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POLUTANT'S CONCENTRATION IN THE LAKE –TESTING AND ANALYSIS OF A MODEL

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ABSTRACT

The modeling of pollutant's concentration in an artificial specific lake, created after coal mining with toxic organic chemicals is the subject of this paper. Typical modeling aim is to predict the pollutant concentration in the lake and its time evolution from field and laboratory observations. The lakes behaves as a completely mixed system with constant concentration everywhere in the lake water and equal concentration in water flowing out from the lake. As we found relevant observations from specific location including collection of sufficient field data, the parameterization of the selected model with calibration, testing and model sensitivity analysis were made.

Keywords: chemicals in the lake, concentration distribution modeling, parameterization and calibration of a model

1. INTRODUCTION

The problem of pollution of the lake formed after the cessation of coal mining exploitation is a common occurrence in some regions of Bosnia and Herzegovina [1]. A typical modeling aim is to predict the pollutant concentration in the lake and its time evolution from field and laboratory observations. The model results can be used to assess the likelihood that the pollutants can exceed a critical level, and how much and for how long, as may be necessary to know for making projects in order to protect the population and the entire environmental system. One simple model based on the mass conservation principle [4] has been developed and solved for pollutant concentration. Location of the selected lake that formed after the cessation of the exploitation of coal ore in the area of southern part of central Bosnia. The lake is pretty shabby, but the local population used for livestock and agricultural purposes.

It is assumed that the concentration of polluting particles is constant throughout the whole lake and equals the concentration in the water flowing out from the lake, actually groundwater. A particular lake has been observed and taken data from the field. The parameterization of the selected model including collection of sufficient field data was also made.

The lake has taken into account a number of tributaries, among which one of them found significantly higher concentrations of chemicals than other. The water flow of this is given in $m^3 day^{-1}$, total water outflow from the lake is also known, and the lake volume as well, constant with time. The laboratory experiments have shown how much the pollutant was biodegradated with a given rate *r* (in our case it is $r = kC$, where C is the concentration of toxic particles and *k* is taken from some empirical data and tested here. A rough initial value for this quantity was taken as 14,6 day^{-1}) . Konstant *k* is much lower in the lake than in the laboratory, as shown in calibration of model [3].

2. MASS-BALANCE MODEL AND SOLUTION FOR POLLUTANT CONCENTRATION

Based on the physical – chemical analysis [2] of problem we made the conceptual model of the mass balance, where the degradation rate was expressed from dimensional analysis, and set over the mass of pollutant relation with its concentration. The mass balance equation is [4]

$$\frac{dm}{dt} = Q_{main}C_{main} + Q_{trib}C_{trib} - (Q_{main} + Q_{trib})\frac{m}{V} - k\,m \qquad (1)$$

where indices „main“ and „trib“ refer to all tributaries and highly polluted one, respectivelly. The highly polluted tributary has been represented separately. The mass inputs come from tributaries and expressed as products of water flow rate *Q* and concetration of pollutant, *C*. The mass outflows are the water outflow that drain from the lake. *V* is volume of the lake, and *km* is degradation rate.

Knowing the values for the parameters at steady state d*m*/d*t*=0, Cout can be determined (*C*out = *m*/*V*) as

$$C_{out} = \frac{Q_{main}C_{main} + Q_{trib}C_{trib}}{Q_{main} + Q_{trib} + kV} \qquad (2) \qquad\qquad C_{out} = \frac{a}{b}(1 - e^{-bt}) \qquad (3)$$

If we want to know how long it takes to establish this concentration level, we need to find solution of the equation (1), analytically or by setting up a SIMILE model **[3]**. Analytical solution is given by equation (3) with constants

$$a = \frac{Q_{main}C_{main} + Qt_{rib}C_{trib}}{V} \quad \text{and} \quad b = \frac{Q_{main} + Q_{trib}}{V} + k\,. \qquad (4)$$

It can be seen that true steady state concentration can not be never reached, only could be approached. Figure 1. shows a SIMILE implementation model and actual time evolution of the pollutant concentration, as solution of equation (1) given by eq. (3) with main parameters and results which are given in the Table 1.

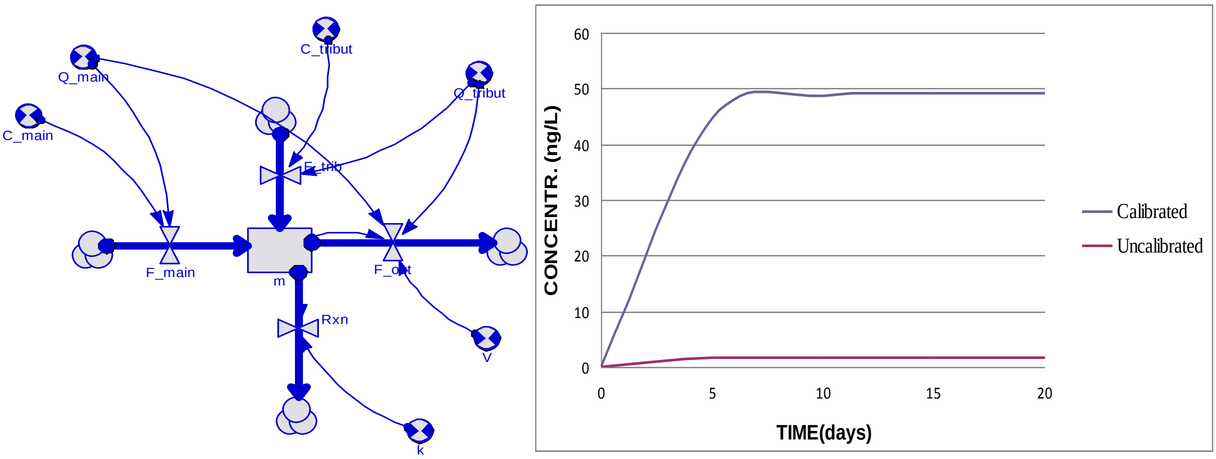

Figure 1. Model for a pollutant in lake with two types of tributaries and a degradation process: Left) SIMILE mass-balance model and Right) Modelled time evolution of the pollutant concentration in the lake with model parametrisation with respect to field findings.

We assumed that field observations reflect steady state situation with rate constant which is about 3% of the rate constant from laboratory findings. Than, our non-calibrated model gives concentration lower for mor than an order of magnitude. This can be associated with a slower rate of degradation in the reality than in laboratory, as the laboratory findings were used to quantify the degradation rate in the model. Here, the calibration of rate constant has made to the field data [2,5](see Figure 1. Right)). At the calibration the rate constant has been solved from equation (2) as the follow expression

$$k = \frac{Q_{main}C_{main} + Q_{trib}C_{trib}}{C_{out}V} - \frac{Q_{main} + Q_{trib}}{V} \qquad (5)$$

Table 1. Parameters for calibrated and non-calibrated model

	For calibrated	For uncalibrated	*t* (day)	*Cout* (ng/L) /Calibrated/	*Cout*(ng/L) /uncalibrated/
Qmain (m^3/day)	25	25	0	0	0
Qtrib (m^3/day)	0,2	0,2	5	44,5526409	1,589804
V (m^3)	14000	14000	10	48,7635200	1,589804
k (day^{-1})	0,47	14,6	15	49,1615099	1,589804
Cmain (μg/L)	5	5	20	49,1991258	1,589804
Ctrib(μg/L)	1000	1000			
A	2,3214E-05	2,3214E-05			
B	0,4718	14,6018			

3. THE MODEL TESTING

The accuracy of the model and its setting can only be tested with an independent set of data that are not used to create, parameterize or adapt the model. Usually, such „secondary „complete data are not available. As a possible suggestion, time-series observations have been divided into two parts, where the first part is used for parameterization of the model and settings, and the second part for the model testing.

In our case the second part of data was available. We assumed that pollutant was deposited with mine sludge in a small accumulation, and degradated by the same mechanism as in the case with the lake. There were no inflows of the pollutant into the accumulation except the waste after mining of coal, which get results for the known concentration of the pollutant in the pond water, known volume *V* and flow rate through the accumulation per day. Based on the assumption that all the pollutants get into the water immediately and using a constant rate of degradation we get the time evolution of the pollutant concentration in the pond.

This is actually the simplified model for the pond, for which the mass-balance equation has the form

$$\frac{dm}{dt} = -(Qout)\frac{m}{V} - km \tag{6}$$

The analytical solution of this equation is $m = m_0\, e^{-(\frac{Qout}{V}+k)t}$ (7)

where m_0 is the initial mass of pollutant in the accumulation. As $C = m/V$ we get

$$C = C_0 e^{-(\frac{Qout}{V}+k)t} \tag{8}$$

We also tested the model according to equation (8) and get the rationale behind approximate results from a given example. On the basis of the results we have seen that it is possible to predict the concentration of a pollutant in the lake , as well as the assessment of increasing its concentration in time. Used parameters were: C_0=0,1 mg/L, *Qout* = 20 m^3/day, *k* = 0,47 day^{-1}, *V* = 400m^3.

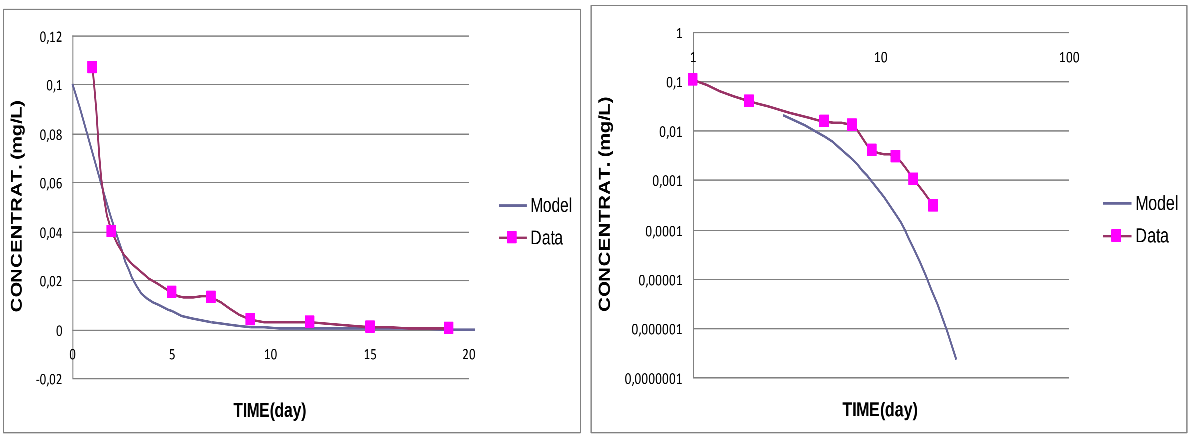

Figure 2. Modelled and observed concentrations of pollutant in the pond vs. time: LEFT-linear plot and RIGHT-logarithmic plot

The Figure 2. shows predictions for pollutant's concentration time evolution for linear and logarithmic function. The results on Figure 2 seems to indicate a fair agreement, but if we look the grapf RIGHT) on this figure., where the same results have been plotted in a logarithmic diagram, we can see, for relatively long times, the model systematically predicts a lower concentration than what was actually observed. In the percentage the discrepancy could be acceptable, as this occurs at very slow concentrations and for not so long time period. Depending of the use of the model results, this may or may not be acceptable.

4. MODEL SENSITIVITY, DOMINANT PHENOMENA AND CONCLUSION

The most important processes and parameters are those that have the greatest impact on the model results.One way of making a sensitivity analysis is to change the value of the parameter around it's expected value [3]. In the model for the lake we used a number of parameter values for modeling steady state concentration and conducted a sensitivity analysis expressed by percentage of change in concentration depending on the percentage of change in parameter. The diagram given on the Figure 3. shows results of this analysis. This indicates that the model has the same sensitivity to k and V, Qmain and Cmain and Qtrib and Ctrib, pair-wise. It means that these three groups of parameters are important than the individual values of parameters. The explanation lies in the fact that the expression of concentration is given over grouped products of mentioned parameters ($C_{out} = \frac{Q_{main}C_{main} + Q_{trib}C_{trib}}{kV}$). From this it can be possible to derive important conclusions of the sensitivity analysis model to parameter values and influence of „mathematics“ of the sensitivity analyses to dominant phenomena contribution.

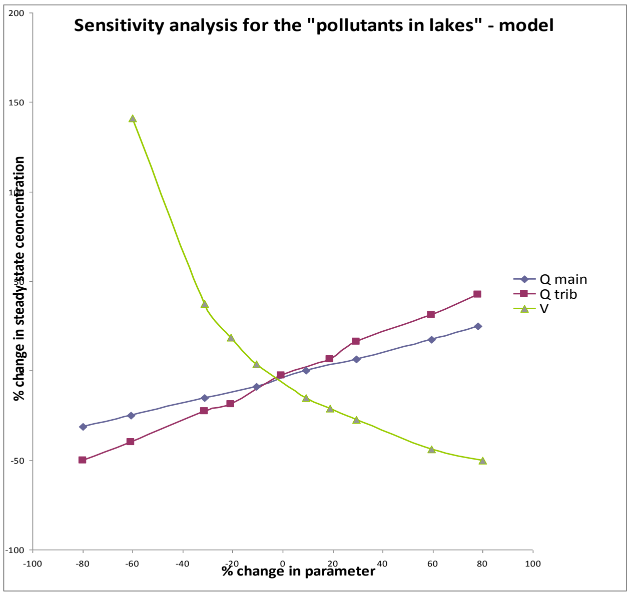

Figure 3. Sensitivity analysis-response in modelled C_{out} to change in parameter values at steady state and given k

As a conclusion it can be stated that collecting data from the field required for the establishment of a conceptual model, as well as the way how to reach this data for parameterization of the mathematical model is very demanding job.

Model has been adjusted by field observations, where this setting is actually an adaptation of the parameter values. The model results are most sensitive to the dominant processes and their parameterization. This has been searched by a sensitivity analysis, which actually helped deducing the uncertainty in the model results.

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