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DIGITAL TECHNIQUES FOR WATER POLLUTION CONTROL

Nina Sava*, ORCID ID: 0000-0001-6827-2721,
Galina Marusic, ORCID ID: 0000-0002-2984-2055

Technical University of Moldova, 168, Stefan cel Mare bd., Chisinau, Republic of Moldova
*Corresponding author: Nina Sava, *nina.sava@ati.utm.md*

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Abstract. This paper is a detailed description and analysis of the most popular techniques digital for water quality control nowadays. It is illustrated how these techniques can be applied to solve problems that have arisen as a result of water pollution of aquatic ecosystems in different countries of the world. The advantages and disadvantages of using dynamic simulation software tools are presented and are based on an analysis of their operation. For each software product are highlighted the water quality parameters that can be simulated. It also presents the analysis of software products regarding the type of simulated aquatic ecosystem, as well as spatiotemporal modelling. The realization of these techniques is based on mathematical models. The development of digital techniques at the regional level may take into account certain characteristics specific to a particular aquatic ecosystem. The models can only cover a limited number of pollutants. In the process of selecting the parameters for the model, pollutants must be chosen which are a concern in themselves and which would also represent a wider set of substances that cannot be modelled in detail. Although the digital techniques examined to provide a particularly accurate estimate of water quality, the behaviour of pollutants in aquatic ecosystems remains an area of active and current research.

Keywords: *pollutants, river, simulation model, software package, water quality.*

Introduction

Water resources are an important source for the existence of everything alive. Ensuring water quality has been and remains the main priority of any society.

Currently, however, there is a continuous degradation of aquatic ecosystems in most regions of the globe, water quality is increasingly influenced by pollution with various chemicals, physical and biological substances. The problem of water pollution is also typical for the main rivers of the Republic of Moldova.

Awareness regarding the toxicity and environmental behaviour of chemicals could help to reduce or even avoid the side effects that these substances may produce [1].

To solve the problems of analysis and control of water quality, it is necessary to perform the processing of a large volume of information about physical, chemical and biological parameters. Achieving high-precision results in an acceptable period of time requires the application of mathematical methods and computers.

This knowledge is fundamental for the development of solutions to ensure the possibility of developing scenarios for predicting the pollution of aquatic ecosystems of the "river" type [1].

Various digital techniques have been applied to control water pollution lately, the application of which is an effective method in determining the spatiotemporal evolution of pollutants [1].

Various dynamic simulation software tools can be used to model the spatiotemporal evolution of contaminants in “river” aquatic ecosystems. Such software is already made by many US companies, such as Atlantic Ecology Division, Office of Research and Development (AQUATOX program), US Environmental Protection Agency (WASP, QUAL2E programs), ANSYS company from Canonsburg, Pennsylvania, USA (ANSYS CFX program), MapTech Company in Blacksburg, Virginia, USA (GWLF program), Institute of Freshwater Ecology and Inland Fisheries, Berlin, Germany (MONERIS program), Aquaveo company in the USA (WMS, SMS programs), US Army Hydrologic Engineering Centre (WQRRS program), etc. [2].

1. Problem formulation

"River" type aquatic systems are an important source of drinking water, so their pollution poses a risk to human health. The flow in the mentioned systems represents a turbulent flow, being a complex phenomenon, characterized by the variation in time and space of the local speeds, the irregular trajectory, and the intersection of the current lines of the water particles.

Pollutant dispersion and transport processes are also complex processes. The dispersion of pollutants is the result of the simultaneous action of a phenomenon of molecular diffusion of the polluting substance with a convection-advection phenomenon, due to the existence of a velocity field in the field in which the pollution takes place. The concentration of the pollutant in the water is influenced by the nature of the porous medium, the flow regime, as well as by the nature of the pollutant.

Due to the complexity of the phenomena that occur in aquatic ecosystems, the analytical solution of turbulent flow problems, as well as the determination of the field of pollutant concentrations, is quite complicated. Therefore, it is very important to collaborate with experts in different fields, especially: chemistry, physics, biology, hydrology, mathematics, and computer science. A considerable contribution in solving the problems related to the determination of water quality, as well as the elaboration of scenarios for predicting water pollution, belongs to the specialists in the field of applied informatics.

Proceeding from the above, the problem of analyzing digital techniques for determining the spatiotemporal evolution of pollutants was formulated.

2. Solutions

The use of models or software packages has highlighted many previously unresolved scientific issues. This is a particularly flexible tool to adapt to other conditions through modification and improvement. With their help, it is possible to reconstruct and perform simulations of the processes to which chemical compounds have been subjected in the past, also to predict the future cycle of chemicals through different ecosystems both globally and regionally and for different time intervals [4].

AQUATOX – simulation model for aquatic systems. AQUATOX predicts the fate of various pollutants, such as nutrients and organic chemicals, and their effects on the ecosystem, including fish, invertebrates, and aquatic plants [5].

The AQUATOX model has been used successfully to quantify the impacts induced by insecticides on ecosystem services provided by a lake from toxicity data for organism-level targets. The simulations showed how exposure to an insecticide could affect aquatic species populations (eg, abundance of recreational fish) and environmental properties (eg, water clarity) which in turn would affect the delivery of ecosystem services [6].

Using the AQUATOX-EFDC model, a short-term environmental impact was assessed for scenarios of 30-30,000 kg of toluene runoff in South Korea's Jeonju River. The result of the AQUATOX-EFDC simulation showed a significant ecological impact, finding that in the scenario in which 3000 kg of toluene were leaked for one day, a substantial change was expected in the range 0-640 m from the accident site. Besides, for a leak of 30,000 kg, a substantial change was expected in the range 0–2300 m from the site of the accident, and the greatest damage was observed for the group of fish species, the apex predators [7].

WASP – a program for simulating water quality analysis, being an improvement of the original WASP (Di Toro et al., 1983; Connolly and Winfield, 1984; Ambrose, R.B. et al., 1988). This model helps users to interpret and predict responses to water quality, natural phenomena, and man-made pollution for various pollution management decisions. It is a dynamic compartment modeling program for aquatic systems, including both the water column and the underlying benthos [8].

It allows the user to investigate 1, 2, and 3 dimensional systems and a variety of types of pollutants. It is one of the most widely used water quality models in the United States and around the world. It might be connected with hydrodynamic models and river basins, which allows multi-annual analyses in various weather and environmental conditions. It has been applied to all major estuaries in Florida [8].

The Water Quality Analysis (WASP) simulation program was used to simulate nutrients, dissolved oxygen (DO), and chlorophyll dynamics in the Shenandoah River Basin, Virginia. The results of a sensitivity test show that the model error decreases with increasing model complexity and sensitivity. The model predicted DO values that tended to be close to the measured data, while total nitrogen and phosphorus tended to be overemphasized. The results highlight the importance of temperature, flow, and speed in influencing water quality between seasons and levels on different sections of the river basin [9].

CE-QUAL-W2 – a two-dimensional, longitudinal/vertical, hydrodynamic, and water quality model. Because the model assumes lateral homogeneity, it is best suited for relatively long and narrow water bodies with longitudinal and vertical water quality gradients. The model has been applied to rivers, lakes, reservoirs, and estuaries [10].

The CE-QUAL-W2 model was evaluated using Xiaxi River data collected in 2007 and 2008. The model results show that CE-QUAL-W2 can predict the total Hg and methylmercury concentrations observed for the Xiaxi River. This application also demonstrated the ability of the CE-QUAL-W2 model in predicting the complex transport and cycling of Hg species in water bodies [11].

As the total dissolved solids (TDS) in the Tigris River in Baghdad and downstream cities can reach 1000 mg / L exceeding both drinking water and irrigation lines, a hydrodynamic and water quality model has been developed, CE- QUAL-W2, of the river. A sensitivity study suggested that an increase in river flow upstream by 15% results in a decrease of about 5% in TDS concentration. It was recommended to maintain an average annual flow in the Tigris River in Baghdad above 420 m^3 / s to keep the total dissolved solids concentration below 500 mg / L and to strictly control the flows through Lake Tharthar and the return flows of irrigation in the main trunk of the river Tigris [12].

The two-dimensional model (CE-QUAL-W2) was used to model water quality in a reservoir of Uiam Lake in Korea that receives nutrients from both non-point and point sources. The result of the scenario simulations showed that reducing the P of the STP effluent from 0.9 mg / L to 0.1 mg / L would effectively reduce the chlorophyll concentration in the lake by 62%. The effect of phosphorus loading can have quite different effects on phytoplankton growth depending on the runoff pattern and the hydrological characteristics of the receiving water bodies [13].

Ansys CFX – industry-leading fluid dynamics calculation software for turbomachine applications. It is known for its accuracy, robustness, and outstanding speed. It is easy to use, but extremely powerful and precise for applications such as pumps, fans, compressors, and gas and hydraulic turbines [14].

Ansys CFX 17.1 and the Telemac 3D Solver were used to show how two different numerical codes simulate the propagation of turbidity currents. It is known that turbidity currents can be a relevant lever to manage the accumulation of fine sediments in tanks. The simulations were performed on two configurations. The first case concerns the modeling of the sinking of a turbidity current. The second model consisted of testing the turbidity current ventilation as a solution for managing the sedimentation of the tank. The advantages and limitations of both approaches are discussed to provide guidelines for modeling turbidity currents in real tanks [15].

QUAL2K (or Q2K) – a water quality model for rivers and streams that are intended to be a modernized version of the QUAL2E (or Q2E) model (Brown and Barnwell 1987). Q2K is similar to Q2E in the following aspects: one-dimensional, the channel is well mixed vertically and laterally [16].

Simulation of water quality parameters of the Dez River in Iran (electrical conductivity, dissolved oxygen, carbon dioxide oxygen demand, NH4-N, NO3-N, and pH) were assessed using the water quality model (Qual2k). The data observed in July 2012 and March 2013 were used for the calibration and validation of the Qual2k model, respectively. The water quality index was assessed over a period of 8 years in terms of industry growth and drought. The calculated water quality index in Iran showed values of 70,1−85. In conclusion, the Qual2k model has been proposed as an appropriate tool for future water quality assessment and forecasting [17].

To propose nitrogen pollution control strategies in a sparsely populated stream in Shixi Creek, southeast China, a simulation-optimization approach based on the QUAL2K model has been developed. The model showed good agreement with field observations from 22 sampling sites sampled between March 2017 and February 2019, with a normalized objective function (NOF) of less than 0,360. For more than 80% of the surface in Shixi Creek to meet the grade III water quality standard, an optimized approach is to reduce more than 55% of N pollution due to point source and 10% of nonpoint point source pollution [18].

GWLF – is a model for predicting the loading of the river basin of medium level, developed to evaluate the nonpoint source flow and the loading of sediments and nutrients from urban and rural river basins. The model offers the ability to simulate runoff, sediment, and nutrient loads (N and P) from a river basin considering areas of varying sizes (eg agricultural, forested, and developed land). It is a continuous simulation model, which uses daily time steps for weather data and water balance calculations [19].

The improved model of generalized river basin loading functions (GWLF-E) has been used to simulate water budgeting, field erosion, and stream erosion along a gradient of agricultural to urban land cover from 1997 to 2015 in the Indian Mill Creek watershed in Michigan, USA. The results showed that GWLF-E could have overestimated the discharge into sub-pools. Evaluation with current strip erosion data found that GWLF-E may have difficulty capturing the complexity of erosion rates, including cases where sediment is deposited on current banks from upstream sources and underestimates current bank erosion in hydrographic basins, sometimes over an order of magnitude [20].

The RGWLF river basin model, which is coupled with a widely recognized multi-objective optimization algorithm and the non-dominant genetic sorting algorithm II (NSGAII), was applied in the Luanhe river basin to search for spatial BMPs (Best Management Practices) for dissolved nitrogen (DisN). The results indicated that at a minimum cost of 9,09 × 107 yuan, the DisN load is 3,1 × 107 kg, and at a maximum cost of 1,77 × 108 yuan, the total dissolved nitrogen load is 1,31 × 107 kg; with the scenario without measures, the DisN load is 4,05 × 107 kg [21].

MONERIS – a model that calculates nitrogen and phosphorus emissions into surface water, in different ways, as well as flow retention in the surface water network.

The application of the MONERIS approach (modeling of nutrient emissions in RIver systems) has been successful in modeling nutrient inputs from the Danube basin. It is a semi-static emission model for point and diffuse nutrient sources that can also be adapted to cope with heavy metals and priority substances (eg lindane) [22].

Modeling studies (MONERIS) allowed the calculation of nitrogen (N) and phosphorus (P) emissions in the Vistula and Oder basins (Poland) and facilitated the estimation of N and P retention in these basins in 1995-2015. The increase of 5,3 times and 3,5 times of N and P emissions in the Oder basin, with the maximum (135,000 tons N year - 1; 14,000 tons P year - 1) observed at the beginning of 1980/1990 was due to population growth and the intensification of agriculture. Pro-ecological activities during the economic transition period (since 1989) have covered various sectors of the economy, including agriculture, environmental protection, for example, the construction of a large number of wastewater treatment plants. Consequently, in 1985-2015, the emission in the Oder basin decreased from the above-mentioned maximums to 94,000 tonnes N year - 1 and to 5,000 tonnes P year - 1, while in 1995-2015, the emission in the Vistula basin decreased from 170,000 to 140,000 tons N year - 1 and from 14,200 to 10,600 tons P year - 1 [23].

WMS – a graphical system for simulating hydrographic and hydraulic basins in two-dimensional space. It can be used to model both the quantity and quality of water. WMS was developed in the early 1990s at Brigham Young University, USA [2].

SMS – a software package for surface water modeling. It was developed by US experts from Aquaveo Company. It can solve dynamic and static problems. It is widely used in process simulation in "river" type water systems, as it manages the entire modeling process: from importing topographic and hydrodynamic data to visualizing and analyzing solutions. The modeling process includes river hydrodynamics, rural and urban flooding, wave modeling, following the dynamics and physical properties of water particles, determination, and analysis of pollutants [3].

To identify tidal characteristics and currents in Lemong waters, Lampung province, as parameters for coastal protection planning, the analysis of current and tide by numerical modeling was performed on the RMA2 module of the Surface Water Modelling System (SMS) software. The modeling was performed using the online nesting method, with four levels of network resolution with the highest resolution at 1 x 1 km^2 near the waters of Lemong beach. The modeling results show that the tide in the Lemong Beach area reaches 1,4 m with a dominant mixed semi-diurnal type. The model also shows that the current pattern in Lemong Beach waters moves predominantly southeastward during flows and northwestward during ebb [24].

WQRRS – a model developed by the United States Army Corps of Engineers, simulates DO, total dissolved solids, P, NH_3, NO_2-, NO_3-, alkalinity, total carbon, organic components and a range of aquatic biota, including plankton, algae, bacteria coliforms, and several species of fish. It shapes the hydrodynamic shape, determines depths and speeds [3].

The water quality of Lake LaFarge, Wisconsin, was investigated using a reservoir version of the Ecological Water Quality for River Systems (WQRRS) model. The study focused on concentrations of temperature, dissolved oxygen, and algae. The tests indicated that, in essence, all the nitrogen and soluble phosphorus in the river were in available forms for algae growth and that phosphorus was most likely the limiting nutrient in the proposed network. The simulations indicated that Lake LaFarge will probably be thermally stratified from May to September [25].

There are different systems for modeling the transport of pollutants in rivers. These include complete hydrodynamic models implemented in MIKE11 (DHI Water & Environment), InfoWorks-RS (Innovyze), and HEC-RAS (USA), and conceptual tank-type models [26].

MIKE 11 – a professional engineering software package for simulating flows, water quality, and sediment transport in estuaries, rivers, irrigation systems, canals, and other water bodies. It is a one-dimensional, easy-to-use, fully dynamic modeling tool for detailed analysis, design, management, and operation of both simple and complex river and canal systems [27].

The MIKE 11 NAM conceptual hydrological approach was used to develop a leak simulation model for the Arpasub Basin in the Seonath River Basin in Chhattisgarh, India. The results of calibration and validation show that this model can define the process of drainage of precipitation from the basin and thus predict the daily flow [28].

The analysis of the sensitivity of the roughness coefficient of Manning, n on the water level of the Delta Mahanadi rivers was performed with the help of the one-dimensional hydraulic modeling package MIKE11. The results showed that the model is sensitive to the roughness coefficient. The value "n" increases with the growth of the stage [29].

InfoWorks ICM (Integrated Catchment Modelling) – the first-ever software platform on the market for complete and truly integrated 1D / 2D hydrodynamic modeling of both rivers and sewage systems [30].

The InfoWorks Integrated Catchment Modeling (ICM) model was used to simulate hydrographs at the outlet of a basin (drainage area 8.3 ha, with 95% permeable areas) in Shenzhen, China. The model incorporating the direction of the quasi-linear double reservoir has been shown to have a greater effect on simulated hydrographs for precipitation events with greater depths and longer durations than the US EPA's nonlinear reservoir steering method [31].

To optimize the locations of water quality storage tanks, a new design strategy was proposed using the InfoWorks ICM model. Thus, its application in the design of decentralized storage tank locations in Fuzhou, China, has shown that the proposed strategy can reduce the total volume of decentralized storage tanks to 0.38 times that of a terminal tank [32].

The need to monitor and map floods has become a mandatory cause of their negative impact on natural resources. In L'Île-Bouchard, this phenomenon occurs frequently, and people living in the flood-prone areas of the Vienne are extremely vulnerable to floods. An analysis of the flood hazard map and the risk map of a river sector for the Vienne river that crosses this commune was made using the InfoWorks ICM software and ArcMap. The results indicated that the model can simulate the actual depth of flooding so that flood hazard maps and flood risk maps were developed [33].

HEC-RAS – software that allows the user to perform a constant one-dimensional flow, non-uniform flow calculations in one and two dimensions, sediment transport / mobile bed calculations, and water temperature/water quality modeling [34].

A numerical model of water quality (HEC-RAS) was developed to simulate the carbonaceous biochemical oxygen demand (CBOD) and dissolved oxygen (DO), in a selected area extended to approximately 25 km in the Diyala River and 22 km in the river Tiger.

The results showed that the Diyala River was polluted in the region downstream of the Al-Rustimiya wastewater treatment plants (treatment plants) with CBOD values ranging from 18 to 25 mg / L and DO ranging from 1 to 3,1 mg / L for the wet season and dry seasons.

While for the Tigris River, CBOD values decreased from 17 to 18,1 mg / L in the dry season and from 3 to 5 mg / L in the wet season [35].

The HEC-RAS model was used to analyze the cleaning of a bridge on the Kabul River near Peshawar, Pakistan. The results showed that the square pillars resulted in a greater cleaning depth compared to the circular pillars. The same trend was observed in the case of hole sizes. A comparison of the experimental results with the hydraulic software (HEC-RAS) showed that they subsequently gave slightly higher cleaning depth values under similar conditions. But this difference decreased with increasing discharge [36].

TLM – the transmission line matrix model can be used to predict the spatiotemporal evolution of a pollutant in natural flows for effective and rapid decision making in case of emergency [37].

All software tools analyzed in this paper have several advantages, but also disadvantages that are presented in Table 1.

Table 1

Advantages and disadvantages of dynamic simulation software tools

Advantages	Disadvantages
They allow the investigation of 1, 2, and 3 dimensional systems and a variety of types of pollutants	Model building and implementation of dynamic simulation software tools requires in-depth knowledge in the field of mathematics and information technology

Continuation Table 1

Ensures the modelling of both the quantity and quality of water	Simulation modeling and analysis can be time-consuming
They are characterized by multiple functions (eg AQUATOX)	Simulation software vendors have developed many packages that contain templates that require only inputs, ie only templates
Have the ability to calculate the two-dimensional velocity field for narrow systems that are stratified (eg CE-QUAL-W2)	The results of the simulation can sometimes be difficult to interpret
They have a high degree of accuracy, robustness and outstanding speed, are easy to use (eg Ansys CFX, MIKE 11, etc.)	

It also differs according to the number of simulated water quality parameters, information that is represented in Figure 1. From the diagram can be noticed that the WQRRS model allows the simulation of the largest number of water quality parameters.

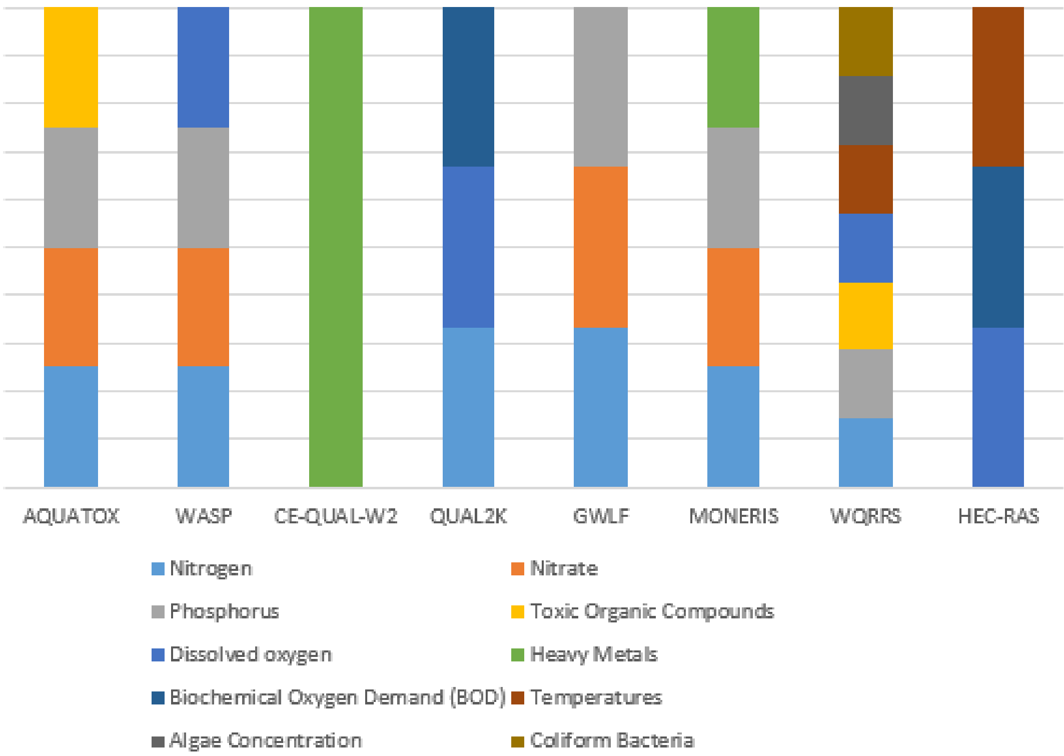

Figure 1. Comparative analysis of software tools for dynamic simulation of water quality parameters.

Another difference is the way it manages the spatial and temporal dimensions for example the SMS and InfoWorks ICM software packages, as well as the way it models the transport processes of the Ansys CFX, WMS, MIKE 11, and TLM software packages.

Thus, following the analysis performed on the use of different software tools for dynamic simulation of aquatic ecosystems, can be observed that not all models can be applied in all conditions.

Conclusions

An analysis of digital water pollution control techniques was performed. A comparative analysis of software tools was performed based on the number of model parameters, which allowed us to find that those software tools that model a larger number of parameters are more complex, i.e. include a larger number of functionalities. Another important element in the analysis process was the degree of complexity of the analyzed aquatic ecosystems, so the simulations for each aquatic ecosystem require different specific software tools. Of major importance in the process of using digital techniques to control water pollution are both spatial and temporal details.

The advantages and disadvantages of the analyzed digital techniques were determined. It has been established that not all products analyzed can be applied under all conditions.

Mathematical and numerical modelling of aquatic systems is applied both in the pre-design stage and in the practical use process.

It has been found that digital techniques are a powerful tool for determining water quality, as well as developing scenarios for predicting water pollution.

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