# Multidisciplinary Digital Solutions for Predicting the Environmental and Cumulative Behaviors of Contaminants in the Danube River Basin Ecosystems

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**Abstract:** Water quality is a key issue for the sustainable development of the world. At present, in most regions of the globe, there is a continuous deterioration of water quality. To stop this process, it is necessary to initiate complex studies and actions by specialists in various fields. According to the Water Framework Directive 2000/60 / EC, approved by the European Commission, it is necessary to ensure the "very good" condition for all water bodies. In this paper, we will briefly present: methods, techniques, and algorithms for a sustainable database on water quality parameters, mathematical models and numerical methods of pollutant transport and dispersion.

**Keywords**: Digital Solutions; the Danube River; Ecosystems

## Problem Statement

To be used, the water must be clean, meet water quality standards. According to the Water Framework Directive, approved in 2000 by the European Parliament and the Council, by 2015, with the extension of the deadlines until 2021 and 2027, it is necessary to achieve a good level of water quality. Unfortunately, lately, there is more and more continuous degradation of water quality. This is true for all aquatic ecosystems, especially river ecosystems, including the Danube River basin ecosystems.

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According to the Report of the European Court of Auditors in 2015 (targeting four EU Member States in the Danube river basin: Romania, Slovakia, Czech Republic, and Hungary) on water quality in the Danube river basin, types and sources of pollution of Danube River basin ecosystems are the following:

- organic pollution, having as sources the wastewater coming from households and industrial installations;
- pollution with nutrients (nitrogen and phosphorus) from agricultural land;
- pollution by dangerous substances, having as source urban and industrial wastewater, use of pesticides in agriculture, contaminated sites and mining sites;
- hydromorphological alterations caused by hydroelectric installations, navigation works, and flood protection infrastructures.

It was found that during the years 2009-2015 the ecological and chemical condition of water bodies has improved very little. Progress has been made on the implementation of the Water Framework Directive, but further efforts are needed. A recommendation of the Report concerning states that to have accurate information on the situation and source of pollution, it is necessary for Member States to ensure better monitoring of water quality. (Raportul special nr. 23 // 2015 Calitatea apei în bazinul hidrografic al Dunării/ Special report no. 23 // 2015 Water quality in the Danube river basin).

In the *Management Plan Of The Danube-Prut And The Black Sea Hydrographic Basin* Cycle I, 2017 - 2022, within the limits of the Republic of Moldova, developed by the Institute of Ecology and Geography of the Academy of Sciences of Moldova in accordance with Directive 2000/60 / EC of the European Parliament and of the Council of 23 October 2000 and the Water Law no.272 of 23.11.2011, discusses the pollution of the mentioned aquatic systems and the main sources of pollution, as well as their impact. Regarding point pollution, in the Prut basin only 1% of Rivers were estimated as possible at risk, and in the Danube-Black Sea basin due to much lower river flows and poorer conditions of treatment plants, registered 15.8% of Water Bodies Rivers exposed to risk. Diffuse pollution is generated by agriculture and animal waste. Under the impact of diffuse pollution at risk are 96% of Rivers of Water in the Prut basin and 94.7% of the Danube-Black Sea basin, within the borders of the Republic of Moldova. Under the impact of hydromorphological pressures, 31.3% of Rivers in the Prut basin and 63.2% of the Danube-Black Sea basin, within the limits of the Republic of Moldova, are at risk. (http://www.apelemoldovei.gov.md/public/files/Plan_Prut-Dunarea_01_11.2016._3.pdf).

An important aspect for determining the dispersion of pollutants in aquatic ecosystems, determining and ensuring water quality, including the development of scenarios for predicting water pollution is the monitoring of all parameters on water quality. There is currently a monitoring network on the aquatic systems mentioned, but at the same time, the existing system also contains some deficiencies, such as technical inability and insufficient financial resources to provide chemical reagents and consumables suitable for the activity, lack of monitoring program for a longer period, etc. (http://www.apelemoldovei.gov.md/public/files/Plan_Prut-Dunarea_01_11.2016._3.pdf).

Based on the above, results in the problem statement of determining the most efficient methods and techniques for calculating the spatio-temporal evolution of pollutants in the Danube River basin ecosystems, as well as the prediction of pollution scenarios.

## Mathematical and Numerical Modeling of Water Quality

An essential tool in calculating the water quality class, as well as determining the spatio-temporal evolution of pollutants in order to prevent exceptional situations, is the mathematical and numerical modeling of river systems. Choosing the appropriate mathematical model and simulation program will allow the correct assessment of water quality (Marusic, 2013, pp. 38-42; Mannina, 2011).

In order to adequately describe the evolution of the studied system, the mathematical model through numerical methods is transformed into a numerical model. Numerical modeling is performed by CFD techniques, with the help of which the partial differential equations are transformed into systems of algebraic equations, the solutions of which represent an approximation of the state quantities in the defined nodes of the computational domain (Anderson, 2012), (Ferziger & Peric, 2002).

There are currently attempts and proposals for modeling water quality in rivers. In these papers, different approaches are proposed regarding the combination of mathematical models, GIS systems, and software techniques. (Filote, Ciufudean, Alaci, Marusic, & Cozgarea, 2012, pp. 243-246) (Marusic, 2013, pp. 80 – 89).

A Decision Support System (DSS) has been developed for water quality management in the Songhua River Basin, China. This system was presented by incorporating a numerical water quality modeling system into a water quality management system with the following components: geographic information system

(GIS), WebGIS technologies, databases, and network technologies. The application system includes information management and water quality modeling management. The developed system allows the calculation of various water quality management scenarios, and also the interpretation of modeling results in order to make those decisions. (Zhang, Yin, & Ling, 2010, pg. 400-403)

A geoinformation system for modeling and forecasting surface water status has been developed in Russia based on GIS technologies. A synthesis of mathematical models was performed, following which a database was created, composed of water quality models. The system allows the collection and classification of information, research of the dynamics of the ecosystem in time and space, elaboration of thematic maps based on the analysis performed, modeling of natural processes in different environments, estimation of the situation, and forecast of the ecological situation. The model of pollutant transport for the Zea river is presented. The water pollution index is calculated, based on which the water quality index is determined (Kozlov, 2010, pp. 58-62).

A system for modeling the spatio-temporal evolution of hydrodynamics and water quality characteristics has been developed for the Severnaia Sosiva River in Russia. Topographic maps of the studied river sector were discretized using the ArcGIS system. Based on the numerical model of hydrodynamics and water quality CE-QUAL-W2, the 3-D model of the studied river sector was built and the numerical simulation of hydrodynamics was performed (determination of the velocity field of water particles and the vertical turbulent diffusion coefficient ). At the same time, a series of scenarios were performed to simulate the calculation of the speed of water particles in the surface layer of the river during floods. It was found that the characteristic sizes of hydrodynamics largely depend on the detailing of the model geometry. The model for determining water quality characteristics calculates a large number of water quality parameters. It has been established that the process of transport and dispersion of pollutants critically depends on the velocity field of the water particles and the degree of turbulence of the water flow (Pusistov, 2006).

The dynamic simulation of the prediction of accidental pollution on a sector of the Someş River downstream of the Romanian city of Cluj-Napoca is presented in the paper (Cristea, Bagiu, & Agachi, 2010, pg. 985-991). A CFD program called COMSOL Multiphysics is applied, which uses the finite element method when discretizing the domain. Two approaches are used: diffuse pollution (which assumes that the pollutant is distributed along the river bank) and point pollution. The k-ε turbulence model and the advection-dispersion equation were used. The effects of adding a neutralizing agent in order to reduce the concentration of pollutants were investigated (Cristea, Bagiu, & Agachi, 2010, pg. 985-991).

A methodology for the mathematical modeling of the flow of the Ural and Sakmar rivers in the Orenburg region, Russia was developed using GIS technologies. For this purpose, the hypsometric surface of the Orenburg region and the relief model was elaborated, taking into account the location of the river network. Level data were taken from the US Geological Survey's GTOPO30 database. The basic equations used are part of a system of equations deduced from the Navier-Stokes system of equations:

$$\omega \frac{\partial V}{\partial x} + V \frac{\partial \omega}{\partial x} + \frac{\partial \omega}{\partial t} = q,$$

$$\frac{\partial V}{\partial t} + V \frac{\partial V}{\partial x} + \frac{g}{\omega} \frac{\partial (\overline{H}\omega)}{\partial x} + \frac{V.q}{\omega} = g(I - I_T),$$

where ω is the cross-sectional area of the river; V - average flow rate; q - the tributary per unit length; x - spatial coordinate; t - time; g – gravitational acceleration of free fall; I - the slope of the river; I_T - hydraulic gradient; H - the distance between the water surface and the center of gravity of the water section.

This system is called the Saint-Venant system of equations. The solution was performed using a parallel programming algorithm, implemented through the Borland Delphi 7.0 programming environment. This environment contains a special type of object-flow, upon activation of which the system independently creates a new flow within an application. After calculating the output data on water consumption or speed, each stream can receive new input data from the previous stream on water consumption or speed (Vlatskii, 2010, pp. 104-109).

A discrete ternary mathematical model of hydrodynamics is presented in the paper (Cisteacov, 2010, pg. 66-77). The model was developed based on the Navier-Stokes equations and the continuity equation:

$$u'_t + uu'_y + vu'_y + wu'_z = -\frac{1}{\rho} P'_x + (\mu u'_x)'_x + \left(\mu u'_y\right)'_y + (\nu u'_z)'_z + 2\Omega(v sin\theta - w cos\theta),$$

$$v'_t + uv'_x + vv'_y + wv'_z = -\frac{1}{\rho} P'_y + (\mu v'_x)'_x + \left(\mu v'_y\right)'_y + (\nu v'_z)'_z - 2\Omega u sin\theta,$$

$$w'_t + uw'_x + vw'_y + ww'_z = -\frac{1}{\rho}P'_z + (\mu w'_x)'_x + \left(\mu w'_y\right)'_y + (\nu w'_z)'_z + 2\Omega u cos\theta + g,$$

$$u'_x + v'_y + w'_z = 0,$$

where $V = \{u, v, w\}$ are the components of the velocity vector; $p$ - hydrodynamic pressure; $\rho$ - density; $\Omega$ - angular velocity of rotation of the earth; $\theta$ - the angle between the angular and vertical speed; $\mu$, $\nu$ - horizontal and vertical components of the turbulence coefficient.

The approximation of the boundary conditions is discussed and it is found that the sources of error in the mathematical model are often the input data. These errors cannot be reduced in the calculation process. That is why all input data must be approximately the same accuracy. A discrete model was obtained, in which the boundary nodes have the same order of approximation of the error with the inner nodes (Cisteacov, 2010, pg. 66-77).

The study of hydrodynamic and morphological processes taking place in the Karnaphuli Riverbed in Bangladesh is presented in the paper (Sarfaraz & Abdul, 2013, pp. 40-48) The mathematical model was developed based on the Navier-Stokes equations and the advection-dispersion equation. With the help of the Delft3D-FLOW program, the hydrodynamics, the morphological processes and the transport of pollutants in the mentioned riverbed were simulated. The model was calibrated and validated based on available data.

The modeling of the interactions of the "river-lake" systems by means of numerical models is presented in the paper (Tidenov, 2013). The mathematical model is described based on the Navier-Stokes system of equations and the equilibrium equation for salinity in the lake. The discretization of the studied field is performed based on the finite volume method. An iterative numerical algorithm was developed in order to determine the hydrodynamics and the temperature field and good results were obtained compared to the in situ data.

A method for solving Navier-Stokes equations based on finite differences for a compressible viscous fluid is discussed in the paper (Usov, 2008, pp. 464–476). The finite difference scheme proposed in the paper does not impose severe time constraints and is valid for structured networks, and the Navier-Stokes equations are divided into 3 systems of finite difference equations, which can be solved independently. The proposed method was tested on case studies on modeling hydrodynamics in small rivers in the Rostov region of Russia.

Based on the WASP6 system (Water Quality Analysis Simulation Program, Version 6.0), which is intended for dynamic modeling of aquatic ecosystems, a water quality simulation model has been developed for the Argazi-Miass-Şerşni water basin in Russia. The basic equation of the model is that of advection-dispersion:

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(U_x C) - \frac{\partial}{\partial y}(U_y C) - \frac{\partial}{\partial z}(U_z C) + \frac{\partial}{\partial x}\left(E_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(E_z \frac{\partial C}{\partial z}\right) + S_L + S_B + S_K$$

where *C* is the concentration of the water quality indicator; *t* - time, $U_x, U_y, U_z$ - speed of advection in the longitudinal, lateral and height direction; $E_x, E_y, E_z$ - longitudinal, lateral and vertical diffusion coefficients; $S_L$ - distributed loading speed; $S_B$- speed of filling the border layer; $S_K$ - speed of total kinetic transformation.

The researched object was divided into segments, the hydrodynamics of the studied sector being calculated using a module from WASP6 - DYNHYD5. Water quality was determined from the water concentration of the indicator substances, which are calculated for each segment. Boundary conditions include concentrations of water quality indices at the beginning of the modeling process (Iulaeva, Raznopolov, & Suharev, 2005, pp. 89-94).

## Solution Approach

An essential factor for the correct assessment of water quality, as well as the elaboration of pollution prediction scenarios, is the choice of the mathematical model and the simulation program appropriate to the studied aquatic ecosystem.

Most flows that occur in nature have a mixed character, an important component of which is turbulence. A turbulent flow can be seen as a nonstationary flow with a disordered structure. There are several definitions of turbulence, but all of them reflect only some of the properties of this complex phenomenon (McDonough, 2007).

The most essential characteristics of the turbulence phenomenon are the following: irregularity, diffusive character, large Reynolds number, three-dimensionality, dissipative character, independence from the nature of the fluid (Pope, 2003).

Flow in river systems is a turbulent flow, which is described using the Navier-Stokes equation system, composed of the Navier-Stokes equations (1) and the continuity equation (2).

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

$$\frac{\partial \rho}{\partial t} + \nabla(\rho\mathrm{v}) = 0, \qquad (2)$$

where $\nabla$ is the Hamilton operator; $\Delta$ - the Laplace operator; $t$ - time; $\nu$ - viscosity coefficient; $\rho$ - 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 (Temam, 1981).

The process by which the movement and scattering of the pollutant occurs is called dispersion. The mechanism of the mentioned process is very complex and can be explained by the simultaneous action of the molecular diffusion phenomenon of the polluting substance and the convection-advection phenomenon. 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 concentration. The phenomenon of dispersion is described with the help of the fundamental equation of advection-dispersion:

$$\frac{\partial C}{\partial t} + \frac{\partial (u_i C)}{\partial x_i} = D\frac{\partial^2 C}{\partial x_i^2}, \qquad (3)$$

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

In order to model different fluid flow processes, including turbulent flow, and to determine flow parameters, *computational fluid dynamics analysis* (CFD) has been widely used lately, using approximate numerical calculation techniques. The advantage of using CFD is the ability to obtain detailed and highly accurate information about the simulated system.

Solving a problem with the help of CFD involves completing the following steps: modeling the geometry of the studied field, discretizing the domain, defining the model, setting properties, establishing initial and limit conditions, solving, analyzing the results (Wilcox, 1994), (Launder, 1974, vol. 3, Issue 2).

Solving by applying CFD involves solving numerical flow equations. Dynamic simulation software techniques are used for this, for example, WASP (Water Quality Analysis Simulation Program), QUAL2E, ANSYS CFX (Computational Fluid Dynamics Software), GWLF (Generalized Watershed Loading Function), MONERIS (Modeling Nutrient Emissions in River Systems), WQRRS (Water Quality for River Reservoir Systems), WMS (Watershed Modeling System), SMS (Surface-water Modeling System), etc. (Marusic, 2013).

The proof of the efficiency of the mentioned methodology regarding the combination of the mathematical and numerical modeling of the studied aquatic ecosystems also results from the results disseminated through scientific papers, a short presentation that follows.

The problem of mathematical modeling of the dispersion of pollutants in the Danube river is discussed in the paper [1]. Numerical modeling of pollutant dispersion was performed using the FlexPDE program. This program is used to solve partial differential equations by the finite element method. The simulations were performed on a sector of the river with a length of 143 km and a width of 0.5 km. The obtained results allow the evaluation of the degree of river pollution (Andrei, 2011).

The SOBEK Rural 1D, 2D program was used in the *Research Report on the Management of Aquatic Ecosystems and Water Resources under multiple stress for the elaboration of hydrological scenarios on risk and flood risk assessment*, and the AQUATOX 3.1 model was used to assess pollution stress of the aquatic ecosystems of the Danube Delta. The AHP (Analytical Hierarchy Process) model was used to evaluate the water quality of the lakes. (http://ddni.ro/wps/wp-content/uploads/2017/11/RST_Faza-II_2015.pdf).

The hydrographic basin of the Prut River is a special geographical and geopolitical importance. The current state of research on the water quality of the Prut River is presented in the paper [27]. A thorough analysis of the bibliography on the water quality of the Prut River was performed and argued the need to develop mathematical models for determining and predicting water quality for river systems. A case study is also presented to determine the dispersion of the pollutant for a sector of the Prut River in Ungheni, which was loaded with water polluted with petroleum products from its tributary Delia River (Marusic & Ciufudean, 2013, pp. 177 – 180).

Mathematical and numerical modeling of the transport and dispersion of pollutants on some sectors of the Prut River have been carried out in a series of works. The hydrodynamics of the river were modeled using the Navier-Stokes system of Reynolds equations. At the base of the pollutant dispersion modeling process is the two-dimensional shape of the fundamental advection-dispersion equation, applied to turbulent flow. The problem of water pollution with copper products is examined in the paper (Marusic & Moraru, 2012, pp. 86-98). For the case study, a sector of the Prut River from the locality of Ungheni was chosen, given the fact that at that time the CMA exceeded the copper products in that sector. The simulations were performed using the SMS program, in dynamic mode. It was found that the transport of pollutants becomes stationary after 5 hours and 30 minutes from the moment of confluence with water (Marusic & Moraru, 2012, pp. 86-98).

The problem of mathematical modeling and numerical simulation of the fluorine dispersion process in river systems is presented in the paper (Marusic, Sandu, & Filote, 2015, pp. 503-506). Fluoride has a special role for human health, being a chemical element necessary for the proper development of teeth and skeletal bones, but human health depends on an optimal amount of fluoride. It presents the negative effects of fluoride on the human body and the results of numerical simulations obtained using SMS software (Marusic, Sandu, & Filote, 2015, pp. 503-506).

The problem of iron water pollution was studied in the paper (Marusic, Filote, & Ciufudean, 2012, pp. 95-98), elucidating the consequences of using iron polluted water for human health, developed the mathematical model of hydrodynamics and iron dispersion for river aquatic systems, based on which models were generated for a sector of the Prut River in the city of Ungheni (Marusic, Filote, & Ciufudean, 2012, pp. 95-98).

## Analysis of Results

Based on the above, we find that in order to obtain a model suitable for the real system, it is necessary to know deeply the ecological system and the processes subject to modeling, based on which we will be able to solve the following problems:

- elaboration of the conceptual and numerical model of the hydrodynamics and water quality of the studied river system;
- practical implementation of the models obtained in water quality management.

The mathematical and numerical modeling of the spatio-temporal evolution of the river type systems in order to estimate the water quality parameters represents a decisive factor in determining the water quality with a higher accuracy. Rivers are a complex aquatic system, so their modeling requires a detailed study for each case. The theoretical basis for the mathematical modeling of water quality in river-type systems is the Navier-Stokes differential equation system and the advection-dispersion equation, and in some cases, the mathematical modeling of water quality in river-type systems can be done using Streeter-Phelps and Saint-Venant equations. The best results for determining water quality are obtained by combining GIS technologies, mathematical models, databases, and various packages of specialized programs. The generation of numerical models based on mathematical models is an important tool in water quality prediction and management.

## Conclusions

The paper analyzed different methods and techniques for determining water quality parameters, including determining the spatio-temporal evolution of pollutants in river-type aquatic ecosystems. To solve this problem, it is necessary to use the effort of specialists in several fields, such as mathematics, computer science, chemistry, biology, etc. A considerable contribution lately is the digital solutions, especially the combination of mathematical modeling and Computational Fluid Dynamics (CFD), in order to obtain numerical models on the phenomena addressed.

Following the analysis of the aspects regarding the mathematical and numerical modeling of the river type systems in order to determine the spatio-temporal evolution of the pollutants, it was established that the water flow in the river type systems represents a turbulent flow, which is described using the Navier-Stokes equation system in the form of Reynolds. For the description of the pollutant concentration field, the fundamental advection-dispersion equation is used. In order to obtain numerical models on the hydrodynamics and dispersion of pollutants in the studied river sectors, different packages of specialized programs are applied. This successful approach can and will be applied to determine the spatio-temporal evolution of pollutants in the Danube River basin ecosystems, as well as the prediction of pollution scenarios. The results of the application will be disseminated in the following works.

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