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APPLICATION OF HENRY-MICHAELIS-MENTEN KINETICS TO 2D ECOLOGICAL PROBLEM

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Abstract. ***In this work two-dimensional hydrodynamic model coupled with four-stages Henry-Michaelis-Menten kinetics was applied to simulate process of the lake simultaneous contamination and decontamination. In the process are involved the following species: the substrate S-contaminant, enzyme E-water cleaner , intermediate complex C, which arrives and finally disappears .The model is described by four coupled partial differential advection-reaction equations with known advective velocities U, V and kinetical parameters for direct and reverse chemical reactions k_1, k_{-1} and k_2, . The model captures the essential features encountered interaction between different chemical waste and enzyme-like cleaners of the lake. Known widely used model concentrates on the two-stage interaction for the species S and P .The main objective is obtaining an improved insight on waste contamination and decontamination for the lake.***

Keywords: lake, contamination, Henry-Michaelis-Mentenkinetics ,water decontamination.

1 INTRODUCTION

Water pollution is a very dangerous process. It occurs when the body of water is adversely affected due to the addition of large amounts of materials to water. There are different types of water pollution: toxic substances, organic substances and industrial waste etc. Also the pollution can occur from neighborhoods with poor residential loan quality, from not disposed garbage and large agricultural areas that use chemicals as fertilizers and pesticides, which runoff into a body of water contribute release of toxic materials into rivers, lakes and the ocean. Without proper filtration of these pollutants, they can harm animals, plants, oceanic ecosystems, soils and other natural resources of the earth. Today over half a billion people live in areas where they consume and rely on polluted water for their survival. It was estimated that thousands of marine mammalians are killed every year by pollution. In our paper we provide some mathematical instruments to obtain an improved insight on the condition of water contamination and decontamination processes. In the case when the pollutant is modelled as dispersed down a shallow stream, the concentration is a function of time and just one space variable and time. The fundamental equation describing transport of chemicals and microbes in the environment for such a case is advection-reaction equation [1],[2]. If the pollutant was dispersed in a shallow lake's surface, the concentration is a function of time and two space variables. Thus the set of the coupled advection-reaction equations would be a suitable tool.

2.GOVERNING EQUATIONS

Consider problem on chemical waste transfer and degradation in a shallow lake .The waste were dispersed in the lake by the wind with velocities U, V [3],[4]]

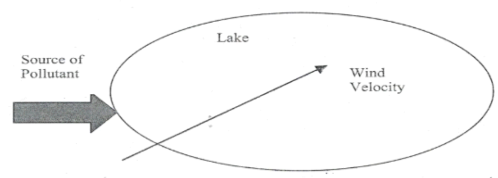

Fig.1.Scheme of the pollutant transfer in an arbitrary-shaped lake .

Its reaction scheme is known as Henry- Michaelis-Menten (HMM) scheme [5],[6] which is depicted using chemical notation as follows:

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} SE \xrightarrow{k_2} P + E.$$

It is suggested that four species are involved in the reactions chain: the substrate S-contaminant which is a source of lake pollution, enzyme E, representing the water cleaner from the contaminant, intermediate complex C- which arrives and disappears and decontaminated product P. Respectively, the mathematical model is described by four advection-reaction equations with known advective velocities

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U, V and kinetical parameters for direct and reverse reactions k_1, k_{-1} and k_2. For simplicity we choose a rectangular lake which length and width are measured in the kilometers. In such a case the governing equations are four advection-reaction equations written as follows:

$$\frac{\partial S}{\partial t} = U\frac{\partial S}{\partial x} + V\frac{\partial S}{\partial y} - k_1 ES + k_{-1}C \quad (1)$$

$$\frac{\partial E}{\partial t} = U\frac{\partial E}{\partial x} + V\frac{\partial E}{\partial y} - k_1 ES + (k_1 - k_2)C \quad (2)$$

$$\frac{\partial C}{\partial t} = U\frac{\partial C}{\partial x} + V\frac{\partial C}{\partial y} - k_1 ES - (k_1 + k_2)C \quad (3)$$

$$\frac{\partial P}{\partial t} = U\frac{\partial P}{\partial x} + V\frac{\partial P}{\partial y} + k_2 C \quad (4)$$

Here: t, x, y are the time and Cartesian coordinate. Initial conditions are given as zero concentrations of the species at time $t = 0$, i.e.

$$\begin{cases} S(x,y,0) = 0, & E(x,y,0) \\ C(x,y,0) = 0, & P(x,y,0) = 0 \end{cases} \quad (5)$$

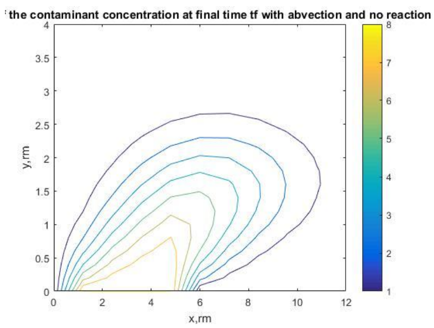

Fig.2.Plane view of the isolines for the contaminant *S* concentrations with *HMM* reaction at the duration time *T*.

The only exception is the upwind boundary of the lake where the Dirichlet boundary conditions are prescribed as follows:

$$S(x,y,t) = S_0, \quad (y = 0, a, x, b)(6)$$

$$E(x,y,t) = E_0, \quad (y = 0, a, x, b)(7)$$

$$C(x,y,t) = C_0, \quad (y = 0, a, x, b)(8)$$

$$P(x,y,t) = P_0, \quad (y = 0, a, x, b)(9)$$

Here $y = 0$ and $a < x < b$ are the coordinates of the dumping site for chemicals placed at the southern upwind boundary of the lake.

Conditions (7)-(9) for the equations (1)-(4) on the dumping site are imposed following approach applied for investigation of the three –members chemical species chain in the soil [7].Similar approach was developed [8] for the constant flow rate boundary conditions.

In the present work is introduced the duration time *T*,in hours. It is the time sufficient for contaminant starting at the dumping site to arrive close to the right boundary of the lake. Thus *T* is used to determine model run duration in the numerical experiments.

3.NUMERICAL SOLUTION

Equations (1)-(4) subjected to the boundary conditions (6)-(9) were solved numerically by means of the explicit method described in details in works [3],[4] using MATLAB-2016 computational package. Input data for the model are summarized below in the Table 1.It should be noted that system (1)-(4) could be reduced to the system of two equations for substrate *S* and product *P* assuming that concentrations of the enzyme *E* and complex *C* are the constant values during the duration *T* of modeling [9].In this work MATLAB-2016 solves non-reduced four-equations system. Thus model output also includes data on the time-dependent concentrations for *E* and *C* behavior which o may be of special interest for better understanding of the contamination and decontamination processes

RESULTS AND DISCUSSION

Scenario 1. The advective velocities U, V are non-zeros but reaction constants k_1, k_{-1}, k_2 are all zeros. Calculations show that the concentrations of the $S-$specie at time T are redistributed with strong dependence on the wind velocities as is depicted in the attached Fig.2.It can be concluded from the Fig.2 that near the dumping site *S*-isolines are triangularly-shaped curves.

Scenario 2. The advective velocities U, V and reaction constants k_1, k_{-1}, k_2 are non-zeros. Full model consists from four coupled transient $2D$ advection-reaction partial differential equations describing simultaneously concentrations of the contaminant, cleaner, intermediate complex and clean product: $S, E, C., P$ .Solutions of the equations at above mentioned duration time T is obtained by explicit method [3],[4]. Concentration isolines for product P are given at the Fig.3 as a set of the closed curves.

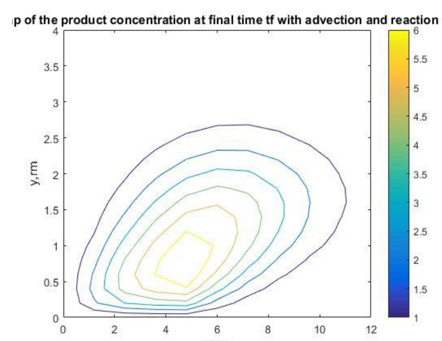

Fig.3.Plane view of the isolines for the product *P* concentrations with *HMM* reaction at the duration time *T*.

Table 1. Variables and parameters values

No.	Parameter	Dimension	Value
1.	L-length of the lake	kilometer	12
2.	W -width of the lake	kilometer	4
3.	U – velocity of the wind in the x-direction	kilometer/hour	0.5
4.	V -velocity of the wind in the y-direction	kilometer/hour	0.2
5.	T-duration of the model run	hours	10
6.	S_0 -substrate concentration on the waste dumping site	mole	8
7.	E_0 -enzyme concentration on the waste dumping site	mole	4
8.	C_0 -complex concentration on the waste dumping site	mole	0.3
9.	P_0 -product concentration on the waste dumping site	mole	0.1
10.	k_1-direct first reaction rate	1/(mole*hour)	2
11.	k_{-1} -reverse first reaction rate	1/hour	1
12.	k_2 - second reaction rate	1/hour	1.5

Results of the computer simulations performed at the Scenario 2 for *E* and *C* concentrations isolines are depicted in the Fig.4 , Fig.5 and Fig.6 which are given below . Note that both *E* and *C* are valuable resources applied in the industrial works for the sustainable lake environment. Thus obtained information on these species could be important from the economical point of view.Fig.6 presents isolines for the contaminant *S* concentrations at the duration time *T*. Comparison between Fig.6 and Fig.2 could be used for evaluation of the effectivity of the cleaning process.

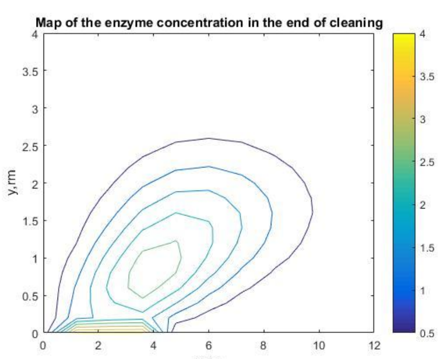

Fig.4. Plane view of the isolines for the enzyme *E* concentrations with *HMM* reaction at the duration time *T*.

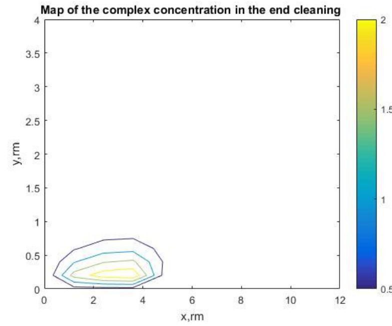

Fig.5.Plane view of the isolines for the complex *C* concentrations with *HMM* reaction at the duration time *T*.

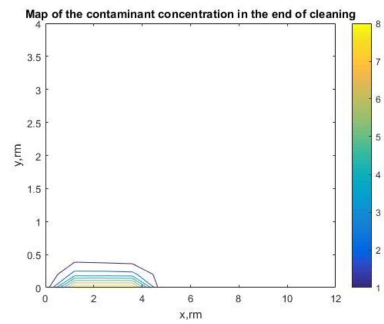

Fig.6. Plane view of the isolines for the contaminant *S* concentrations at the duration time *T*.

Consider together Fig.2 for the substrate *S*-isolines and Fig.3 for the product *P*-isolines. There is no strong dependence on the wind for product *P* -isolines with comparison to the substrate *S* - isolines. It may be explained in such a way that at the duration time *T* advection term is partially suppressed by the reaction term in the equation (4).

5.CONCLUSION

In present work the coupled problems of simultaneous chemical contamination –decontamination of a shallow lake is considered following approach developed by Henry, Michaelis and Menten. Results give a new insight and may be useful for understanding of the complicated processes accompanying dumping of the waste in lakes. Obtained solution for *E* -species may be explained by suppression of the advection term by chemical term in the equation (4).This could be taken into consideration for proper design measures for the lake environment protection from the chemical contamination.

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