fluent. The results highlight the capability of ANSYS Fluent to determine critical parameters required for subsequent simulations, enabling accurate assessment of pollutant concentration distributions.

Keywords: *hydrodynamics, river, CFD, ANSYS Fluent, numerical modeling, pollution, water quality.*

Rezumat. Predicția și monitorizarea eficientă a poluanților din sistemele acvatice de tip râu sunt esențiale pentru protejarea ecosistemelor acvatice și a sănătății publice. Acest studiu prezintă o metodologie pentru modelarea numerică a hidrodinamicii în sistemele acvatice folosind produsul program ANSYS Fluent. Rezultatele demonstrează potențialul ANSYS Fluent în determinarea parametrilor critici necesari pentru simulările ulterioare în scopul obținerii câmpului de concentrații a poluanților.

Cuvinte cheie: *hidrodinamică, râu, CFD, ANSYS Fluent, modelare numerică, poluare, calitatea apei.*

1. Introduction

Moldova's freshwater resources are under increasing pressure, and river flow zones have undergone significant changes due to centuries of human activity. This has caused environmental changes in river ecosystems, such as water pollution from various sources of pollution such as petroleum substances, nitrites, nitrates, etc., loss of biodiversity, landscape deterioration and coastal erosion.

The water quality of the Dniester River is not only a concern for the Republic of Moldova, but also for the entire region and Europe in whole, especially because it flows into the Black Sea and the quality of the river's water influences both the country's ecosystem as well as the entire region [1]. There has been strong regional and international cooperation for several decades, achieved through various organizations and conventions. Various directives are being developed to regulate the quality of river waters in Europe and in the associated countries [2]. The need to predict pollution and monitor it is an important step in the process of protecting and improving water quality.

Water pollution prediction is an important thing in the management of aquatic environment for the prevention and control of water pollution. At present, there are several prediction methods for monitoring the pollution of aquatic systems, which are selected depending on the need and the type of aquatic system. The competent organizations choose the monitoring application program according to their own needs. According to the different mechanisms of the different water pollution prediction methods, they can be divided into statistical prediction method [3], intelligent prediction method and mechanism model prediction method [4].

As it was mentioned, the major concern is the quality of river water. It is not enough to monitor the water, to detect the pollutant through different sensor networks, it is necessary to predict and prevent the evolution of the pollutant concentration downstream [5]. It is expensive and isn't cost-effective to use a multitude of sensors, therefore, implementing different applications that would facilitate the prediction and monitoring the pollutants is appropriate. These applications could significantly help to improve the quality of water in aquatic systems [6].

2. Numerical modeling of river-type aquatic systems

The study of water quality in river-type ecosystems is extremely important. This issue becomes especially important when rivers are a major source of drinking water, water for irrigation, and water for industrial use. River pollution is currently one of the most serious environmental problem. After entering the river, pollutants spread rapidly. The process is determined by molecular motion, turbulence and non-uniform distribution of velocity in the cross section of the flow. Thus, contaminants disperse on the water surface and are transported downstream by the water flow

Understanding the mechanisms of pollutant transport in different types of rivers contributes to the correct numerical modeling for effective management of pollution situations in the aquatic ecosystem. The study of these processes represents an essential component of environmental engineering. The transport of pollutants in rivers is fundamentally described by the advection–dispersion equation [7].

Numerical modeling provides a very important tool in obtaining water quality prediction scenarios. With the help of numerical models, it could be analyzed the dispersion of pollutants in time and space. The input data for numerical models regarding the dispersion of pollutants are the hydrodynamic parameters, therefore the first step is to obtain the hydrodynamics. Specialized software products are used to obtain the hydrodynamic parameters [8].

Computational fluid dynamics (CFD) is a branch of fluid mechanics that uses numerical methods and data structures to analyze and solve problems involving fluid flows. CFD simulates and analyzes the behavior of liquids or gases in an environment and to describe the physical processes that occur due to this interaction. This approach allows solving complex problems, for which analytical methods are difficult to apply. Over the years, numerous software have been developed that provide better and more accurate solutions, which are necessary for solving complicated problems.

CFD is also a flexible, accurate and widely applicable tool that is applied in solving problems related to fluid dynamics and especially in flowing fluids such as river-type aquatic systems [9].

Using an application for predicting pollutants in aquatic ecosystems requires in-depth knowledge of the real system, the physicochemical laws, in order to correctly configure the software and to achieve the goal of prediction the water pollution.

Various software have been developed to identify sustainable solutions for water resource management and to improve the prediction of pollutant dispersion. Water quality models are important decision support tools for water pollution control. These models are applied to study the aquatic ecosystems health, and assessing the effects of point and diffuse pollution. Water quality models are complex software, which are usually not easy to learn and apply.

These software programs are developed by various state organizations, but also by various research centers, universities, and software development companies. These models are of different types, such as: models for assessing exposures in groundwater, surface water, food chain, etc. Such software are: SWAT, HSPF, AQUATOX, QUAL2K, WASP, TOXSWA, SWASH, MODFLOW 6, HEC-RAS, iRIC, HYDRUS, ANSYS Fluent, AGNPS, SMS and many others [7].

SWAT – (The Soil and Water Assessment Tool) is a small-scale watershed model used to simulate the quality and quantity of surface and groundwater and to predict the environmental impacts of land use, land management practices, and climate change [10].

HSPF - (Hydrologic Simulation Program Fortran) is a comprehensive package for simulating watershed hydrology and water quality for both conventional and toxic organic pollutants, allowing integrated simulation of soil contaminant runoff processes with flow-hydraulic and sediment-chemical interactions.

AQUATOX - is a simulation model of the evolution of various pollutants, such as nutrients and organic chemicals, and their effects on the ecosystem, including fish, invertebrates and aquatic plants.

QUAL2K - one-dimensional model intended to represent a well-mixed channel both vertically and laterally, with a hydraulic system in steady state, constant non-uniform flow rate and the amount of kinetic heat of the water quality.

WASP – (The Water Quality Analysis Simulation Program) for interpreting and predicting water quality from natural phenomena and human-caused pollution [11].

TOXSWA – (TOXic substances in Surface WAters) is a pseudo-2-dimensional model, which describes the behavior of pesticides in a water layer and its underlying sediment at the field edge scale [12].

SWASH - (Surface WAter Scenarios Help). It is an easy-to-use software product developed to perform various surface water pollution scenarios [13].

MODFLOW 6 - is an object-oriented program and framework developed to provide a platform for supporting multiple models and multiple model types within the same simulation [14].

HEC-RAS - the numerical model uses gradient and topography to estimate flow depth, velocity, and flooded areas. It is also useful for calculating sediment transport and water temperature [15].

iRIC – (International River Interface Cooperative) developed for numerical simulation of river flow and morpho-dynamics. It is a tool for analyzing river flow and morpho-dynamics, but also to predict flood, rainfall runoff generation, tsunami propagation [16].

HYDRUS - is a Windows-based modeling software suite that can be used to analyze the water flow, heat, and solids transport in variably saturated porous media (e.g., soils) [17].

AGNPS – (AGricultural Non-Point Source Pollution Model) The model predicts water, sediment by particle size class, erosion source, and chemicals—nitrogen, phosphorus, organic carbon, and pesticides [18].

SMS - (Surface-water Modeling System) is used for hydrodynamic modeling and substance transport in aquatic environments. The software generates 1D, 2D and 3D models in the field of surface waters, allowing to develop versatile models, grid generation and three-dimensional visualization of results [19].

ANSYS Fluid - used for numerical simulation of fluid flow and heat and mass transfer phenomena. The software allows modeling the complex processes, including turbulent flows, chemical reactions, and pollutant transport in fluid media. The tool is widely used in research and engineering to analyze the optimization of hydrodynamics and thermal processes [20].

Analyzing the multitude of researches that are carried out globally, it has been demonstrated with certainty that numerical modeling through software programs is an effective solution for current research.

The paper [21] proposes a new method for numerical simulation of pollutant transport in rivers, applied to the Severn River (Great Britain). The method uses the finite volume method for numerical solution and a multilayer neural network for estimating the longitudinal dispersion coefficient, used as an input parameter in the advection–dispersion equation. Validation by comparing simulated results with measured data demonstrated high model performance. The use of neural network significantly improved the accuracy of the simulation of pollutant transport in the river.

Modeling the aquatic systems for better monitoring of pollutants is carried out in many regions. In the article [22], the dynamics of pollutants in the Prut River system in the Giurgiulesti locality sector was examined and using the SMS software and it was developed a simulating model of the spatio-temporal evolution of pollutant dispersion. The obtained results highlight that computational methods are effective for analyzing and predicting the behavior of pollutants.

In the paper [23], it was proposed a complex of qualitative mathematical models with dynamic parameters for the assessment and forecasting the aquatic environment in Latvia. All constructed models are described in terms of differential equations and mathematical physics and are considered to be evolutionary models.

In [24], the QUAL2Kw model was subjected to calibration and validation tests. This model was implemented in the Tungabhadra River, India, and it was studied the dissolved oxygen concentration in the river water. The following were the basis of these studies: the ability to increase the flow, to oxygenate the source and to modify the volume of pollution.

In [25], the QUAL2E water quality model, a continuously stirred tank reactor method, was used to model the flow of the Beylerderesi River, Turkey, as a dynamic model, and the kinetic parameters were determined applying the optimization methods. For the optimization step, a secondary sequential programming method was used. The model prediction showed that the obtained results were consistent with the experimental data. The parameters of the Beylerderesi River model were estimated by SQP optimization, using a MATLAB code, and the dynamic simulations were performed with a rigid Runge-Kutta explicit integrator. The physicochemical data were analyzed in SPSS 22 by ANOVA for mean comparison, providing useful information to predict the impact of industrial investments on water quality and to measure environmental effects.

In the research paper [26], was accomplished the modeling and simulation on the Măleia River (Hunedoara County, Romania). The purpose of this research is to simulate general and accidental pollution. Using the SMS software, it was modeled the spatio-temporal evolution and dispersion of pollutant transport for surface aquatic systems. The developed numerical models estimated the dispersion of ammonium, nitrites and nitrates in the studied sector. Based on the results of the numerical simulation, it was established that the obtained, calibrated and validated numerical models can be used for any pollution scenario in emergency situations and accidents.

In [27], was investigated turbulent flow in an open channel affected by rigid vegetation. Numerical modeling was performed in Ansys Fluent, solving the RANS equations for turbulent flow and using the standard κ-ε model for turbulence. The free water surface was captured by the VOF method, and the volume discretization and numerical schemes were chosen for stability and accuracy. The study demonstrated the applicability of ANSYS Fluent in simulating complex flow in natural channels and constitutes a methodological basis for extending it to pollutant transport and dispersion models, even though pollutants were not directly integrated in the respective article.

Analyzing the implementation of different numerical models, we conclude that they are important tools for predicting the adverse effects of water pollution and can help guide practical investments for better management of the aquatic systems quality. In water quality models, it is necessary to optimize the parameters determined by trial and error to ensure the reliability of the model.

3. Problem formulation

The importance of water for human health was underlined in the mentioned above research, as well as the role of software in solving problems related to the pollution of aquatic systems. For the Republic of Moldova, the most important source of drinking water is the Dniester River. According to laboratory data of the Agency of Environment [28], regarding the water quality of the Dniester River from 2019-2024, it was found that the lower sector of the Dniester River has become increasingly polluted. Increased concentrations of pollutants were identified in the preliminary data, especially ortho-phosphates and suspended matter. For this reason, the Dniester River area near the locality Olănești was selected to obtain the hydrodynamic parameters. Table 1 presents the pollutants that were analyzed as well as their harmful impact on the environment and humans.

Table 1

Pollutants and their impacts

Pollutant	Main source	Environmental impact	Impact on humans
Orthophosphates (PO_4^{3-})	Fertilizers, detergents, wastewater	□ Moderate eutrophication, algae growth, oxygen depletion	☒ Slightly harmful directly
Suspended matter	Sediments, organic and inorganic particles	☒ Decreases light, affects photosynthesis, deposits on the bottom of the water	☒ Can transport heavy metals and pathogenic microorganisms

Continuation Table 1

CCO -Cr	Biodegradable and non-biodegradable organic matter	☒ High oxygen consumption, affects aquatic fauna	☒ Indirectly harmful, indicates the presence of organic pollutants
BOD_5	Biodegradable organic matter, wastewater	☒ Reduces dissolved oxygen, affects fish and the ecosystem	☒ Indirectly unsafe for consumption
Nitrogen nitrite (NO_2^-)	Partial oxidation of ammonia, reduction of nitrates	● Toxic to fish, reduces available oxygen	● Highly toxic; methemoglobinemia to infants, affects blood oxygenation
Nitrogen nitrate (NO_3^-)	Fertilizers, agriculture, wastewater	☒ Contributes to eutrophication and algae proliferation	☒ At high concentrations, methemoglobinemia to infants, cardiovascular problems

☒ – Low toxicity level / minor impact, ☒ – Moderate level, ☒ – High level, ● – Very high / critical level

Monitored data show increased values of nitrates, ortho-phosphates, suspended matter, BOD5 and CCO-Cr, which indicates a consistent pressure on the aquatic ecosystem. The main cause is the accumulation of pollutants from upstream sources: local discharges, both domestic and industrial, insufficiently treated, plus pollutants from intensive agricultural activities, which transport nutrients and sediments into the river, especially during periods of precipitation or snowmelt. In addition to these are the hydromorphological conditions specific to the lower sector, characterized by a low slope and slow flow, which reduce the natural self-purification capacity of water and favor the persistence of pollutants [29]. The choice of the sector near the Olănești locality for analysis reflects the cumulative impact of human activities in the entire upstream area and will allow the evaluation of the impact of pollutants on water quality.

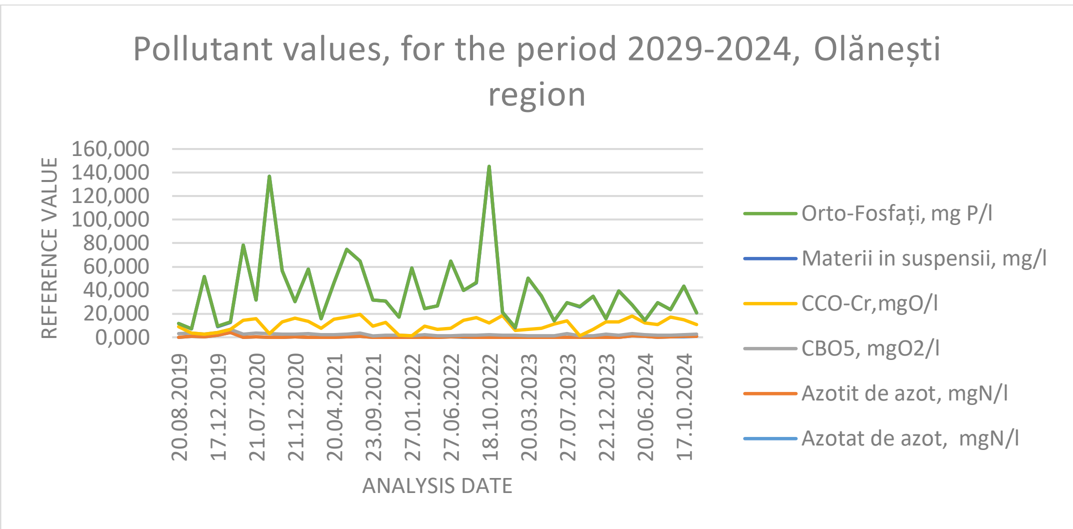

Figure 1. Pollutant values in Olănești (2019-2024).

In Figure 1, can be noticed the increases of ortho-phosphate concentrations, which indicate surface runoff from fertilized agricultural lands. Pollutants are transported to the river throughout the year, but during rainy periods and during snowmelt, the pollutant concentration increases. High values of COD-Cr and BOD_5 indicate pollution with wastewater of domestic and industrial origin that has not been properly treated. These types of pollution are frequently encountered near populated areas, where intensive agricultural activities take place, as well as direct discharges into river waters or discharges that are not subjected to an adequate treatment process.

4. Solving the problem

Since the beginning of its development, modeling has established itself as one of the most powerful and flexible tools supporting decision-making processes. Numerical models are extremely numerous and varied. Modeling techniques are implemented in various fields of activity. Effective decisions are based not only on modeling and simulation, but on a comprehensive system analysis. The made researches led to the conclusion that the ANSYS software is one of the most reliable tools that can provide accurate results. ANSYS Fluid provides accurate quantitative predictions regarding fluid-compound interactions, and solves a wide range of CFD simulation challenges to obtain reliable results in predicting pollutant dispersion in river-type aquatic systems.

ANSYS Fluid combines extended pre-processing and post-processing capabilities. In the Fluid environment, it is possible to model the following elements: fluids in a uniform and temporary state, laminar and turbulent flow, the range of fluid flow: subsonic, transonic and supersonic, heat transfer in thermal radiation, flotation; non-Newtonian fluid; multiphase fluid, the cavitation effect. ANSYS Fluent enables advanced analyses and modeling, as well as high-quality visualization and animation. The use of the ANSYS Fluent software in modeling pollutant behavior in aquatic systems represents an efficient and well-justified solution. This software accurately reproduces hydrodynamic processes and pollutant transport mechanisms in aquatic environments. In aquatic ecosystems, pollutant dynamics is simultaneously governed by flow, dispersion, turbulence, and physico-chemical and biological reactions, and these mechanisms are integrated into the numerical modeling framework of ANSYS Fluent.

Another advantage is the possibility of simulating three-dimensional flows, areas with velocity variations, turbulence effects. This aspect is particularly important in modeling real rivers because the dispersion of pollutants is influenced by several factors such as: riverbed morphology, aquatic vegetation, inhomogeneous turbulence. Ansys Fluent offers the possibility of simultaneously simulating several types of pollutants (nitrogen compounds, phosphorus, organic substances). This is important in water quality analysis, since the interaction between different substances, since the interaction between them determines processes such as eutrophication or the consumption of dissolved oxygen.

In aquatic ecosystems, the transformations between different pollutants can be numerically modeled by this software, which has the ability to integrate chemical reactions and biochemical processes. Thus, simulations can be used both for analyzing the current situation and for predictions depending on flow, temperature, types of pollutants. So, Ansys Fluent can perform predictive analyses for aquatic systems, such as evaluating the impact of discharges and assessing measures aimed to reduce pollution.

Ansys Fluent has advanced numerical accuracy, flexibility in modeling physicochemical phenomena and the possibility to simulate real pollution scenarios, which gives it an advantage in practical use. These features make it an effective tool for studying the behavior of pollutants in river ecosystems and for implementing modern strategies for aquatic environmental protection [30].

In order to solve the formulated problem, CFD simulations were performed using the ANSYS Fluent package. The simulated river sector is located between Nezavertailovca and Tudora, with a focus on the Olănești locality. The used hydrometric data [31] come from the Nezavertailovca and Tudora locations, as they are the closest and most relevant for the analyzed segment. These measurements allowed the definition and calibration of the boundary conditions necessary for building the 2D model. Compared to the geodetic distance of 6,414 m, the actual length of the riverbed is 10,153 m, indicates significant sinuosity. The riverbed is 58% longer than the direct path, which indicates the presence of well-defined meanders. This increases the water travel time and promotes lateral mixing in the river flow.

Table 2

General and obtained data of the Nezavrtailovca point (2021)

Hydrological / Geometric Parameter	Value	Unit	Observations
Flow	124	m^3/s	Measured value (2021).
Water level	1,17	m	Average depth in section.
Estimated average speed	0,37	m/s	Calculated from Q and an estimate of the cross-sectional area.
Riverbed length	10153	m	The actual length of the course on the winding route.
Geodetic distance	6414	m	The straight-line distance between points.
Sinuosity coefficient	1,58	-	Indicates a watercourse with moderate sinuosity.

The geometric data for the section between Olănești and Tudora clearly highlight the sinuous nature of the riverbed. With an effective length of 24,658 m, compared to 8,301 m in a straight line, the riverbed presents well-defined meanders, indicating a remarkable sinuosity.

Table 3

General and obtained data of Tudora point (2021)

Hydrological / Geometric Parameter	Value	Unit	Observations
Flow	466	m^3/s	Measured value, indicating a high flow regime. (2021).
Water level	4,67	m	Significant level, corresponding to a high flow rate.
Estimated average speed	0,75	m/s	Increased speed, reflecting a more energetic flow.

Continuation Table 2

Riverbed length	24658	m	Actual length of the extremely winding course.
Geodetic distance	8301	m	The straight-line distance between points.
Sinuosity coefficient	2,97	-	Indicates a watercourse with very pronounced sinuosity

The sector of the Dniester River in the Olănești locality is characterized by a sinuous riverbed, with an actual length of 4,372 m compared to 2,324 m in a straight line, resulting in a degree of curvature of 1,88, typical of plain meanders. The riverbed narrows from 77,1 m at the entrance to 49,3 m at the exit, which accelerates the flow and raises the water level downstream. The hydraulic parameters were determined by interpolation and empirical relationships, using real upstream and downstream data: the flows (124–466 m³/s) and water levels (1.17–4.67 m) were adjusted proportionally to the position of Olănești, and the velocity was estimated by the formula $V \approx 0{,}342 \cdot H^{0{,}51}$. The widths of the riverbed were taken from satellite images, and the compatibility of the section and velocity with the calculated flow was verified. This approach allowed obtaining a coherent set of parameters for numerical simulation, without direct measurements in the sector, these values were presented in Table 4.

Table 4

Shape and dimensions of the riverbed in the Olănești sector

Geometric Parameters	Value	Unit	Observations
Actual length of the river	4372	m	The river has a curved shape.
Straight line distance	2324	m	-
Degree of Bending	1,88	-	A value greater than 1.5 indicates a river with bends.
Riverbed length at Inlet	77,1	m	The river narrows (by 28 meters, or ~36%) along the village.
Riverbed length at Outlet	49,3	m	

Given the predefined data, the hydraulic parameters of the given sector were calculated and are represented in Table 5.

Table 5

Calculated hydraulic parameters in the sector of interest

Hydrological Parameter	At the entrance to Olănești	At the exit from Olănești	Main Effect
Average water speed	0.49 m/s	0.54 m/s	The water is accelerating.
Water level	2.08 m	2.47 m	The water level rises slightly downstream,
Estimated flow rate	213 m3 / s	251 m3 / s	The amount of water is increasing; it is due to small streams

Numerical simulation of the Dniester River sector in the Olănești locality, characterized by a curved riverbed configuration, was performed using ANSYS Fluent. The results of the numerical simulation are presented in Figure 2.

Figure 2. Turbulence intensity (%) on the 2D plane of the Olănești locality, Dniester River.

From Figure 2 can be seen the spatial distribution of the turbulence intensity, expressed in percentage. The maximum values seem to be located mainly on the outer part of the curves, where the fluid velocity increases and the velocity gradient becomes more pronounced. This distribution is consistent with the known hydrodynamic behavior of natural rivers, where kinetic energy and mixing processes are more intense in these areas.

Overall, the image suggests a realistic modeling of the interaction between the bed geometry and the turbulent flow regime. The modeling obtained can be used for the analysis of sediment transport or pollutant dispersion, since turbulence controls the mixing and dilution processes in aquatic systems. The numerical model regarding the magnitude of the Nistru River water flow velocity in the Olănești locality sector was also obtained, which can be observed in Figure 3.

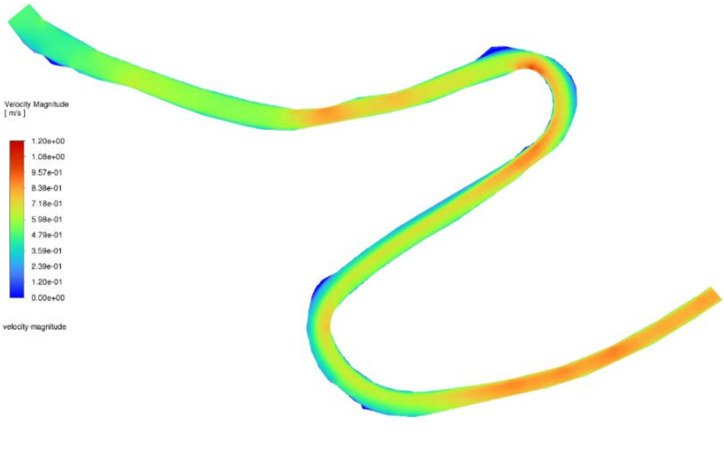

Figure 3. Velocity magnitude (m/s) of the Olănești locality sector.

Velocity magnitude distribution can be noticed in Figure 3, it indicates and average velocity of approximately 1,2 m/s. The velocity distribution highlights a clear variation between the inner and outer areas of the river bends. In the outer part of the river bend, higher velocity values can be observed, due to the effect of centrifugal force effect and the concentration of the main flow. In the inner part of the riverbed, appear areas with reduced velocities, associated with flow braking processes and possible recirculation areas.

On relatively straight sections, the velocity is distributed more uniformly. This distribution is typical for natural river flow and reflects the direct influence of the riverbed morphology on the velocity field. The obtained results are relevant for the analysis of sediment transport and pollutant dispersion processes, since the current velocity controls both advection processes and the mixing efficiency in the aquatic environment.

The developed numerical modeling confirmed the accuracy of the model and its capability to reproduce the transport and dispersion processes of pollutants. Organic pollutants originating from point sources (BOD_5 and COD -Cr) were significantly diluted throughout the river sector, their concentrations decreasing by over 600 times, which shows the efficiency of natural self-purification processes. In contrast, the pollutants present in the riverbed (TSS and PO_4P) remained relatively constant, suggesting a continuous input or a higher hydrochemical inertia. The model proved to be stable and reproducible, and mass conservation was fully respected. Consecutive testing produced almost identical results, confirming the correctness of the simulations and providing a realistic picture of how the river can reduce pollutant concentrations through natural mechanisms.

5. Conclusions

Numerical modeling of aquatic systems represents a significant step in the process of monitoring the ecological situation of rivers. Predicting water pollution is another important stage of water environment research. Information systems and software products used worldwide highlight the relevance of this ecological problem. The multitude of programs applied for simulation and modeling plays an important role in developing concrete solutions for ecological problems of aquatic systems, but especially rivers, which are the main source of drinking water. Research has also conducted that, at present, one of the most efficient and accurate software tools used for numerical modeling of aquatic systems is ANSYS Fluent. This software offers a wide range of modeling options and could provide answers to the most complex research challenges. The numerical modeling performed on the hydrodynamic parameters confirmed the accuracy of numerical modeling with Ansys Fluent.

The obtained results will be subsequently used to develop numerical models for pollutant transport and dispersion in river-type aquatic systems.

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Citation: Braniște, R. (2026). Numerical modeling of hydrodynamics of river-type aquatic systems. *Journal of Engineering Science*. 2026, 33 (1), pp. 120-132. https://doi.org/10.52326/jes.utm.2026.33(1).08.

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