ELEMENTARY AND COMPLEX SIMULATION OF A RIVER POLLUTION IN ORDER TO RAISE ENVIRONMENTAL TRAINING AND AWARENESS
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SIMULAREA ELEMENTARĂ ŞI COMPLEXĂ A POLUĂRII UNUI RÂU PENTRU INSTRUIRE ŞI CONŞTIENTIZARE DE MEDIU

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Keywords: *simulation, modeling, environmental, awareness, teaching, practice, pollution*

ABSTRACT
This paper shows the role of numerical simulation of physical processes in the environmental awareness and education, emphasizing the right choice of its complexity depending on the level of depth at which should or can be done the exposure. The authors insist on the important role incumbent on incremental simulation (based on mathematical models as simple as possible) in environmental awareness and even in higher education field. The jump to complex simulators can be done only after knowing (which means to know a model and a simulator, that we will try to explain in the paper) the basic models, and the use of complex simulation is effective only within specialist teams including at least 2 -3 or more related fields. These views are supported in the paper with simulators and their use in practical case of pollution of a river simulation.

REZUMAT
Lucrarea prezintă rolul simulatoarelor proceselor fizice in procesul de conştientizare de mediu si in învăţământ, accentuând asupra alegerii potrivite a complexităţii acestuia funcţie de nivelul de profunzime la care trebuie sau poate fi făcută expunerea. Autorii insista asupra rolului mai important ce revine simulatoarelor elementare (bazate pe modele matematice cat mai simple), in procesele de conştientizare de mediu si chiar in învăţământul superior de profil. Saltul către simulatoarele complexe se poate face numai după cunoaşterea (ce înseamnă a cunoaşte un model si un simulator, ne vom strădui sa explicam in lucrare) modelelor elementare, iar folosirea eficienta a simulatoarelor complexe este eficienta numai in echipe de lucru care include specialist in cel puţin 2-3 sau mai multe domenii conexe. Aceste opinii se susţin in lucrare cu exemple de simulatoare si utilizarea lor in cazul practic al simulării poluării unui râu.

INTRODUCTION
After *Bailey and Borwein, 2003* or *Merriam Webster, Learner' Dictionary,* the simulation is something that is made to look, feel, or behave like something else especially so that it can be studied or used to train people:

- a computer simulation of spaceflight
- simulations of body movements
- a simulation of the planet's surface
- computer simulation to predict weather conditions.

After *Pimpunchat et al., 2009* or *Oxford Dictionary*simulate means:

- to pretend that you have a particular feeling;
- to create particular conditions that exist in real life using computers, models, etc., usually for study or training purposes;
- to be made to look like something else;

After *Pimpunchat et al., 2009*, the origin of this word is located in time in the mid of 17th century from the Latin word, simulate that means copied or represented, from the verb simulare, from similis "like".

Very interesting are the definitions given by *Cambridge Dictionaries Online, 2015* for the notion of simulation. After *Cambridge Dictionaries Online,2015*, in British for the simulation are usual the next definitions:

- a model of a set of problems or events that can be used to teach someone how to do something, or the process of making such a model;

- in football, the act of pretending to have been fouled to try to win a penalty or free kick unfairly.

In American, the simulation is used after *Cambridge Dictionaries Online, 2015* preferential meaning: a model of a real activity, created for training purposes or to solve a problem.

Also *Cambridge Dictionaries Online,2015* proposes the usual meanings in business simulation:

- a situation or event that seems real but is not real, used especially in order to help people to deal with such situations or events;

In *http://www.webopedia.com/TERM/S/simulation.html*, the simulation suggests imitation: the process of imitating a real phenomenon with a set of mathematical formulas.

In fact, as with many other words, the simulation has several meanings, acquired a vague and relative sense to areas where it is used. It is certainly a feature of modern language, which as you want exactly, becomes inaccurate, the more are increasingly using many words.

Consequently, by *www.meriam-webster.com/dictionary/simulator,*, a device that enables the operator to reproduce or represent under test conditions phenomena likely to occur in actual performance, is called simulator. This device can be a physical (small-scale simulation model, its electronic one - analogue simulation, a computer) or theoretical (theoretical model with analytical solutions available).

A notion that can replace simulation that when this is done theoretically, is numerical experiments. In this case, the simulator is human mind or more generally, thinking, or computer. According to *Bailey and Borwein, 2003*, the numerical experiment is included in what is called the experimental mathematics. By (*Bailey and Borwein, 2003*), experimental mathematics, *(Weisstein, 2016)* is a type of mathematical investigation in which computation is used to investigate mathematical structures and identify their fundamental properties and patterns. As in experimental science, experimental mathematics can be used to make mathematical predictions which can then be verified or falsified based on additional computational experiments.

Borwein and Bailey (2003) use the term "experimental mathematics" to mean the methodology of doing mathematics that includes the use of computation for:

1. Gaining insight and intuition.
2. Discovering new patterns and relationships.
3. Using graphical displays to suggest underlying mathematical principles.
4. Testing and especially falsifying conjectures.
5. Exploring a possible result to see if it is worth formal proof.
6. Suggesting approaches for a formal proof.
7. Replacing lengthy hand derivations with computer-based derivations.
8. Confirming analytically derived results.

Whatever type of simulation and the simulator, it can be used with confidence only after validation. This means that between the physical quantities involved in the process must be examined, at least within certain limits, relations between same characteristic values of the real process. After validation, the simulator can be used to find new relationships, finding optimal working processes, or improvement in order to generalize.

There are many works written in this field in recent years, among which: *(Tyagi et al., 2012)*, *(Benedini and Tsakiris, 2013)*, *(Marusic, 2013)*, *(Nopparat et al., 2006), (Cakaj, 2010), (Shiffman, 2012)*.

I made a long introduction to define as precisely as possible the instruments whose use tries to comment on the work of environmental and pedagogical awareness.. We try to prioritize their work by the complexity of environmental and educational awareness and pedagogical. Below we give a few examples, and then we draw conclusions.

MATERIAL AND METHOD

We examine a particular case, a pollution of a river, but the most elementary possible, but coupled with interaction with oxygen in the river water. This will give greater scope conclusions.

The mathematical model underlying the simulation, consists of a system of two partial differential non-linear equations, though simple, as the number of equations and shape, boundary condition and initial pose difficult problems to solve. List of model parameters is given in Table 1.

Table 1

List of model parameters, notations, units of measurement and simulation values Neajlov River

Model parameters		Values in model
Notation	**Name (units SI)**	
L	polluted length of the river, m	>10000
D_P	pollutant dispersion coefficient on the variable direction *x* ($m^2 day^{-1}$)	34.56
D_X	dispersion coefficient of dissolved oxygen in the direction of the variable *x* ($m^2 day^{-1}$)	34.56
v	water speed in the direction of the *x*, m day^{-1}	21600
A	normal sectional area of the river, m^2	12.5
q	rate added pollutant along the river, kg m day^{-1}	0.06
K_1	coefficient of pollutant degradation rate at 20^o C	8.27
K_2	de-airing the rate coefficient for dissolved oxygen at 20^o C	44.10
k	halfsaturated concentration ratio of oxygen required to decompose the pollutant, kg m^{-3}	0.007
α	mass transfer of oxygen from air to water, $m^2 day^{-1}$	16.5
S	oxygen saturation concentration, kg m^{-3}	0.01

The equations of the mathematical model are:

$$\begin{aligned} \frac{\partial(AP)}{\partial t} &= D_P \frac{\partial^2(AP)}{\partial x^2} - \frac{\partial(vAP)}{\partial x} - K_1 \frac{X}{X+k} AP + qH(x),\ (x < L \le \infty, t > 0) \\ \frac{\partial(AX)}{\partial t} &= D_X \frac{\partial^2(AX)}{\partial x^2} - \frac{\partial(vAX)}{\partial x} - K_2 \frac{X}{X+k} AP + \alpha(S - X),\ (x < L \le \infty, t > 0) \end{aligned} \tag{1}$$

Where:

P is the pollutant, and *X* is the oxygen concentration in the river water, and:

$$H(x) = \begin{cases} 0, x \le 0 \\ 1, x > 0 \end{cases} \tag{2}$$

is Heaviside function.

Equations (1) add initial and boundary conditions that will result for a particular case. Nonlinearities make the system of equations to not be solved analytically on the initial form (system solutions are possible only in numerical form, at least currently). Basic analytical solutions can be obtained in individual cases which although possible, are generally rare in nature. However, these solutions are the first that can validate theoretical model, then opening the door to other analytical and numerical investigations.

Particular solution

According with the authors of *(Pimpunchat et al., 2009)*, is consider only the steady-state solution in the case when dispersion can be take negligible, D_p=0, D_x=0. For this case the system (1) became:

$$\begin{aligned} \frac{d(vAP_s(x))}{dx} &= -K_1 \frac{X_s(x)}{X_s(x)+k} AP_s(x) + q,\ (x > 0) \\ \frac{d(vAX_s(x))}{dx} &= -K_2 \frac{X_s(x)}{X_s(x)+k} AP_s(x) + \alpha(S - X_s(x)),\ (x > 0) \end{aligned} \tag{3}$$

with boundary conditions:

$$P_s(0) = 0, X_s(0) = S \tag{4}$$

In addition, to linearize equations is needed also the hypothesis that the half-saturated oxygen demand concentration for pollutant decay is negligible (k=0). In these circumstances, the solution is obtained:

$$P_s(x)=\frac{q}{K_1A}\left(1-e^{\frac{-K_1x}{v}}\right),\ X_s(x)=S-\frac{K_2q}{K_1}\left(\frac{1}{\alpha}-\frac{1}{\alpha-K_1A}e^{\frac{-K_1x}{v}}\right)-\frac{K_2qA}{\alpha(\alpha-K_1A)}e^{\frac{-\alpha x}{vA}} \quad (5)$$

As a consequence of assumptions, the solution (5) does not depend on time and is valid only for $x>0$ for $x<0$ with: $P_S(x)=0$ and $X_S(x)=S$. Asymptotic behaviour of the solution is given by:

$$\lim_{x\to\infty}P_s(x)=\frac{q}{K_1A},\lim_{x\to\infty}X_s(x)=S-\frac{qK_2}{\alpha K_1} \quad (6)$$

A graphical representation of the solution to facilitate awareness

For application, I have got Neajlov River, Giurgiu County. The spill occurs near the bridge over the Neajlov, the settlement Calugareni. The graphical representation of the solution is given in Fig.1. It was the first level of complexity of the pollutant transport on the river phenomenon simulator.

In *(Pimpunchat et al., 2009*), the authors make another application through analytical results, but with a broader hypothesis, however improbable characteristics of situations in reality. Next we preferred to generalize the result to situations more likely in reality to solve numerically the problem (1) - (4).

We constructed a simulation using Mathcad software facility (can use Matlab, Mathematica, FlexPDE, COMSOL, and many other well-known software programs).

The results of this simulator can be given in Fig.1 or in separate graphical representations.

This is the second level of complexity of the simulator phenomenon of pollutant transport on the river. The third level of complexity begins with complex software programs, specialized, such as WASP, ISIS, FLO-2D and 3D SoilVision, etc. This category of simulators includes, also, those created in programs that made complex simulation for a wide range of physical phenomena *(Cristea et al., 2010)*.

There are approaches earlier in this issue, with results which must be reconsidered *(Bouchard and Duplex, 1994; Shagalova, 1996)*.

In this article we shall merely list them and show the difficulties of use.

RESULTS

A first result obtained using the mathematical model (Eq.1-4) in the simplifying assumptions that allow analytical solution (Eq.5) is given in Figure 1. This result allows an awareness and education of good quality, fast and useful, but not technically accessible than only to university level.

Figure 1 shows overlapping plots of solution component variations over river aerial photograph of the area that aims phenomenon of pollution: pollutant concentrations and dissolved oxygen. On the aerial photo of the area are marked places for distance measurement reference to river axis.Marking labels appear on the horizontal axis of the graphs of variation in pollutant concentrations and dissolved oxygen.The map in Figure 1 can be used for delimitation of the river zone where certain species of animals or plants are in danger of losing their life, to determine the location where remediation might make optimal aeration for delimitation of any prohibited areas access to people and animals.

Map of Figure 1 represents an important public awareness on how the phenomenon takes place, especially around the affected area residents can identify their homes or workplaces.

Using experimental values, presented in table 2, were drawn charts of variation of the average values for the coefficient of static friction and the angle of natural slope for the six grist fractions analyzed, using MS Excel program version 12 (fig. 2).

Values of bulk density, specific surface, porosity and mean diameter of the grist fractions analyzed are presented in table 3.

Based on the data obtained and presented in Table 3, were drawn, as graphic, variations of bulk density, density, specific surface and porosity of grist intermediate products analyzed.

As can be seen from the analysis of data from table 3, and of charts in figure 3, bulk density of fractions resulted at sorting of grist in plansifter compartment C2 has a random variation, it depends such on the type of sieve frame fabric, and the size of apertures of the working sieve, but also on the initial granulation of grist or on shell content adhesive on the semolina particles subjected to grinding.
In Fig. 2-6 simulator results are given, namely pollutant transport phenomenon along a river, in the context of the phenomenon of aeration as a remedy.

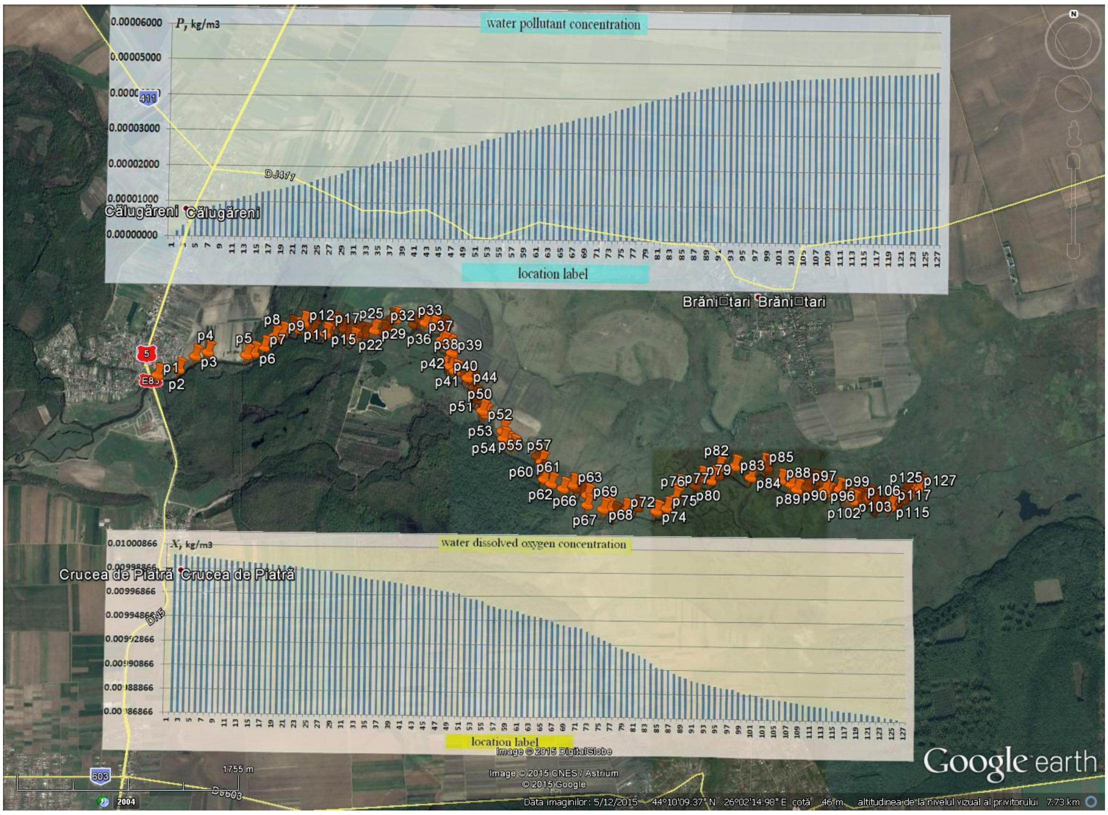

Fig.1 - Variation in pollutant and water dissolved oxygen concentrations along a section of river

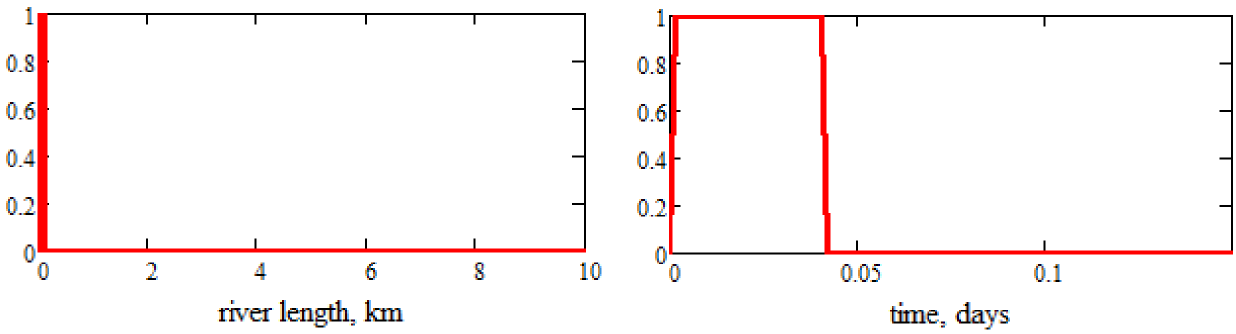

Fig.2 - Space (left) and time (right) history of the time and space factor control (discharge function)

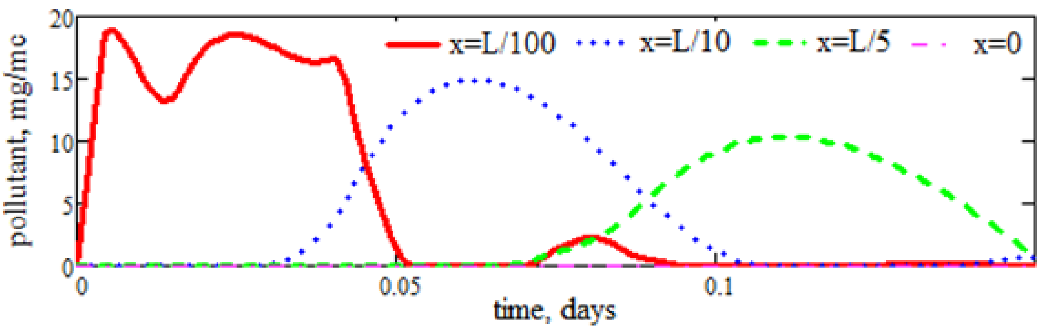

Fig.3 - Time history of the pollutant concentration in four locations along the river

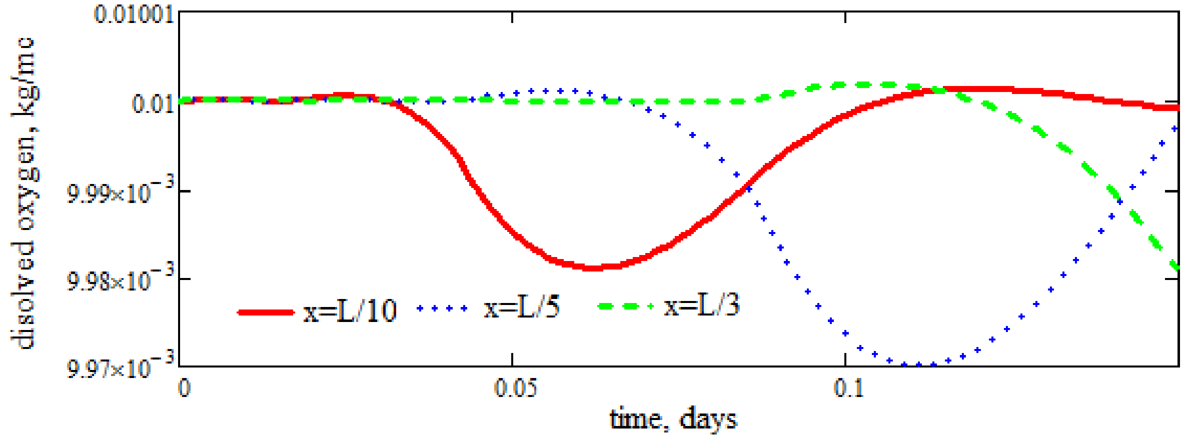

Fig.4 - Time history of the dissolved oxygen concentration in three locations along the river

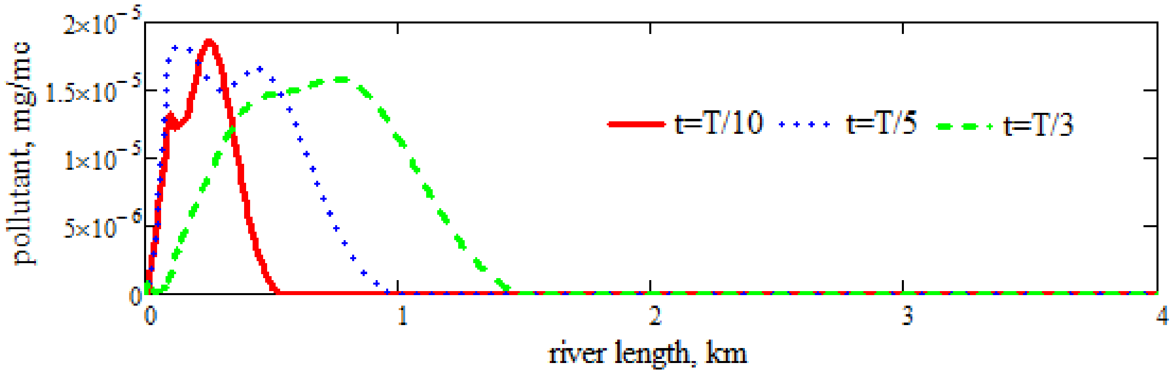

Fig.5 - Variation along the river of the pollutant concentrations at three time points

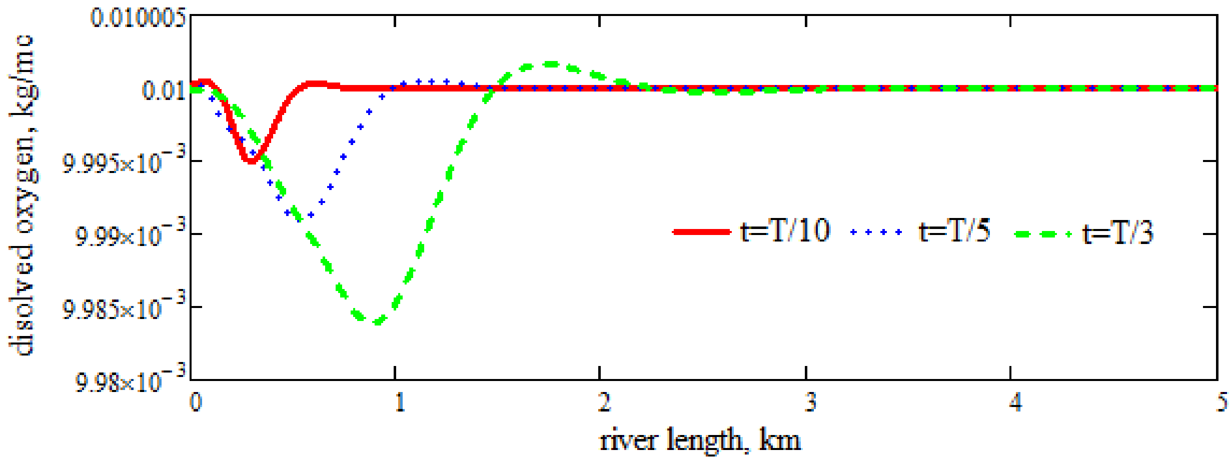

Fig.6 - Variation along the river of the dissolved oxygen concentrations at three time points

The function of discharge shall form a constant multiplied by factors trapezoidal in time and space, factors that delimit the range of temporal and spatial discharge occurs. Temporal and spatial variation of the discharge function are given in fig. 2. Spill (pollutant discharge) occurs on a portion of length 99 m starting from 1 m elevation (center area under the bridge at Calugareni over Neajlov) for one hour at a rate q = 0.06 kg m^{-1} day^{-1}.

History of the pollutant concentration of 3.6 hours in four locations in the river (100 m, 1000 m, 2000 m and 0 m) is given in Fig.3. History of the water dissolved oxygen concentration of 3.6 hours in four locations in the river (100 m, 1000 m, 2000 m and 0 m) is given in Fig.4.

Changes in concentrations of pollutants over the first four kilometers of river measured from the central area under the bridge at three time points, is given in Fig.5. Varying the concentration of dissolved oxygen in the water during the first four kilometers of the river measured from the central area under the bridge at three time points, it is given in Fig.6.

To achieve these results was considered a maximum length of riverbed observable L= 10 km (until the first tributary whose appearance made inoperative model). Model characteristic parameters were fixed at values in Table 1.

Calculation program has run a total of 100 temporal steps and 1500 steps in space.

There are some fine points of the solutions (right solution must be positive and after cancel remain zero until the end if other leaks do not occur) that must meet to obtain the correct solution.

CONCLUSIONS

Several conclusions can be drawn even if a description of the same level computing very complex models cannot be included in this article.

First, it is clear that at the level of awareness or learning, mathematical models and simulators based on them are more useful than the complex software programs which include among other facilities the contaminant transport simulation.

1D mathematical model is simple and easily verified by our intuition about the phenomena of dispersion and propagation of attenuated wave. The results of these models allow the assessment of the time before a dangerous pollutant concentration reaches a certain distance from the spill site. This is the time available for intervention. Some of the results are readily accepted and even obtained an audience that is not technical background. The operation of the simulator is not recommended however, without further instructions. In contrast, students in technical and specialized audience, we recommend using these simulators and the confrontation of the results with the intuition and reality. Doing so can see advantages and disadvantages of these models and simulators. The use of elementary models and simulators facilitates the understanding of the logic of complex programs that solve such problems. Even the simple model presented in this work is not the easiest, because it includes parameters that characterize the flow of water, oxygen and pollutant dispersion and their interaction. Therefore, to ensure the accuracy of results are required qualifications for modeling dispersion and hydraulic phenomena in the transport of substances, and (in the least) in numerical calculation. A basic model of the 1D cannot play a series of important aspects of pollutant concentrations difference between the central area of the riverbed and banks, concave geometric concentration in certain areas (ports, piers, river basins in communication with) etc. Other issues on which model they contain are not exposed to the influence of thermal field, the influence of atmospheric pressure, influence the quality of river fluid (density, viscosity, speed side) interaction with river tributaries, normal variation riverbed section, additional flows from rainfall etc. To account for these phenomena, enter third level of models and simulators, namely complex software programs. These problems coupled fluid flow problem with the transport of substances and energy problem, the problem of heat transfer and biomass and contain empirical relationships between certain parameters of the model. To give a brief idea on how these programs can address demands an example of the WASP program is offered for free.

Inputs include: geometry riverbed, the necessary data integration (start time and end time, minimum step, the method of integration, etc.), system polluted with their main properties, constants parts to the surface and pores data about fluid flow and how it is done downloading pollutant, boundary conditions, Time for loading and border conditions, the output. Therefore the use of this program required knowledge in different domains, consequently a number of specialists in various fields. For this reason it is not recommended to use such simulators in awareness activities and training specialist's formation. These programs are recommended by specialist teams already trained in the necessary fields.

ACKNOWLEDGEMENT

This work has been done within the project "Network and web platform to improve the public awareness on environmental management and protection in the cross - border area Giurgiu - Rousse and adjacent cross - border areas" funded by "Romania – Bulgaria Cross-Border Cooperation Programme 2007 – 2013" *(www.envirobg.eu)*.

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