STUDY ON NUMERICAL MODELING OF WATER QUALITY IN „RIVER-TYPE” SYSTEMS

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INTRODUCTION

Water from rivers is used in most fields of human activities, so water quality maintenance is a global problem. It is monitored by the Water Framework Directive 2000/60/EC (Amended by Directive 2008/32/EC), approved by the European Commission, stating that by 2015 it is necessary to provide the state "*very good*" for all Water Bodies [1].

Lately, information systems have been widely used for assessing processes that occur in “*river-type*” systems and determining water quality. These systems consist of two main components: mathematical models and software packages [2].

A study on mathematical modelling of water quality in aquatic systems of "*river-type*" is presented in [3].

There is now a wide range of software packages used to model the environment, which can be classified into 3 types: based on spreadsheets, based on solving equations and based on dynamic simulation [4].

The purpose of this paper is the analysis of software packages and the study on numerical simulation of water quality in "*river-type*" systems.

1. SOFTWARE FOR NUMERICAL MODELING

Some packages based on spreadsheets include: Excel®, Quattro® Pro[7] and Lotus®[8]. They have incorporated a wide range of mathematical, statistical and logical functions. Also, they contain a lot of options for storing, keeping and sorting data, plotting, analyzing and exporting data. However, the above packages do not contain advanced mathematical functions and numerical procedures and are not able to perform the operations of differentiation and integration [4].

For environmental modelling, mathematical packages are used, such as Mathcad®, Mathematica®, MATLAB®, and TK Solver. These arrays have incorporated operating functions, complex numbers, animation, interpolation and numerical procedures. Not all listed packages have drawing tools, but they have the ability to import graphical format from other applications [4, 5, 6].

Lately, for modelling environmental systems, dynamic simulation packages have been used, such as Extend™[9], ithink®[10], Simulink®[11], ANSYS CFX, WASP (Water Analysis Simulation Program), CE-QUAL-W2, WMS (Watershed Modelling System), AGNPS (Agricultural Non-Point Source Pollution), GWLF (Generalised Watershed Loading Function), MONERIS (Modelling Nutrient Emissions in River Systems), QUAL2E, WQRRS (Water Quality for River Reservoir Systems), SMS (Surface - Water Modelling System), etc.

Extend™[9], ithink®[10], and Simulink®[11] have a flow GUI and support modelling linear and nonlinear systems in continuous or discrete time. The main features of these packages are animation, customizable GUI, sensitivity analysis and optimization. The downside is that they do not automatically maintain dimensional consistency [7].

ANSYS CFX is a program of finite element analysis. It is used for simulation in engineering, such as fluid flow calculation, electronic and electromagnetic optimization. It was used for numerical simulation of pollutant dispersion in rivers Argeş and Dâmboviţa in Romania. The pollutants dispersion discharged from the two points on the surface was simulated. The obtained numerical models allow tracking pollutants concentration in time and space and distance estimation of the polluted river [8].

A water quality model was developed for water basin "*Argazi - Miass - Shershni*" in Russia. WASP6 dynamic simulation program was used, developed by the Environmental Protection Agency of USA. It is designed for the analysis and prediction of water quality in various sources of surface water supply. This program incorporates two special submodules: TOXI, for modelling, taking into consideration toxic substances and EUTRO, for modelling water quality by standard indicators. Mathematical apparatus of WASP6 contains 171 equations. The program allows choosing equations used for modelling, depending on model objects, input data available and established boundary conditions. The obtained model allows analyzing the actual situation, predicting changes and taking decisions for an appropriate management [9].

The results of hydrodynamics and water quality modelling for river Severnaia Sosiva from Russia is presented in [10]. It was developed a modelling system, the nucleus of which is the numerical simulation program of water quality, CE-QUAL-W2. This program was developed by the U.S. Army Corp of Engineers. A 3-D model of the studied sector was made by means of ArcGIS program. Based on data from hydrological stations Sosiva and Sartini, a database was developed with the following modules: Meteorology, Hydrology and Hydrochemistry. The obtained model calculates water quality parameters [10].

A water quality monitoring system was developed for the river Neva in Russia. The main components of the system are: the mapping of the river studied sector, "*Neva*" database, simulation model of the pollutants dispersion. The mapping was developed with ArcInfo version 9.1 program, which has been connected to "Neva" database. The numerical simulation model was developed based on the "*Ghidroecoprognoz*" version 2.97.001. The obtained results allowed state estimation of the water system in real-time, with the condition of changing various modelling parameters [11].

An information system was developed for Teleczkoe water basin and the estuary sector of the river Chiulyshman from Russia. The hydrodynamic and water quality model was developed. The developed system contains three modules: WMS basin modelling system, 3.5 version of the model CE-QUAL-W2, the database. The database is composed of lake bathymetry, the relief of the shore, meteorology, hydrology, water quality parameters [12].

The AGNPS program is very useful for forecasting loading basins with nutrients from agricultural sources and forecasting water quality. It was developed by the Research Center for Agriculture and Natural Resources Center USA [13, 14].

The evaluation of nitrogen and phosphorus emissions in surface waters is done using GWLF program. It was applied to the Cannonsville watershed in the USA. The model provides reasonable estimations of monthly flow and nutrient and sediment loading. This program was successfully applied for modelling nutrient export in Choptank River Basin on the coastal plain of the Chesapeakedrainage [15, 16].

MONERIS program is widely used for assessing watershed loading with nitrogen and phosphorus from point and diffuse sources. For example, it was used to assess nutrient and pollutant loading for the German part of the Elbe River basin [17] and for nutrient emissions modelling in "*river-type*" systems [18].

In the United States, QUAL2E water quality model is widely used, which was developed by the United States Environmental Protection Agency (EPA) in 1998. QUAL2E simulates temperature, DO, BOD, chlorophyll, nitrogen (organic nitrogen, ammonia NH_3, and NO_3^- nitrate), organic and inorganic phosphorus and coliform bacteria [19].

Another model, WQRRS, developed by the United States Army Corps of Engineers, simulate DO, total dissolved solids, P, NH_3, NO_2^-, NO_3^-, alkalinity, total carbon, organic constituents, and a number of aquatic biota, including plankton, algae, coliform bacteria, and several species of fish. It models hydrodynamic shape, determines depths and speeds [19].

The disadvantage of the listed programs is that they do not fully support the modelling process, but depend on other programs and systems, including those related to topography and databases.

The most useful software package for modelling water quality in "*river-type*" systems is the SMS system, which is a software package for modelling surface waters. It was developed by the USA experts from Aquaveo Company. It can solve dynamic and static problems. It is widely used in simulating processes in “*river –type*” water systems, as it manages the entire modelling process: from importing topographic and hydrodynamic data up to visualizing and analyzing solutions. The modelling process includes river hydrodynamics, floods in rural and urban area, waves modelling, following the dynamics and physical properties of water particles, the determination and analysis of pollutant dispersion.

SMS program is often used to determine the concentration of pollutants field. This process is done in two steps: first, it is determined the hydrodynamics of the studied sector using the SMS module named RMA2, then the results are used as input data for the module RMA4, in order to determine the pollutant dispersion. The base module of RMA2is the system of Navier-Stokes equations in the form of Reynolds by Cartesian coordinates x and y (1), (2), together with the continuity equation (3) for incompressible fluid in turbulent motion of the free surface:

$$h\frac{\partial u}{\partial t}+hu\frac{\partial u}{\partial x}+hv\frac{\partial u}{\partial y}-\frac{h}{\rho}\left(E_{xx}\frac{\partial^2 u}{\partial x^2}+E_{xy}\frac{\partial^2 u}{\partial y^2}\right)+gh\left(\frac{\partial H}{\partial x}+\frac{\partial h}{\partial x}\right)+$$
$$+\frac{gun^2}{\left(h^{1/6}\right)^2}\times\left(u^2+v^2\right)^{1/2}-\varsigma V_a^2\sin\psi+2h\omega v\sin\varphi=0 \quad (1)$$

$$h\frac{\partial v}{\partial t}+hu\frac{\partial v}{\partial x}+hv\frac{\partial v}{\partial y}-\frac{h}{\rho}\left(E_{yx}\frac{\partial^2 v}{\partial x^2}+E_{yy}\frac{\partial^2 v}{\partial y^2}\right)+gh\left(\frac{\partial H}{\partial y}+\frac{\partial h}{\partial y}\right)+$$
$$+\frac{gvn^2}{\left(h^{1/6}\right)^2}\times\left(u^2+v^2\right)^{1/2}-\varsigma V_a^2\sin\omega+2h\omega v\sin\phi=0 \quad (2)$$

$$\frac{\partial h}{\partial t}+h\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)+u\frac{\partial h}{\partial x}+v\frac{\partial h}{\partial y}=0 \quad (3)$$

Where h is the water depth (m), u - local velocity in the x direction (m/s), v - the local velocity in the y direction (m/s), t - time (s), ρ - density of water (kg/m^3), g - gravity acceleration (m/s^2), E - coefficients of turbulent viscosity (Pa.s or kg / m / s), H - geodetic elevation of the riverbed (m), n - Manning's roughness coefficient, ζ - empirical coefficient on air friction, V_a - wind speed (m/s), ψ - wind direction (degrees counterclockwise from the positive x-axis), ω - angular velocity of rotation of the Earth (rad/s), φ - place latitude.

The base module of RMA4 is the two-dimensional form of the advection-dispersion equation ADE applied to the turbulent flow regime:

$$h\left(\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}-\frac{\partial}{\partial x}D_x\frac{\partial c}{\partial x}-\frac{\partial}{\partial y}D_y\frac{\partial c}{\partial y}-\sigma+kc+\frac{R(c)}{h}\right)=0 \quad (4)$$

Where c is the concentration of pollutant (mg/L), D_x and D_y - turbulent diffusion coefficients in the x and y, k - decay constant (s^{-1}), σ - the local term source of pollutant (unit measure of concentration/s), $R(c)$ - precipitation/evaporation (concentration unit x m/s) [20].

2. NUMERICAL SIMULATION USING SURFACE-WATER MODELING SYSTEM (SMS)

Case studies using SMS program are presented in [21, 22, 23, 24, 25].

An industrial water pollution coming from the textile factory was found for a sector of the river Olt, city of St. George, Romania. The problem of determining the spatio-temporal dispersion of pollutants for the mentioned sector was developed, which was solved using SMS program. Two chemical indicators were analyzed: BOD_5 and COD - Mn. Data were obtained on the lateral and longitudinal dispersion of pollutants coming from the treatment plant. It was found that the SMS package can be applied to a project aimed at wastewater treatment using fitotehnologia [21].

The SMS program was used to determine the spatio-temporal evolution of petroleum products for a sector of the Prut River, Costesti, Moldova. Simulations were performed on a real river section with a length of 2.4 km and 1.2 km wide. It was determined the hydrodynamics and the field evolution of pollutant concentrations in all the finite elements of the studied domain [22].

The dispersion of oil products depending on the time is shown in Fig. 1:

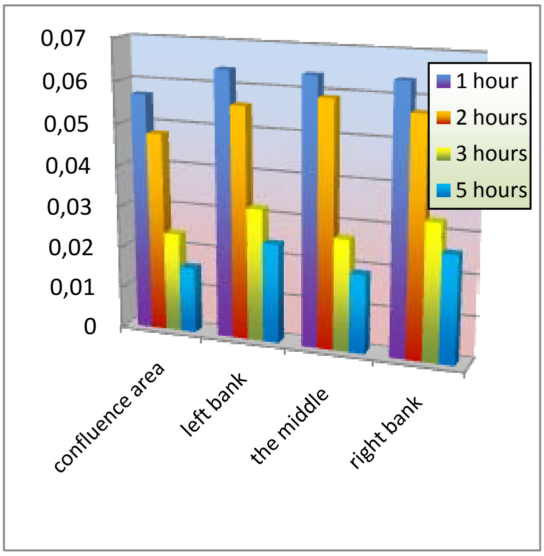

Figure 1. Temporal evolution of the concentration field of petroleum products.

The problem of dispersion modelling of chemical pollutants on a sector of the Prut River in the town Ungheni was made in August 2011, when the mentioned sector was polluted with copper compounds. To solve the problem, we used the SMS program. The simulation was carried out in dynamic way [23]. The dispersion of copper compounds was determined in all finite elements of the studied sector (Fig. 2).

The problem of mathematical modelling and numerical simulation of the process of fluoride dispersion in "*river-type*" systems is developed in [24]. The fluoride influence on the human body is being discussed. The problem was solved by using the SMS program. It was determined the fluoride dispersion for a sector of the Prut River [24]. Fig. 3 shows the temporal evolution of fluoride concentrations field.

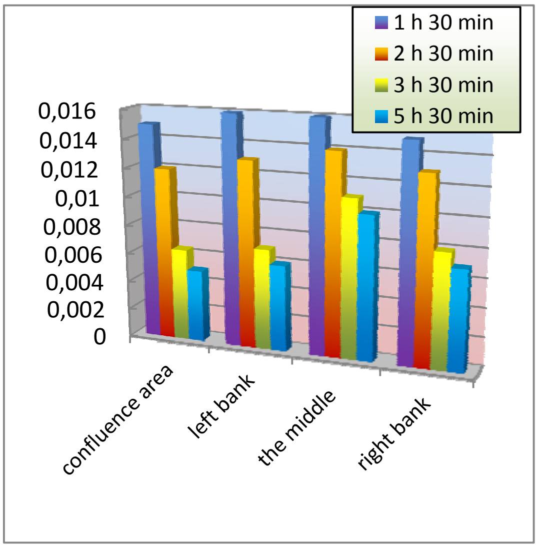

Figure 2. Temporal evolution of the concentration field of copper compounds.

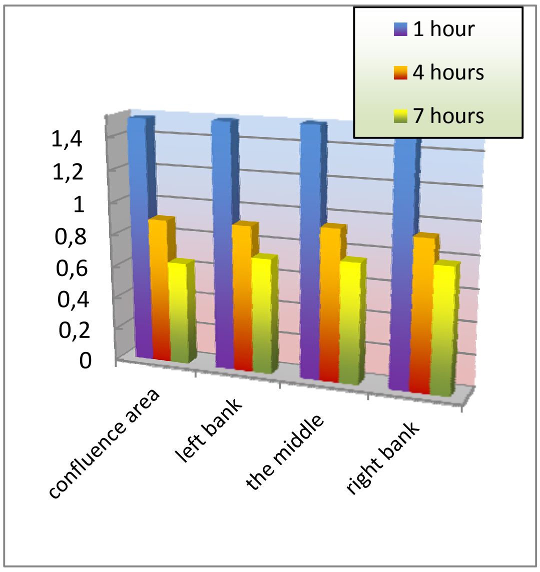

Figure 3. The temporal evolution of fluoride concentrations field.

The negative consequences of iron water pollution are discussed in [25]. The SMS software is used to determine the hydrodynamics and pollutant dispersion for a sector of the Prut River in the town Ungheni, Moldova. The iron dispersion at different time intervals from the moment with water confluence is shown in Fig. 4.

The obtained numerical model allows the determination of iron concentration field evolution in space and time throughout the studied sector.

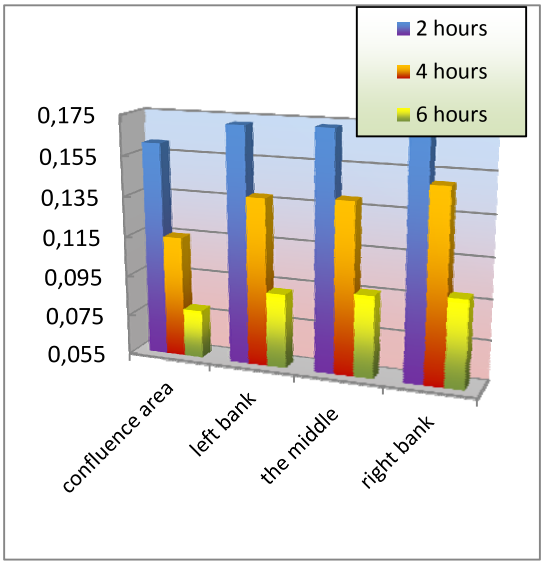

Figure 4. Temporal evolution of the iron concentrations field.

CONCLUSIONS

A review was conducted concerning the software packages used to assess water quality in "*river-type*" systems. It was found that the most optimal software is SMS (Surface-water Modelling System). This observation is argued by the fact that the mentioned system manages the entire modelling process and can be applied in dynamic or static regime.

Taking into consideration the case studies presented in other papers, it can be assumed that applying the mentioned package makes possible to track the spatio-temporal evolution of the pollutant dispersion in all the finite elements of studied sector. This will allow us to determine and forecast the correct water quality and predict pollution exceptional phenomena.

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