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Dynamic Simulation of Someş River Pollution Using MATLAB and COMSOL Models

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The present paper is aimed to river water quality modelling. A numerical and an analytical model have been developed in order to predict the transport of pollutants in the Romanian Someş River. A novel approach for the analytical modelling offers the opportunity to use variable parameters along the river length. Space dependent model parameters have been used for both solutions. The modelling results provide information on the time and space evolution of pollutant concentration. Comparison between results of the two models reveals their incentives and limitations.

Keywords: pollutant transport model; Somes River; numerical model; analytical model.

Prediction of flowing water quality and characteristics is having an important place in the research work at global level due to the need to counteract the effects of the natural disasters or accidents that might take place. The river water quality modelling (WQM) literature is very rich in transport models of specific substances, which may be conservative or non-conservative compounds.

A large part of the WQM publications present only one-dimensional (1D) experimental models useful to a certain river case or focused on only one pollutant. Considering nitrogen as an example, the literature survey shows the existence of several models for the nitrogen compounds [20, 22]. These models are dynamic and include first order kinetics for the transformations. They describe the factors influencing nitrate transport in flowing waters [22] and kinetics of the nitrogen transformations [1, 11, 27 and 38].

However, models on other kinds of pollutants, considering one or several species, which suffer transformation processes during their transport are also available in literature [1, 3, 20, 28, and 29].

Another type of models predicts the evolution of pollutant concentration in rivers and describes water quality parameters for large river lengths, or even for basin scale [10, 16 and 18]. They consider daily or even monthly time-steps for the computation algorithm. These models are useful to assess the situation of the river water quality over long periods of time, but they may be hardly used in cases of severe calamities. For these cases models having smaller computation steps are suitable. Such features are characteristic for the following presented models, developed for the Someş River.

For the simulation of different pollution scenarios several water quality simulators are available [7, 24, 42, 43]. Short reviews of the available WQM software products are presented in several papers [13, 34]. Among them there are two types of software. One type is represented by the simple water quality simulation tools based on a significant number of simplifying assumptions [19]. They take into consideration only few input variables concerning pollution sources or pollutants, use average values for the river hydraulic parameters and take into account simple kinetics for the pollutant transformations or even consider the transport as being conservative.

On the other hand, complex software is also available for making real time predictions, and for presenting biological and chemical processes along with the physical ones (e.g. BASINS, CE-QUAL-RIV1, MIKE11, PC QUASAR, QUAL2K, SWAT, SWIM, QUESTOR). These software products are very useful but they usually do not allow the user the desired access to the underlying equations in order to modify them and make the software suitable for the particular case of interest. Usually, the costs for implementing such software are considerable.

Considering previous research discussed above it was decided to build flexible models suitable for the Someş River, which have the ability to predict both the space (along the river) and time evolution of conservative and non-conservative pollutants concentration.

Screening the literature on the Someş River it was noticed that only few water quality studies have been carried out until now. Some of them show accidents that happened in the last years [23, 25, 3, 36]. Another set of papers presents the state of the water quality [25, 32, 33] or specific aspects related to the chemicals affecting the water [26]. None of these studies has as subject the prediction of the Someş River water quality and the pollutants transport along the river.

Consequently, the development of a specific simulation tool for water quality prediction is of great interest for the environmental management in the Someş River Basin and also for other flowing waters in Romania. They are necessary, taking into consideration that flowing waters in Romania are often polluted [5, 6, 8, and 40].

The present paper considers the transport and transformation of non-conservative pollutants, without aiming to a specific type of pollutant, but rather to develop an efficient software framework for building applications able to cope with different potential pollutants. It is dedicated to pollutant transport modelling by using both (1) numerical methods for solving the underlying PDE and (2) implementation of the analytical solution of the underlying PDE.

Experimental part

The Someş River is the fifth largest river in Romania and the most important in Transylvania. The investigated area considered in the present paper consists in a river length of

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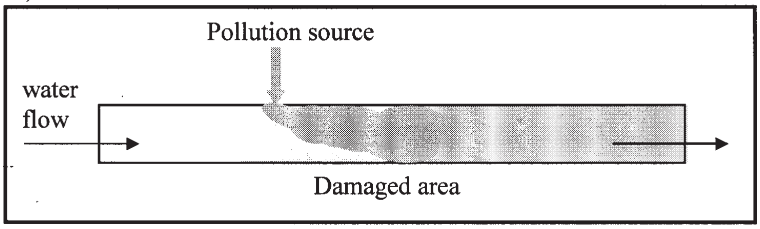


Fig. 1. Transport of pollutant emerging from a point release

Table 1

TRANSFORMATION RATE CONSTANTS AND ALLOWED LIMITS ASSOCIATED TO WATER QUALITY INDICES EMPLOYED IN PREVIOUS STUDIES

Quality indices	**Transformation k [day^{-1}]**	**Allowed limit**	
		in effluents [17] [mg/l]	**in rivers [mg/l] [35] Category: I;II;III;IV;V**
Organic pollutants	Biodegradation 0.40 – 1.30 [14]	Phenols: 0.3 Detergents: 0.5	Phenols: 0.001;0.005;0.02;0.05;>0.05 Detergents: 0.1;0.2;0.3;0.5;>0.5
Nitrate	Denitrification 0.01 – 0.88 [1]	25.00	1;3;5.6;11.2;>11.2

88 km and was chosen after analysing the information regarding pollution sources presence along one of the main branches of Someş River [2].

The upstream end of the investigated river stretch is located at the entrance of the river in the city of Cluj-Napoca and the downstream end is located near the municipality of Dej. The experimental data consists in: concentration measurements collected between years 2001 and 2005 on a monthly basis, information about the discharge of pollution sources in the river, collected during year 2004, and river channel cross sectional profiles.

The reasons for studying this river reach (segment) are related to the high diversity of pollution sources along it, but also to the dense population living in its basin [30, 40]. The pollution sources within the investigated area are: industrial sites, waste water treatment plants, sewage systems, agricultural fields, and livestock farms. Most of sources may be characterised by continuous point pollutant discharge, as shown in figure 1.

When the discharge starts the pollutant is present just in the source vicinity. In time, the pollutant extends across the channel and along its length. Due to convection the pollutant is transported downstream and because of dispersion it is spread in the river channel. The dispersion may also cause the presence of the pollutant upstream the source along a short distance. More details on the convective-dispersive pollutant transport in rivers are available elsewhere [41].

This paper presents a usual pollutant discharge in Somes River. The source is considered as being located in the industrial site of the Cluj-Napoca city at 90 km downstream the river spring, as identified in a previous study [2]. The same study [2] together with other investigations regarding Someş River [30, 40] reveal that among important pollutants of this river stretch there are nitrate, ammonium, organic pollutants, metals. All these species could represent the subject of the simulation scenario presented in this paper, with the specification that characteristic parameters (e.g. transformation rates) should be specified according to simulated pollutant. Transformation rate constants (k [day^{-1}]) associated to some of their transformations are presented in Table 1, as they were employed in previous studies. Maximum allowed limits for these pollutants are also specified. Such parameters for other pollutants are available elsewhere [e.g. 1, 15, 19, 28, 29 and 41].

The pollution source mass flow concentration is 5g/s non-conservative pollutant and is released trough a discharge pipe. It is assumed to be instantly distributed over the cross section of the river.

Results and discussions

Mathematical models formulation

To illustrate the propagation of the pollutant discharged by the continuous point source two mathematical models have been developed. The 1D form of the basic equation (1) for WQM is the common basis for both models and it is describing the pollutant concentration (c [mg/L]) change in time (t [s]) along the river length (x [m]), depending on the mass transport and transformation mechanisms [41].

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_x \frac{\partial c}{\partial x}\right) - \frac{\partial}{\partial x}\left(V_x c\right) - kc \qquad (1)$$

The analytical solution of equation (1) employed in this research was used in other pollutant transport modelling studies as well [36]:

$$c(x,t) = c_0 + \frac{(c_S - c_0)}{2}\left[erfc\left(\frac{x - V_x t}{\sqrt{4D_x t}}\right) + \exp\left(-\frac{xV_x}{D_x}\right) erfc\left(\frac{x + V_x t}{\sqrt{4D_x t}}\right)\right] \qquad (2)$$

In all equations x denotes the distance downstream the pollution source [m]. c_0 [mg/L] is the initial concentration along the river, assuming nonzero initial concentration conditions throughout the river; c_{S0} [mg/L] is the initial concentration at the source (x_S [m]); and c_S [mg/L] is the concentration at the source during the release (t [s]). The convective velocity (V_x [m/s]) and the longitudinal dispersion (D_x [m^2/s]) are depending on the water flow (Q [m^3/s]) and river channel characteristic parameters, as described in table 1. More details on analytical solutions for WQM are provided elsewhere in literature [14, 41].

To the conservative form of equation (2) we added a term corresponding transformation processes. This is expressed through first order kinetics, which takes into account biological, chemical, physical transformations of the pollutant during the transport and any other processes leading to the change of pollutant concentration. Depending on pollutant transformations may cause loss of pollutant (k is positive), and they are named pollutant sinks, or gain of pollutant (k is negative), being named pollutant sources. In this paper both models use constant k value (equal to 10^{-5} s^{-1}) expressing a pollutant sink. Transformations constant is assumed to be independent of water parameters (temperature, BOD, DO, pH), considered in other studies [1, 29].

Models show how mass transport is caused by convection (second term on the right side of eq. (1)) and diffusion (first term on the right side of eq. (1)), not considering other kinds of pollutant transport (e.g. infiltration from the river banks).

For numerical modelling the PDE form of equation (1) is implemented in COMSOL Multiphysics software. The software is able to solve PDEs using the finite element method, taking into account the specified conditions related to river characteristics, the source and boundaries. For analytical modelling equation (2) is implemented in MATLAB software. Both, the numerical and analytical solution have been developed on the same assumptions for the initial and boundary conditions, transformation kinetics and using the same channel parameter values.

According to a high number of published pollutant transport models the river parameters are considered in two ways: (1) as averaged values for the entire modelled segment; or (2) as averaged values assigned specific river segments (reaches), defined according to the non-uniformity of the river channel along the modelled segment [14, 18 and 41]. In contrast with these models an important feature of both models presented in our paper is that river characteristic parameters are variable along the modelled river segment.

It is well known that equations corresponding to analytical solutions for the prediction of pollutant transport along rivers are dependent on the type of pollution source [41]. A distinct form of the analytical solution corresponds to each type of pollution source. Analytical solutions take into account simplifying assumptions which characterize the river by constant values of the hydraulic parameters, and the source as having constant discharge. Models presented in literature consider that the average pollutant concentration or pollutant mass flow at the source is the input at each time and space integration step in order to make predictions of pollutant concentration in the river [16, 19, 36 and 41].

In the present paper, for the dynamic simulator based on the analytical model, a novel approach is implemented in order to offer the possibility of using space dependent river parameters. This approach implies re-evaluating the pollutant mass flow characterizing the polluting source at each computation step. In this novel approach the pollutant mass flow at the source, having the real discharged value at each time step, is used to make predictions in the first computation step according to space (in the vicinity of the source). Afterwards, the pollutant mass flow associated to the computed pollutant concentration from the current space step is used to predict the concentration in the next step. This procedure enables the analytical solution to take into account the space dependent parameters along the modelled river length, but also to compute the solution for time dependent pollutant discharge.

Model parameters

Model parameters have been computed on the basis of field data. Measurements reveal non-uniform channel features and water flow along the investigated river section, as presented in figure 2. The normalized parameters have been obtained by referencing their values to the maximum value of each parameter.

First, channel characteristics (S [m/m], B [m], H [m]) and water flow (Q [m^3/s]) have been evaluated, and afterwards they have been used to compute D_x and V_x. In models these parameters are evaluated by equations presented in table 2.

Channel parameters and flow rate dependence on river length (x [m]) is given by third order polynomials determined with the help of polynomial regression functions in MATLAB. Velocity and dispersion coefficient are computed using relationships proposed in literature [4, 19 and 39]. Mathematical expressions presented in table 2 have been included in both mathematical models, along with k equal to 10^{-5} s^{-1} (0.86 day^{-1}).

Simulation results

Models have been used to simulate the pollution scenario described above, in order to assess consequences of the continuous release of 5g/s of non-conservative pollutant over 24 h. Combined effects of convective-dispersive

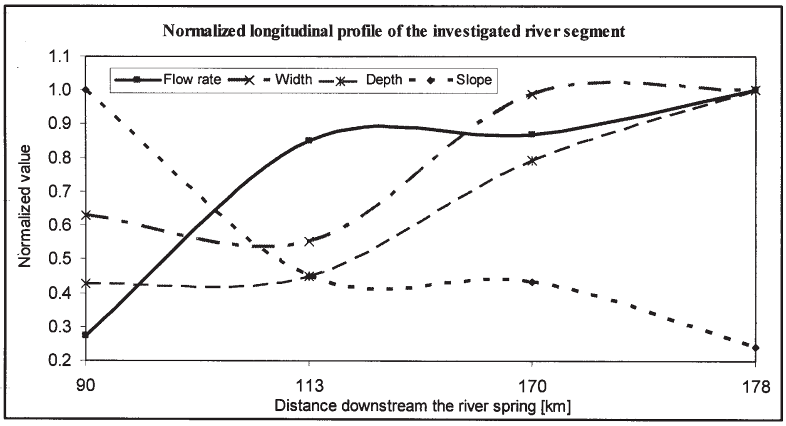


Fig. 2. Normalized channel parameters and water flow along the investigated river segment.

Table 2

REGRESSION EQUATIONS USED TO COMPUTE THE RIVER SPACE DEPENDENT MODEL PARAMETERS

Parameter	Symbol	Measuring Unit	Equation
Slope	S	m/m	$-1.70\cdot10^{-17}x^3+2.41\cdot10^{-12}x^2-1.00\cdot10^{-7}x+2.26\cdot10^{-3}$
Width	B	m	$-1.53\cdot10^{-13}x^3+2.37\cdot10^{-8}x^2-6.59\cdot10^{-4}x+35.90$
Water depth	H	m	$5.49\cdot10^{-15}x^3-4.43\cdot10^{-10}x^2+9.47\cdot10^{-6}x+8.50\cdot10^{-1}$
Water flow	Q	m^3/s	$4.42\cdot10^{-13}x^3-6.72\cdot10^{-8}x^2+3.07\cdot10^{-3}x+19.05$
Longitudinal dispersion coefficient	D_x	m^2/s	$D_x=0.058\frac{Q}{SB}$ [10]
Velocity	V_x	m/s	$V_x=\frac{Q}{HB}$

transport and transformations driving forces on pollutant distribution along the river length are taken into account, as well as the influence of space dependent river parameters. Simulation results are shown as graphical representation of pollutant concentration evolution in both space and time. They reveal similar behaviour of the analytical and numerical models for the simulated release.

Both models allow the assessment of the river distance affected by pollutant at certain moments of time after the release start, as presented in figure 3 and 4. The pollutant concentration in river at the source is 0.26 mg/L (fig. 3 and 4). Pollutant released at source will be transported along all investigated area in less than one day (fig. 3 and fig. 4).

Both models predict a concentration of 0.125 mg/L at the downstream boundary (178 km from the spring), reached after 23 h from the release start. Depending on the simulated pollutant such values (at the sources, at the downstream end) exceed the allowed limits of some metals (e.g. copper, lead); are very close to allowed concentration limits of some organic pollutants (e.g. detergents); or they are very much under allowed limits for some nutrients (e.g. nitrates). Examples of concentration limits are displayed in table 1.

The concentration profile in time at a certain distance downstream the polluting source may also be computed. As an example the time evolution of pollutant concentration at 44 km downstream the polluting source is shown in figure 5.

According to results of the analytical model the pollutant spill reaches the point situated at 44 km downstream the source after 6.7 h from the release start (fig. 5a). Concentration is increasing fast in the next 2.2 h, until it reaches the maximum value of 0.2 mg/l, further maintained constant during the release (if discharged pollutant flow and hydrodynamic conditions of the river are constant). The same concentration value is achieved also according to simulations of the numerical model (fig. 5b).

The computation time needed for obtaining the numerical solution (24 h of the real process time) is 142 s, compared to 43 s simulation time requested by the analytical model. The analytical approach proves to be less expensive and capable to provide simulation results in shorter computation time.

The analytical model requires less time for development, compared to the numerical one, needs less computer resources and is easier to implement. But on the other hand the numerical model is more flexible compared to the analytical one because adding; modifying or crossing out a source of any type is possible and easy to implement at any time. The core of the numerical model (the PDE) remains the same, and the elements to be specified are: location of the source, space distribution of the source, release duration, nature of discharge, initial and boundary conditions. For the analytical model to simulate the pollutant release from another type of source it is needed to implement in the model the PDE solution corresponding to that specific type of pollutant release [41].

Both models may be used to assess the transport of pollutants in Someş River in case of accidental release as well, as any kind of conservative or non-conservative pollutant can be simulated, and the source location can be specified and positioned anywhere along the investigated river section. They offer the opportunity to estimate the effects of pollutant release and to support users in taking decisions in order to manage efficiently necessary counteracting measures.

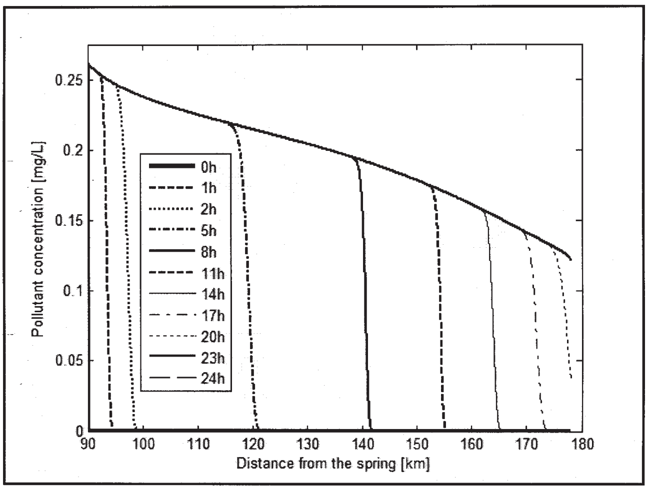


Fig. 3. Simulation results of the analytical model

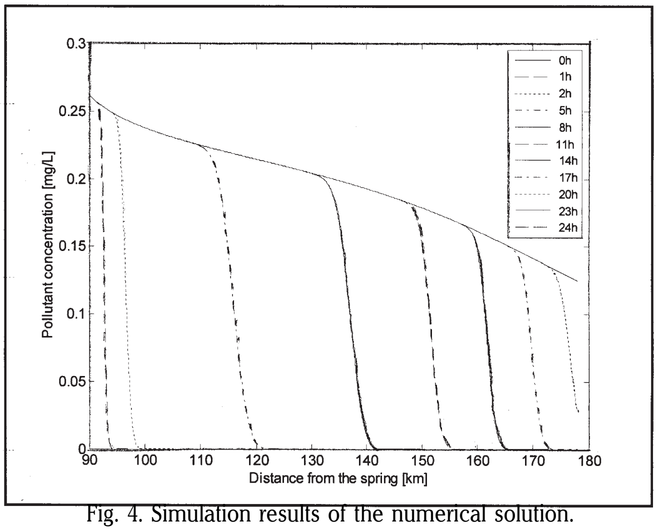
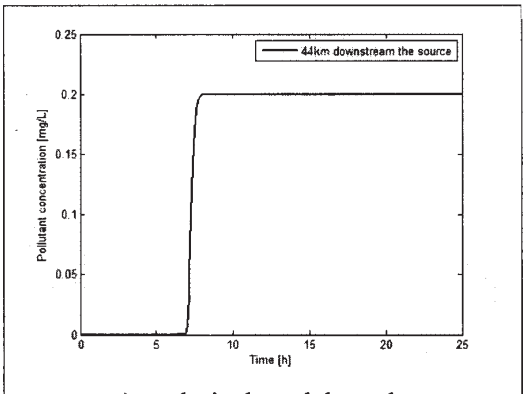
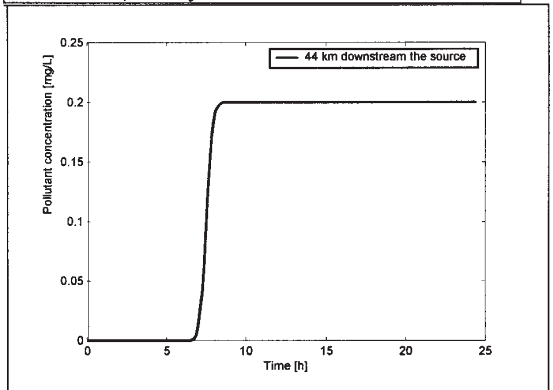


Fig. 4. Simulation results of the numerical solution.



a) analytical model results



b) numerical model results

Fig. 5. Evolution of pollutant spill at 44 km downstream the source (134 km from the spring) for: a) the analytical model and b) the numerical model

Conclusions

For the simulation of a continuous pollutant release in the Romanian Someş River two mathematical models were implemented, using MATLAB (for the analytical model) and COMSOL (for the numerical model). They provided similar results for predicting the time and space pollutant concentration evolution. Analytical model proved to demand less resources and computation time, compared to the numerical model which needed the triple amount of time to simulate the same pollution scenario.

Models use the same initial and boundary conditions and variable parameters along the investigated river segment. The proposed modelling approach based on analytical solution offers the possibility to use space dependent parameters along the modelled river length due to a novel technique of computing the pollutant mass flow released by the source. This approach considers the mass flow released by the source to predict the pollutant concentration in the river at the first computation step. Further, the mass flow of the source is replaced by the mass flow corresponding to predicted concentration from the previous computation step.

The models open up possibilities for the development of new and computation efficient computer tools for WQM and waste water treatment in the Someş River Basin. The numerical model will be further used to develop a system for continuous monitoring and on-line control of pollutant concentration, in order to counteract the negative effects of pollution on the Someş River ecosystem.

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