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Mathematical modeling of multi-input heavy metals in drainage systems

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Abstract— In this paper, a mathematical model of one dimensional advection diffusion equation with sink or source and multi-inputs of heavy metals is introduced in drainage systems. The finite difference method is used to predict the concentration of the heavy metals in certain time and at specific distance for multi inputs at different times.

Keywords —Finite difference; Advection diffusion equation; Multi-input sources.

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1 Introduction

There has been a growing concern in the international community and an increased awareness of the drainage systems pollution problems, particularly with regard to water pollution [1] Many drainage systems have suffered environmental damage due to discharges from manufacturing processes and wastewater from centres of pollution over several decades [2]. In recent years these environmental concerns have made the development of mathematical models that predict the diffusion of pollutants in natural water systems more urgent [3]. The main attraction of such models, in contrast with physical models, is their low cost and the fact that they easily adapt to new situations. Thus the widespread popularity of mathematical modeling techniques for the hydrodynamic and pollutant transport in rivers justifies any attempt to develop new models based on novel and rigorous approaches [4].

This paper describes numerical modelling of heavy metals in a drainage system. It would be necessary to recognize and introduce the heavy metals behaviors and different processes during their transportation along the drainage; for example their sources, chemical and physical reactions, and also introducing the environmental conditions affecting the rate of concentration variability of these substances. The one-dimensional partial differential equation governing equations (PDE) of hydrodynamic and water quality will be fully described with the corresponding numerical solution methods. As a part of water quality PDE equations the one dimension Advection-Diffusion will be described and it will be shown that how the dissolved heavy metals may be numerically modeled through the source term of this equation [5].

Numerical models provide a valuable tool for predicting flow, pollutant and sediment transport process and are increasingly applied by engineers and environmental managers. Accurate numerical model prediction of pollutant concentrations can assist in the planning, design and management of the structures related to the river basins and irrigation and drainage networks. The numerical models provide an approximate solution to the governing partial differential equations, so, using the higher order finite difference accurate schemes has become popular [6].

2 The Governing Equation

The basic governing equation, which is based on the principle of conservation of mass and Fick's law is known as the 'Advection-Diffusion Equation. Fick's law states that the flux of solute mass, that is, the mass of solute crossing a unit area per unit time in a given direction, is proportional to the gradient of the solute concentration in that direction

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[7].

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x} \pm kC \qquad (1)$$

Where,

C = Average heavy metal concentration $\left[ML^{-3}\right]$

D = Longitudinal diffusion coefficient $\left[L^2 T^{-1}\right]$

U = Average velocity $\left[LT^{-1}\right]$

k = Rate of reaction coefficient $\left[T^{-1}\right]$, which may have a positive or negative value as the dissolved heavy metals disappears or accumulates in a given drainage system. The reaction coefficient can be affected by several environmental factors such as: temperature pH and salinity

3 The Finite Difference Method

In this paper we have solved the one dimensional advection diffusion equation with reaction term using finite difference method namely FTCS used by B. Ataie et al [8]. The detail of the method as the following

$$\frac{\partial C}{\partial t} = \frac{C(i,j+1) - C(i,j)}{\Delta t}$$

$$\frac{\partial C}{\partial x} = \frac{C(i+1,j) - C(i-1,j)}{2\Delta x}$$

$$\frac{\partial^2 C}{\partial x^2} = \frac{C(i+1,j) - 2C(i,j) + C(i-1,j)}{(\Delta x)^2}$$

Substituting in equation (1) yield

$$\frac{C(i,j+1) - C(i,j)}{\Delta t} = D\left[\frac{C(i+1,j) - 2C(i,j) + C(i-}{(\Delta x)^2}\right] - U\left[\frac{C(i+1,j) - C(i-1,j)}{2\Delta x}\right] - kC(i,j)$$

Multiplying both sides by Δt and rearranging

$$C(i,j+1) = \left[1 - 2D\frac{\Delta t}{(\Delta x)^2} - k\Delta t\right]C(i,j) + \left[D\frac{\Delta t}{(\Delta x)^2} - U\frac{\Delta t}{2\Delta x}\right]C(i+1,j) + \left[D\frac{\Delta t}{(\Delta x)^2} + U\frac{\Delta t}{2\Delta x}\right]C(i-1,j)$$

In the next subsections, the model will be studied in some different initial and boundary conditions with the constants as in the Table.

Velocity (U)	0.016 m/s
Diffusion (D)	0.2 m^2/s
Reaction coefficient (k)	1e-6 1/s

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3.1 Constant initial condition

In this case the initial and boundary conditions are

$$C(x,0) = 0$$

$$C(0,t) = C_0$$

$$C(\infty,t) = 0$$

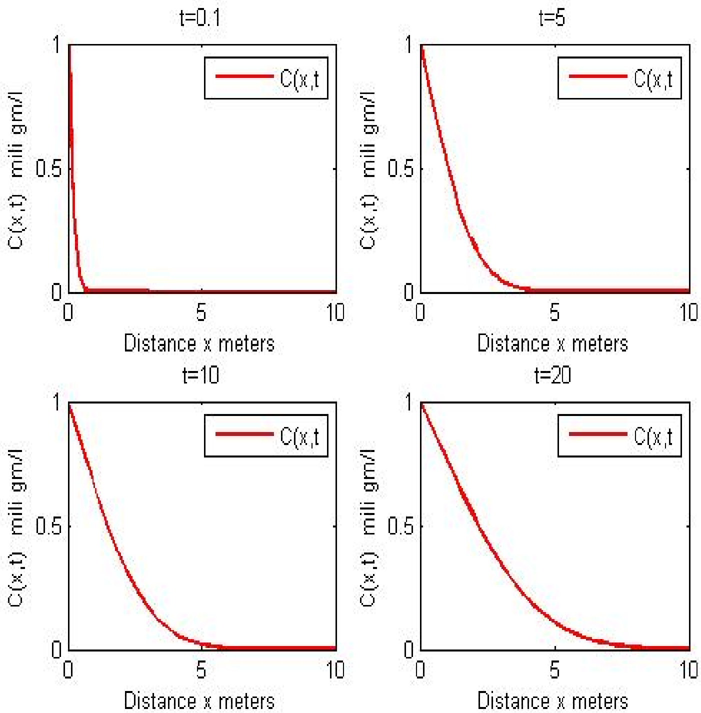

Fig. (1) The relationship between concentration and distance at different times, $C_0 = 1$

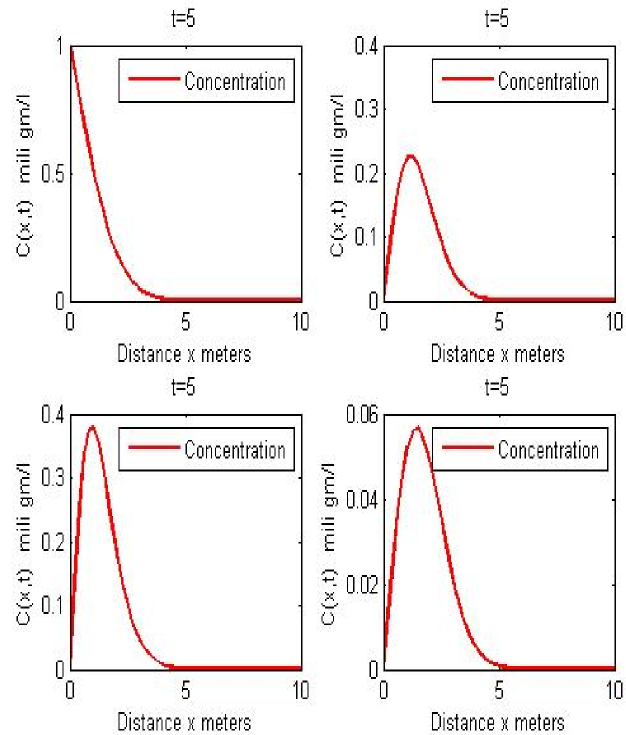

Fig. (2) The relationship between concentration and distance at different times with $t_0 = 5, 3, 4$ and 1 sec

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3.2 Unit step initial condition

$$C(x,0) = 0$$

$$C(0,t) = C_0 U(t - t_0)$$

$$C(\infty,t) = 0$$

In this model the attenuation of concentration with distance is faster than the first one due to the nature of the unit step source input.

3.3 Multi input with constant initial condition

$$C(x,0) = 0$$

$$C(0,t) = C_1, \quad C(x_1,t_1) = C_2$$

$$C(\infty,t) = 0$$

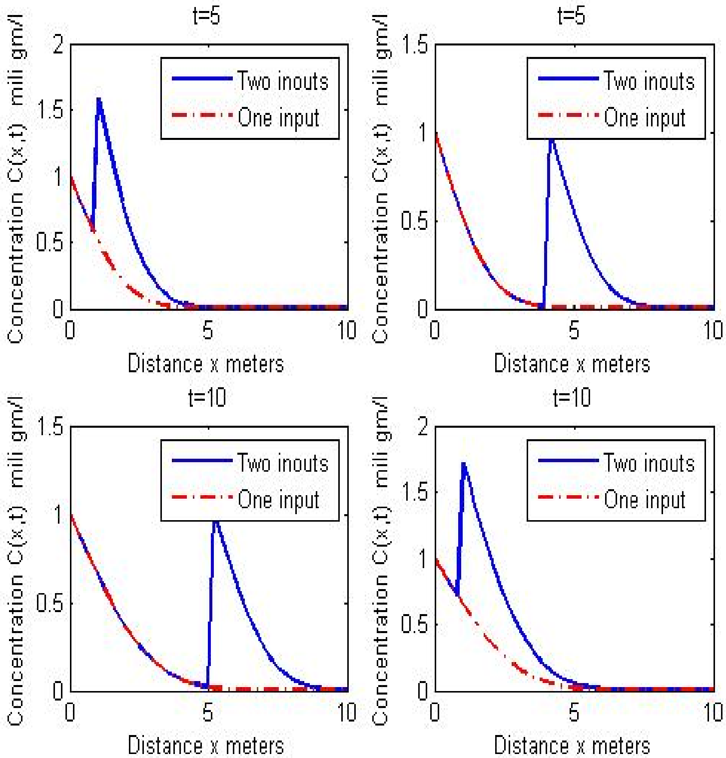

Fig. (3) The relationship between concentration and distance at different times with $\left(x_1,t_1\right)=(1,1),(4,1),(5,5),(1,3)$

In this model, we assume that a second constant source of heavy metals is added to the stream at different distances and times. Due to this second sours the graph show that the concentration is sometimes greater than 1 mg .

3.4 Multi input unit step initial condition

$$C\left(x,0\right)=0$$

$$C\left(0,t\right)=C_1U\left(t-t_0\right),\ C\left(x_1,t_1\right)=C_2U\left(t-t_2\right)$$

$$C\left(\infty,t\right)=0$$

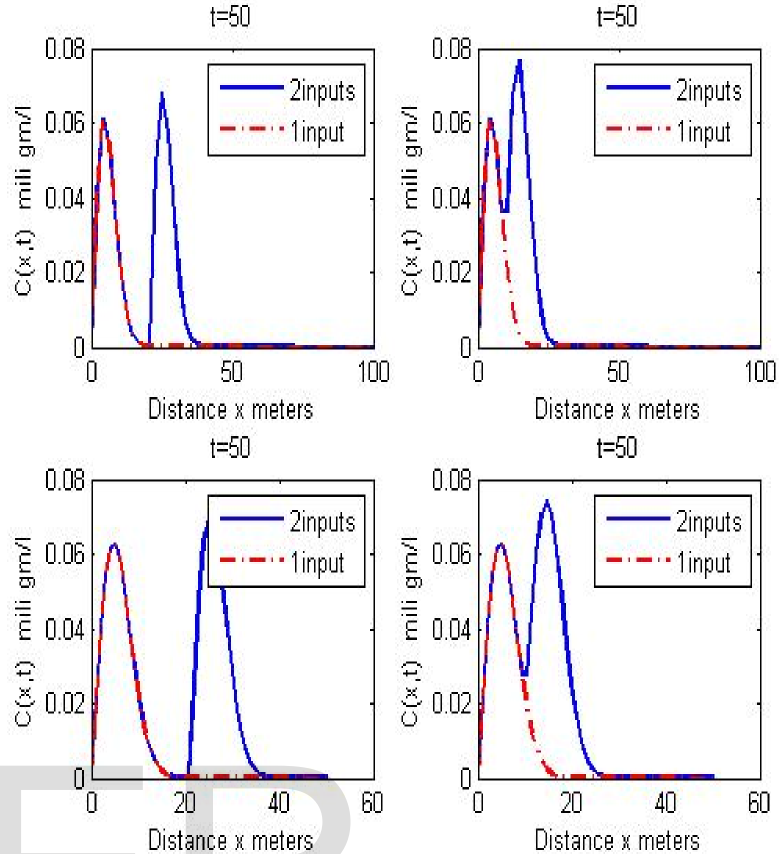

Fig. (4) The relationship between concentration and distance at different times with $C_1=C_2=1,t_0=t_2=10,\left(x_1,t_1\right)=(20,5),(10,5),(20,5),(10,5)$

This model similar to the previous one except that the input sources are not constants.

4. Conclusions

In this work, a finite difference method is used to solve the advection diffusion equation in one dimension with one source input, two sources input of heavy metals at different times and different distances. In the multi input sources the suggested algorithm is used to compute the concentration of heavy metals at position and time where the second source input is installed. The computed concentration is added to the second source and this sum will be considered as an input for the next stage. The concentration of heavy metals is computed for constant and unit

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step initial conditions.

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