Modeling of Spacio-temporal Evolution of Fluoride Dispersion in "River-type" Systems

GALINA MARUSIC[1], ION SANDU[2*], VIOLETA VASILACHE[3], CONSTANTIN FILOTE[3], NINA SEVCENCO[4], MONICA-ANCA CRETU[2*]

[1] Technical University of Moldova, 168 Stefan cel Mare şi Sfant Blv., MD-2004, Chisinau, Republic of Moldova

[2] Al.I. Cuza" Univeristy of Iaşi, ARHEOINVEST Interdisciplinary Platform, 22 Carol I Blv., Corp G Demisol, 700506, Iasi, Romania

[3] "Stefan cel Mare" University of Suceava, 13 Universitatii Str., 720229, Suceava, Romania

[4] State University of Medicine and Pharmacy "Nicolae Testemitanu" of the Republic of Moldova, 165 Stefan cel Mare şi Sfant Blv., MD-2004, Chisinau, Republic of Moldova

This paper presents the modeling evolution of fluoride concentration in "river-type" systems. We discuss the fluoride influence on the human body, taking into consideration aspects of fluoride content in drinking water, deficiency and excess fluoride in the body and others. In order to determine the fluoride concentration, we study the problem of mathematical modeling of two-dimensional dispersion of the pollutant. It offers a case study of the Prut River, for which the numerical model of hydrodynamics and the dispersion of fluoride concentration on one sector of the river are applied. The Navier-Stokes equations in differential form Reynolds are used for modeling, as well as the continuity equation and the equation of the pollutants transport. The Surface-water Modeling System (SMS) v.11.0 was used to develop the numerical models. The results are useful for tracking changes in pollutant concentrations in space and time, in any finite element in the studied river sector (with or without sampling). This will allow greater accuracy in determining water quality.

Keywords: *fluoride, turbulent motion, Navier-Stokes equations, continuity equation, two-dimensional dispersion of pollutants*

The mathematical modeling of spatio-temporal evolution of "river-type" systems has an important role in predicting the behaviour of these systems. Knowing the concentration of the pollutant field distribution in time and space contributes significantly to the prediction of exceptional phenomena.

Fluoride has a special role for human health. This is an important chemical needed for proper development of teeth and skeletal bones [1-3], but human health depends on an optimum amount of fluoride. The lack of this element manifests itself by tooth decay and its excess leads to general intoxication of the body [4-5].

World Health Organization (WHO) has set an allowable limit of fluoride in drinking water of 1 mg/L [6]. In Moldova, the average content of fluoride in drinking water ranges from 0.14 to 0.7 mg/L [7].

Water pollution control in rivers, in most cases, is done through information systems for monitoring the environmental pollution levels in time and space, a main component involved in this approach is modeling and forecasting the state of the examined area [8].

In aquatic systems, pollutants are distributed through input fundamental processes, diffusion and advection. Mathematical models are used to predict their transport [9-10]. Choosing the mathematical model and appropriate simulation program will help to assess and forecast water quality.

Currently, there are various pollutant transport simulation programs for running water, for example: dynamic modeling packages - Extend, iThink, Simulink, which provides a graphical flow simulation, animation and sensitivity analysis; then, AGNPS (Agricultural Non-Point Source pollution), which is used to forecast the load of pollutants from diffuse agricultural sources; GWLF (Generalised Watershed Loading Function), used to assess nitrogen and phosphorus loads and MONERIS (Modelling Nutrient emissions in River Systems), which assesses nitrogen and phosphorus emissions in surface waters [11-12].

The advantage of these software packages is the ability to simulate pollutant dispersion in "river-type" systems, but the disadvantage is that they do not manage the whole process of modeling.

Surface-water Modeling System (SMS), which was designed by specialists of the Aquaveo Company USA, is very useful for effective management of the entire process of modeling surface water: from importing topographic and hydrodynamic data to visualization and solutions analysis (SMS Tutorials, 2011) [13].

The purpose of this paper is to develop the mathematical model of hydrodynamics and pollutant dispersion in "river-type" systems for determining the spatio-temporal evolution of fluoride on a sector of the River Prut, Ungheni (R. Moldova), using the SMS.

Experimental part

Material and methods

River hydrodynamics represents a turbulent flow, which is characterized by variation in time and space of local velocities, irregular trajectory and power lines intersecting the water particles. The physicist O. Reynolds, who demonstrated turbulent flow regime, proposed to add additional terms to the system of Navier-Stokes equation, which have more uniform stress due to turbulence [14, 24].

For water flow modeling on the Prut River study area, the system of Navier-Stokes equations as Reynolds (1) and (2) was used together with the continuity equation (3),

* *email: cretu_monika@yahoo.com; ion.sandu@yahoo.com*

which completely describe the dynamics of water in rivers in a turbulent regime:

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

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

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

In equations (1) - (3) h mean water depth (m), u - local velocity in the x direction (m/s), v - local speed in y direction (m/s), t - time (s), ρ - density of water (kg/m^3), g - gravitational acceleration (m/s^2), E - coefficients of turbulent viscosity (Pa.s or kg/m/s), H - share geodetic bed (m), n - Manning coefficient of roughness, ζ - empirical coefficient concerning the friction with air, 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 [15-16] (Surface Water RMA2, 2011).

Dynamic spread of pollutant in water depends on the nature of porous environment, the flow (the velocity field) and the nature of the pollutant. For mathematical modeling of pollutant transport, the advection-dispersion fundamental equation (ADE) is used, which is a partial differential equation, obtained by applying mass balance to a unit volume of mass in the river [17]. Pollutant dispersion model developed in this work is based on two-dimensional form of the ADE, applied to the turbulent flow regime [18-19]:

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

In equation (4) 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] (Surface Water RMA4, 2011).

Numerical models were developed using the Surface-water Modeling System (SMS) program v.10.1.11, which is a software package for efficient management of the entire process of modeling surface water: from the import of topographic and hydrodynamic data to visualization and solutions analysis.

The development of pollutant dispersion was conducted in two stages. At the first stage, the numerical model of water flow was generated in the program using the SMS Resource Management Associates (RMA) 2.

At the second stage, RMA4 module was applied to the resulting hydrodynamics from RMA2, which determined the field evolution of fluoride concentrations.

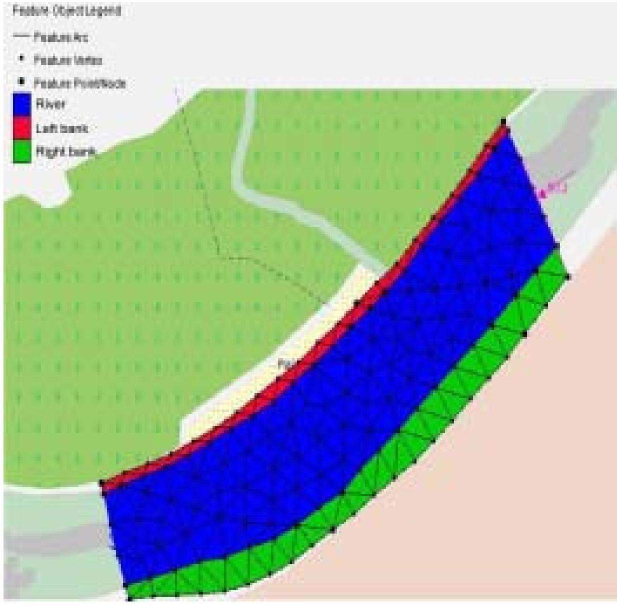

Fig. 1. 2D representation of the domain geometry

The digital image of the Prut River in the town Ungheni was imported into the SMS from www.maps.google.com, and directly digitized into SMS by manually creating objects with parameters such as points, arcs and polygons. On each arc there were created equal segments by redistributing points at an equal distance. Using these arcs, polygons were created and there were established three specific areas: the river, left bank and right bank (fig. 1).

The numerical model of water flow was developed using RMA2 program, which is a horizontal two-dimensional model which uses the system of Navier-Stokes equations as Reynolds after x and y Cartesian coordinates (1), (2) together with continuity equation (3) for incompressible fluids with free surface in turbulent motion. To solve the system of equations, the finite element method was used. The interpolation functions are quadratic for speeds and linear for depths (Surface Water Modeling System - RMA2, 2011).

Turbulence effects are taken into account by using the coefficients of turbulent viscosity, which are used to calculate the Peclet number $Pe=\frac{\rho U dx}{E}$, where $U=\sqrt{u^2+v^2}$ the resulting average speed and dx - length element in the flow direction.

The program carries out the mathematical model of water movement – determines the local velocity field vertically u, and v, the resulting speed as well as depth h.

There were established the following boundary conditions:

- for the arc group at the inflow (top) cross sections, the constant flowrate Q = 50.2 m^3/s was assigned;
- for the arc group at the outflow cross sections the constant geodetic rate H = 4.6 m was assigned.

For the modeling were used:

- simulations on real section of the river of length 700 m and width 76-65 m;
- constant density of water (1.000 kg/m^3);
- Peclet number equal to 20 of fluoride dispersion was determined using RMA4 program that is designed for numerical simulation of advection - diffusion processes from an average depth in an aquatic system (Surface Water Modeling System - RMA4, 2011). RMA4 uses the resulting hydrodynamics from RMA2 and calculates the solution of equation (4) using finite element method. The turbulence influence in the convective field is represented by using turbulent diffusion coefficients in the x and y directions. In

RMA4, to determine these coefficients, two methods are used: direct, where each element receives the respective values of these coefficients, or automatically, using the Peclet's number, which is given by

$$Pe = \frac{Udx}{D} \qquad (5)$$

In formula (5) U is the mean velocity, dx - length element in the flow, D - turbulent diffusion coefficient.

A constant source of fluoride to the concentration C = 1.6 mg/L was introduced on the border of pollutant entry. Numerical simulation was performed for 12 h , time considered sufficient to establish a permanent regime. The analysis of pollutant transport in water was carried out in dynamic regime, which allows the estimation of pollutant evolution at different time intervals.

Results and discussions

In all the finite elements of the geometry of the studied sector there were determined depths h and local velocities in the x and y (including resultant speed U). Figures 2 - 3 present the obtained results [21-23].

From figure 2 we see a scale represented by different colours, which indicates the depth values of the finite points; in the studied river sector.

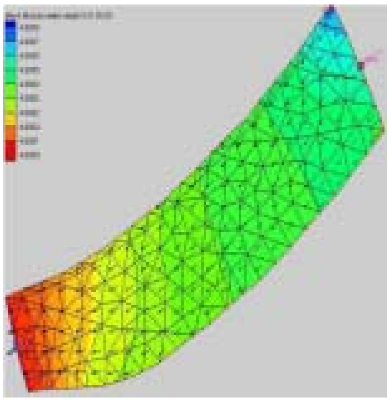

Fig. 2. Depths variation in the studied sector

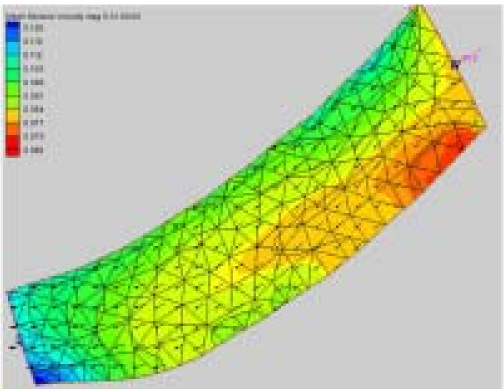

Fig. 3. Resultant velocity vectors distribution

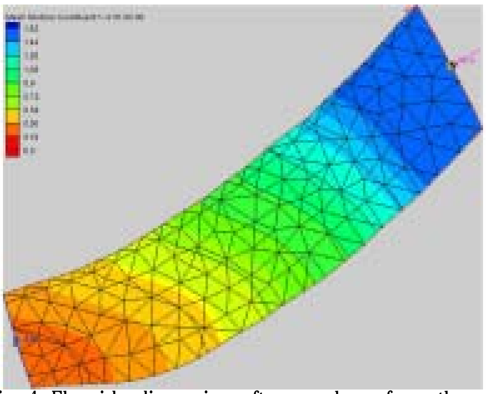

Fig. 4. Fluoride dispersion after one hour from the water confluence

Table 1

RESULTS OF NUMERICAL SIMULATION OF HYDRODYNAMICS IN A SECTOR OF THE PRUT RIVER

Region	*Umin* (m/s)	*Umax* (m/s)	*hmin* (m)	*hmax* (m)
In the confluence	0.074	0.091	4.60049	4.60076
On the left border	0.098	0.112	4.60013	4.60076
On the right border	0.063	0.123	4.60004	4.60047

The resulting velocity field is shown in figure 3.

The characteristic parameters, determined from the numerical simulation of hydrodynamics in the model area are shown in table 1.

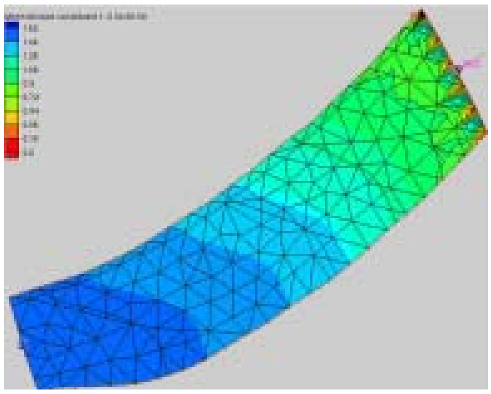

Fig. 5. Fluoride dispersion after four hours from the water confluence

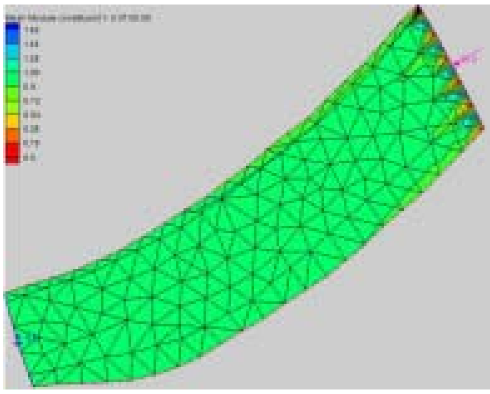

Fig. 6. Fluoride dispersion after seven hours from the water confluence

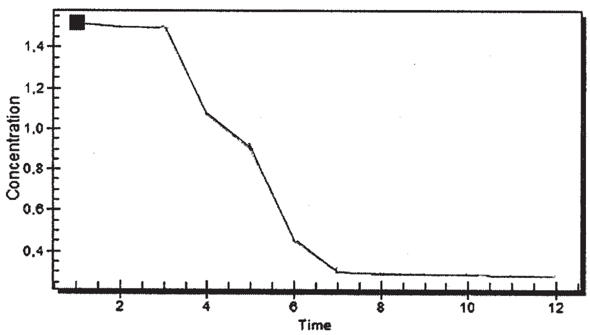

Fig. 7. Fluoride dispersion in the area of confluence.

The field evolution of fluoride concentrations was determined using the hydrodynamics obtained at the first stage.

Fluoride dispersion after 1 h from the water confluence is shown in figure 4.

The polluted river sector with fluoride is being observed for 1 h. The pollutant transport on the studied sector is presented in figures 5 - 7.

From calculations it was found that after 4 h fluoride concentration decreased significantly in the confluence.

After 7 h the pollutant transport has become stationary.

Temporal variation of fluoride dispersion in the confluence is shown in figure 7.

Conclusions

The problem of modeling the evolution of fluoride concentration in "river-type" systems was studied. The influence of fluoride on the human body was discussed, emphasizing the aspects related to the fluoride content in drinking water, fluoride deficiency and excess in the human body.

A conceptual model of the problem was developed, consisting of geometric attributes of the studied area, the forces acting in the area and physical characteristics. From the conceptual model, two numerical models were generated, which have been applied on a sector of the Prut River in the town Ungheni.

The numerical model developed at the first stage determines the field of speeds, and depths for each finite element of the created network.

The obtained results at the first stage were used as input data for RMA4 program, which determined the evolution of fluoride dispersion on the studied river sector. It was found that after 7 h, the pollutant transport has become stationary.

The simulation was carried out in dynamic conditions, which determined water particle hydrodynamics in time and space.

The developed numerical models are useful for predicting pollutants transport in "river-type" systems, for water quality management of the Prut River, and therefore, for the fluorosis prevention.

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