FLUORIDE DISPERSION MODELING FOR „RIVER-TYPE” SYSTEMS

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INTRODUCTION

Determining the spatio-temporal evolution of pollutants dispersion in "*river-type*" systems of has an important role in predicting pollution phenomena. This problem can be successfully solved by developing mathematical models and using software packages for simulating transport pollutants processes.

Fluoride has an important role to human health. It is a chemical element necessary for proper development of teeth and skeletal bones. But human health depends on optimum amount of fluoride. The lack of this element manifests itself in caries and its excess leads to general intoxication of the body, disturbs metabolic processes [1].

The purpose of this paper is to develop the mathematical model of hydrodynamics and dispersion of pollutants in order to determine the fluoride dispersion for a sector of river Prut, the Ungheni town.

1. FLUORIDE ACTION ON HUMAN BODY

Fluoride is found in nature (water, soil, air) or in food. Fluoride enters the body through two main pathways: through the consumption of water and food, and by respiratory route. In water, fluoride is present as fluoride, dissolved or suspended. Fluoride is found in sea water at a concentration of 0.8 to 1.4 mg/L, and surface waters below 1 mg/L. In Moldova, the average content of fluoride in drinking water ranges from 0.14 to 0.7 mg/L [2]. There are regions in the world, such as the USA, South Africa, Italy, India, etc.., where the water has, naturally, a high content of fluoride (naturally fluoridated water), from 20 to 50 mg/L [3, 4].

In the human body, the highest amount of fluoride is found in calcified tissues. In the bones, fluoride is continuously replaced by a dynamic reshuffle, analogue to that of calcium, where the old one is mobilized, removed and replaced. The concentration of fluoride in the bones is altered during life, depending on the amount ingested. Typically, when fluoride saturation was reached, the surplus is eliminated. Thus, it was found that the at the content of 1 mg/L in drinking water, the concentration in the bones reaches 200 mg/L for children of 10 years, or 1.200 mg/L for people over 80 years. However, when the amount of fluoride in drinking water is more than 9 mg/L, the concentration in the bones is of more than 10.000 mg/L [5]. In addition to bones, fluoride is the main beneficiary of the tooth, which becomes more resistant to acid attacks.

Chronic poisoning occurs only in the bones and teeth, clinical manifestation being called fluorosis. The occurrence of fluorosis is related to the amount of fluoride ingested, the time it acted, the ambient temperature (heat is a factor favoring the occurrence of fluorosis), to food (food rich in calcium reduce their frequency), nutritional diseases suffered by the patient etc.

Bone fluorosis occurs to people who ingested fluoride for a long period of time, for more than 20 years and about 10-25 mg/L per day, or industrial exposure. As a rule, these are people affected by consuming fluoridated natural water or workers in industries such as cryolite and bauxite, who are exposed to prolonged sodium fluoride pollution or aluminum fluoride [1, 6].

Negative effects caused by fluoride administration in other organs and tissues have been extensively studied including the fact that its use was and still is challenged for various reasons. In the research conducted in areas with endemic dental fluorosis due to high natural fluoride content of drinking water for over 8 mg/L, there could not be established a definite connection, for example, between the incidence of cancer or heart disease, nerve, skin, eye, endocrine, renal, etc. and the amount of fluoride ingested daily [5, 6].

On the other hand, it appears that, when consuming drinking fluoridated water, there are benefits to the outbreak of fracture and, especially, in patients with osteoporosis. The explanation is that fluoride produces an increasing number of osteoblasts in the fracture, thereby, stimulating the rate of healing and alkaline phosphatase action. It appears that fluoride in drinking water has a beneficial effect in preventing cardiovascular disease, but it requires advanced scientific research [7].

General toxic action of fluoride on the body is proportional to its amount in the body and does not depend on access roads. Also, the specific action of fluoride on the bone and teeth is determined predominantly by the concentration in drinking water. World Health Organization (WHO) has established permissible limit of fluoride in drinking water of 1 mg/L [8].

As demonstrated in the research conducted in many countries, fluoride concentration in drinking water sources considerably exceeds the allowable limit (fig. 1).

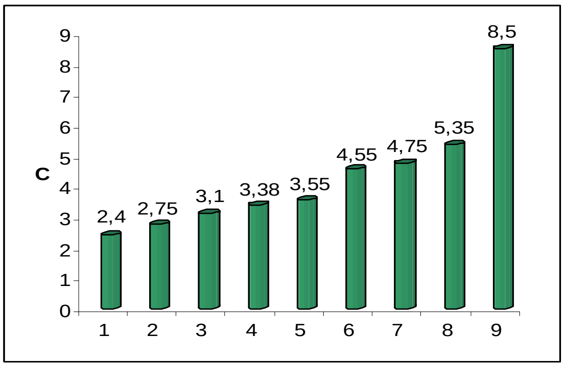

Figure 1. Fluoride concentration in water supplies in some countries of the world.
C - average concentration (mg/L). 1 - the USA, 2 - Romania, 3 - Bulgaria, 4 - Great Britain, 5 - Saudi Arabia, 6 - China, 7 - France, 8 - Denmark, 9 - India.

Ions fluoride concentration in drinking water sources in many regions of Moldova is increased, exceeding the admissible limit set by WHO [4, 9], which is reflected in Fig. 2:

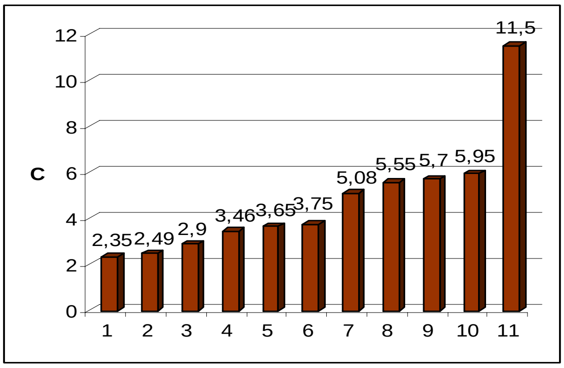

Figure 2. The concentration of fluoride in drinking water sources in some regions of The Republic of Moldova. *C - average concentration (mg/L).*
1 - Anenii Noi, 2 - Cimislia, 3 - Orhei, 4 - Floresti, 5 - Chiadir-Lunga, 6 - Hincesti, 7 - Glogeni, 8 - Camenca, 9 - Ungheni, 10 - Fălesti, 11 - Pîrlița.

2. EXPERIMENTAL

2.1 Mathematical modeling of hydrodynamics and pollutants dispersion

Water dynamics in rivers represents a turbulent flow. This has been established and proven by physicist O. Reynolds [10].

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), 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 [11, 12, 13].

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 [15]. Pollutant dispersion model developed in this work is based on two-dimensional form of the ADE, applied to the turbulent flow regime [15]:

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

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) [16].

2.2. Materials and methods

To generate the numerical models, the Surface-water Modeling System (SMS) v.10.1.11 was being used, which was developed by the AquaVeo specialists from the United States. This system is very useful for effective management of the entire process of modeling surface water: from importing topographic and hydrodynamic data, to visualizing and analyzing solutions.

In order to determine the fluoride dispersion, the river hydrodynamics was found out first, using a SMS module named Resource Management Associates (RMA 2). Then the results were used as input for RMA4 module, with which the fluoride concentration of field evolution was determined.

To define the geometry of the studied domain, the digital image of the Prut river from Ungheni town was imported from www.maps.google.com site and digitized directly into the SMS manually creating the parameters objects such as points, arcs and polygons (fig. 3).

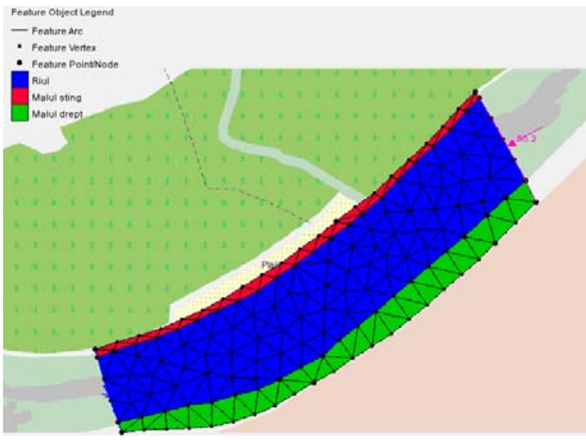

Figure 3. 2D representation of the domain geometry.

2.3. Numerical modeling of hydrodynamics and fluoride dispersion

The numerical simulation of hydrodynamics was performed using RMA 2 program which solves the system of equations 1-3 by finite element method [13].

The following boundary conditions were established: flow rate Q = 50,2 m^3/s and H = 4,6 m geodetic rate.

For the modeling were used simulations for the real river section of length 700 m and width 76-65 m.

The numerical simulation of fluoride dispersion was performed using RMA 4 program, which uses the resulting hydrodynamics from RMA2 and calculates a solution of the equation (4) using the finite element method [16].

The following scenario was simulated: at the input boundary the pollutant was introduced with a constant source of fluoride concentrations C = 1.6 mg/L. The numerical simulation was carried out for 12 hours. Water pollutants transport analysis was performed in dynamic conditions.

3. RESULTS

Depths variations in the studied sector is shown in Fig. 4.

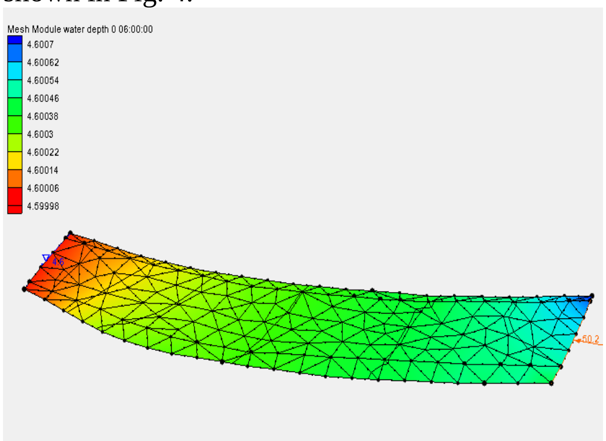

Figure 4. Depths variation in the studied sector.

Fig. 5 shows the velocity field distribution of water particles.

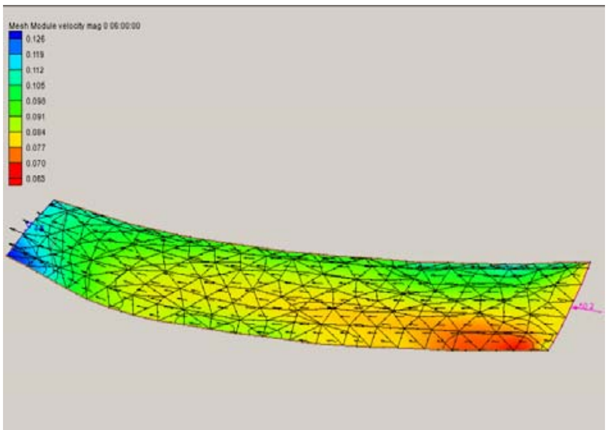

Figure 5. Resultant velocity vectors distribution.

Particle velocity in the confluence area is shown in Fig. 6.

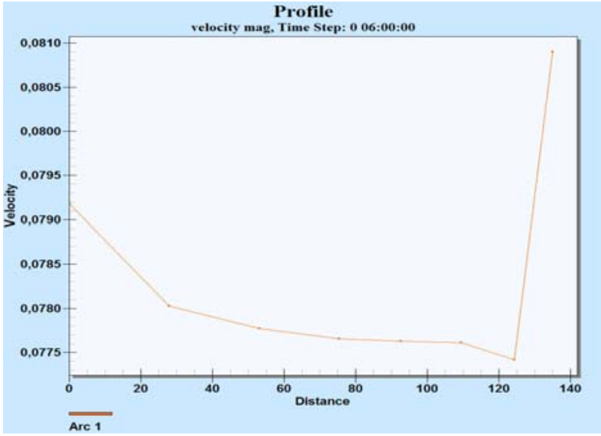

Figure 6. Resultant velocity vectors distribution in the area of confluence.

Speed particles near the left bank at different time intervals is shown in Fig. 7.

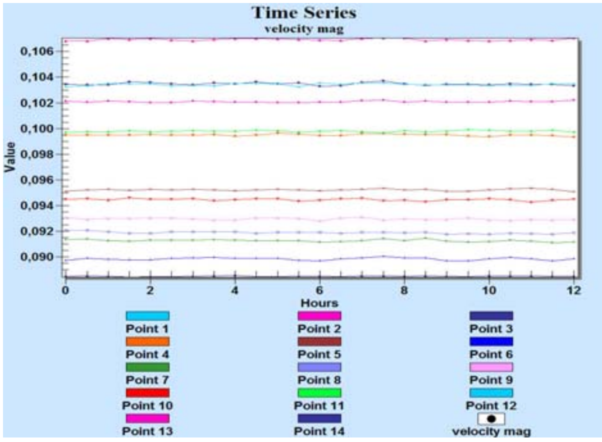

Figure 7. Resultant velocity vectors distribution near left bank.

The dispersion of fluoride in different intervals of time from the water confluence is shown in Figure 8-10.

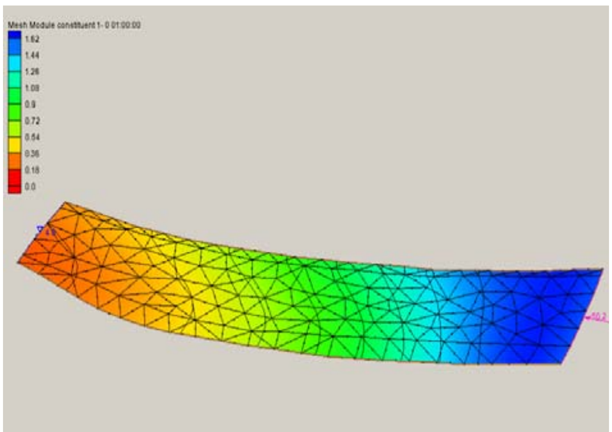

Figure 8. Fluoride dispersion after 1 hour from the water confluence.

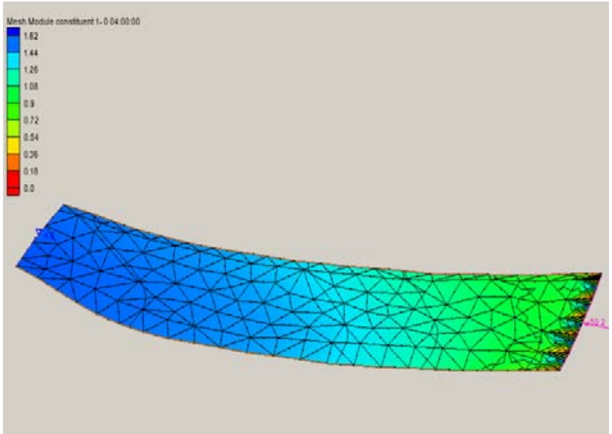

Figure 9. Fluoride dispersion after 4 hours from the water confluence.

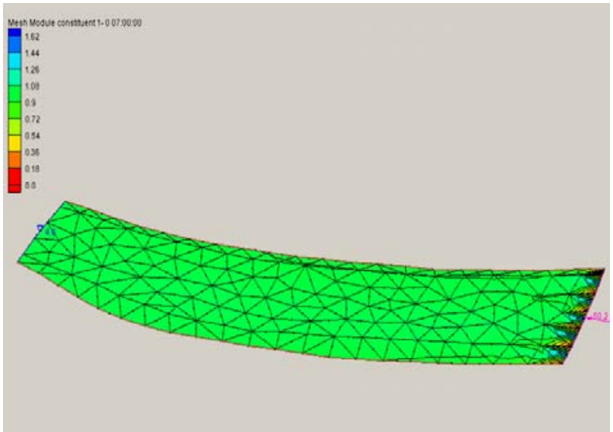

Figure 10. Fluoride dispersion after 7 hours from the water confluence.

Fluoride dispersion near the left bank is shown in Fig. 11.

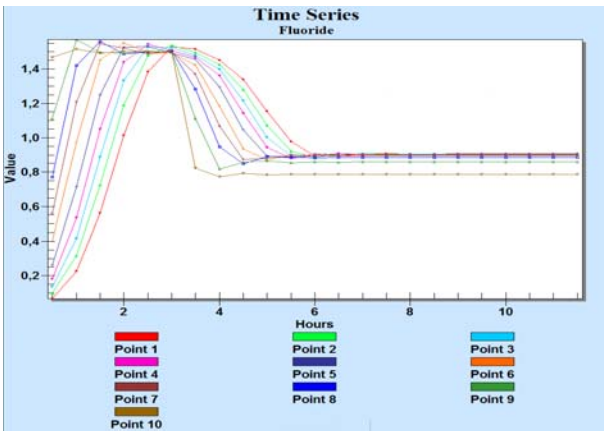

Figure 11. Fluoride dispersion near the left bank.

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.

A numerical model of hydrodynamics was generated, which helps to obtain the numerical model of fluoride dispersion.

The simulation was performed in a dynamic regime, this allowed the determination of spatio-temporal evolution of velocity field**.**

The obtained model can be used for modeling any other sector of the Prut river and is useful in predicting and preventing emergency situations.

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