Numerical Analysis of Heavy metals transport through soil media with second order decay

Arpita Deodikar[1], Dr. Avneesh Kumar[2]

1: Research Scholar, Department of Applied Sciences, Dr. K. N. Modi University, Newai, Rajasthan.

2: Assistant Professor, Department of Applied Sciences, Dr. K. N. Modi University, Newai Rajasthan.

ABSTRACT:

A mathematical model to analyse heavy metals dispersion in homogeneous, isotropic aquifer under the influence of a second order decay with constant seepage velocity is presented. A finite difference implicit scheme (ADI) has used to solve 2- dimensional transport equation. Numerical experiments were carried out for two different time dependent source input. The influence of different values of second order decay parameter (μ) on the transport of contaminants plume has been studied for two, four and six years of simulations. The results obtained by the present study indicate that as decay parameter increases, spreading of contaminant reduces significantly. The disposal scheme for short duration with higher concentration (scenario II) is found to be better option in comparison with the disposal scheme for longer duration with less concentration (scenario I).

Key words: Mathematical modelling, porous media, ADI scheme, disposal scheme, differential equation

INTRODUCTION:

The importance of this study concerning of chemical substance decay is apparent with current problem of pollution in the environment. It has been a common practice to discharge the waste material in the soil. Due to dumping of such hazardous waste viz, heavy metals, fertilizers and radioactive substances increase in groundwater pollution has been observed. In order to control the contamination concentration in ground water the understanding of the rate of contaminants dispersion and its decay are necessary.

Several researchers have presented numerical and analytical solutions to one-dimensional and two-dimensional chemical transport problem. Van Genuchten (1981) have presented complete set of solutions for adsorption, zeroth order production and first order decay considering it as one-dimensional problem. The method of obtaining analytical solution for chemical transport in two-dimensional aquifer is presented by Latinopoulos et. al. (1988) without considering any of these terms. As the decay mechanism reduces the strength of concentration naturally, this has been accounted in the present model by considering second order decay. Kool et. al. (1994) has studied subsurface transport of degrading contaminant from land disposal sites by using composite modelling approach. Das et. al. (2000) has presented a numerical model for two-dimensional solute transport in porous media with first order chemical reaction at the upper boundary under various types of disposal schemes. Although various numerical models for contaminant transport are being widely used, the numerical model with second order decay to minimize the contaminant concentration in an aquifer is of special interest.

The numerical model developed for solving chemically active contaminant transport may find its application in making initial estimate on the extent of aquifer contaminant and for selecting suitable source disposal source scheme.

STATEMENT OF THE PROBLEM:

Consider a homogeneous, isotropic plane aquifer of length “L” under the constant seepage velocity with a finite strip of contaminant source of length “a” aligned along y-axis from the top. We apply a cartesian co-ordinate system in which x-axis is in longitudinal direction and y-axis is along the depth of the aquifer (Fig1).

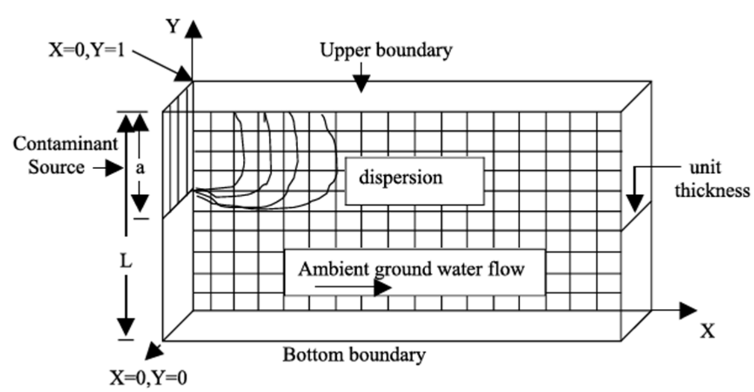

Fig 1: Schematic cross-sectional representation of contaminant transport in an aquifer

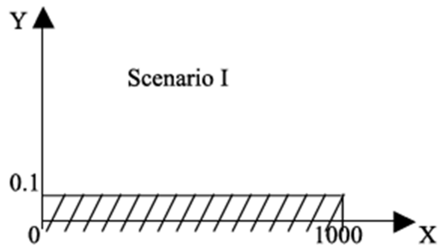

Fig 1(a): Input with longer duration
and less concentration

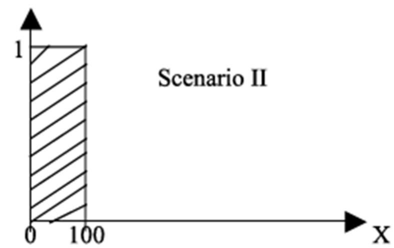

Fig1(b): Input with short duration
and higher concentration

The partial differential equation describing two-dimensional chemical transport with second order decay can be described as,

$$D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} - \vartheta \frac{\partial c}{\partial x} - R \frac{\partial c}{\partial t} = \gamma c^2 \qquad (1)$$

Where c is the solute concentration (M/L^3), v is average seepage velocity (L/T), R is the and γ is the decay coefficient. D_x and D_y are longitudinal and vertical dispersion coefficient respectively (L^2/T).

The corresponding initial and boundary conditions can describe as

$$c(x, y, 0) = c_i \qquad (2a)$$

$$c(x, y, 0) = c_{input} \qquad y>L-a,\ t \geq 0$$

$$= c_i \qquad \text{otherwise} \qquad (2b)$$

$$\lim_{y \to L} \frac{\partial c}{\partial y} = 0 \qquad \lim_{x \to \infty} \frac{\partial c}{\partial x} = 0 \qquad \lim_{x \to 0} \frac{\partial c}{\partial x} = 0 \qquad (2c)$$

Where c_i is the initial concentration of the aquifer and c_{input} is the source concentration. Normalizing the aquifer dimensions and variables, the transport equation reduces to

$$D_L \frac{\partial^2 C}{\partial X^2} + D_T \frac{\partial^2 C}{\partial Y^2} - \frac{\partial C}{\partial X} - R \frac{\partial C}{\partial T} = \mu C^2 \qquad (3)$$

Where

$$X = \frac{x}{L}\ ,\ Y = \frac{y}{L}\ ,\ C = \frac{c}{C_0}\ ,\ T = \frac{tV}{L}\ ,\ D_L = \frac{D_x}{LV}\ ,\ D_T = \frac{D_y}{LV}\ ,$$

$$\mu = \frac{\gamma C_0 L}{V}\ ,\ C_i = \frac{c_i}{C_0}\ ,\ C_{input} = \frac{c_{input}}{C_0}\ ,\ A = \frac{a}{L} \qquad (4)$$

The corresponding initial and boundary conditions in the dimensionless form are

$$C(X, Y, 0) = C_i \qquad (5a)$$

$$C(X, 0, T) = C_{input}\ , \quad Y > 1 - A\ ,\ T \geq 0$$

$$= C_i \quad \text{otherwise} \qquad (5b)$$

$$\lim_{y \to 1} \frac{\partial C}{\partial Y} = 0 \qquad (5c)$$

$$\lim_{x \to 0} \frac{\partial C}{\partial X} = 0 \qquad \lim_{x \to \infty} \frac{\partial C}{\partial X} = 0 \qquad (5d)$$

The governing equation (3) described is solved by using initial and boundary conditions described in equation (5a)- (5d) and employing finite difference scheme, specifically by using Alternate Direction Implicit (ADI) method.

The idealized problem presented here deals with the comparative study between two simple contaminant disposal schemes.

Scenario I:

In this scenario, a constant concentration of 1000 ppm has been considered for 1000 days of input (Fig. 1a)

Scenario II :

To keep the total volumetric inflow concentration to be same, 100 days released with input concentration equal to 10,000 ppm has been considered (Fig 1b).

It is assumed that the solute rate inflow is proportionally analogous to the input concentration in both of these cases.

NUMERICAL COMPUTATION:

Owing to the complexity of analytical solution of equation (3) with respect to the boundary conditions, Alternate Direction Implicit (ADI) scheme of finite difference technique is adopted.

This is based on implicit approach of the Douglas Rachford difference scheme. The details of the scheme and its finite difference representation are described by Das et. al. (2000). To get an insight in to the dispersion process, numerical computation has been carried out by assuming the values of various parameters as, $D_L = 0.5,\ D_T = 0.05,\ A = 0.5,\ \Delta T = 0.0025,\ R = 1.0$.

Initially the aquifer is free from contaminant i.e $C_i = 0$. The concentration released from the strip source of length 'a' along y-axis from the top is considered for both the scenarios I and II. The model area covers non-dimensional distance varying from 0 to 0.5 along the length of the aquifer and 0 to 1.0 along the depth of the aquifer. A square grid cell with $\Delta X = \Delta Y = 0.1$ is considered for which the total number of grid cells along (X, Y) direction becomes (50, 10). The resulting finite difference equations become simultaneous linear algebraic equations with tridiagonal coefficient matrix of the form,

$$P_1 C_{i,j-1}^{n+1} + Q_1 C_{i,j}^{n+1} + R_1 C_{i,j+1}^{n+1} = S_j \quad (6)$$

In Y-sweep,

Where $P_1 = R_1 = \frac{D_T}{(\Delta Y)^2}$ (7)

$$Q_1 = -\left(\frac{R}{\Delta T} + \frac{2D_T}{(\Delta Y)^2} + \mu\, C_{i,j}^{n}\right) \quad (8)$$

And

$$S_j = -\left(\frac{1}{2\Delta X} + \frac{D_L}{(\Delta X)^2}\right) C_{i-1,j}^{n} + \left(\frac{2D_L}{(\Delta X)^2} - \frac{R}{\Delta T}\right) C_{i,j}^{n} + \left(\frac{1}{2\Delta X} - \frac{D_L}{(\Delta X)^2}\right) C_{i+1,j}^{n} \quad (9)$$

Similarly in X-sweep,

$$P_2 C_{i,-1,j}^{n+2} + Q_2 C_{i,j}^{n+2} + R_2 C_{i,-1,j}^{n+2} = S_i$$

Where

$$P_2 = -\left(\frac{1}{2\Delta X} + \frac{D_L}{(\Delta X)^2}\right) \quad (11)$$

$$Q_2 = \left(\frac{2D_L}{(\Delta X)^2} + \frac{R}{\Delta T} + \mu\, C_{i,j}^{n+1}\right) \quad (12)$$

$$R_2 = \left(\frac{1}{2\Delta X} - \frac{D_L}{(\Delta X)^2}\right) \quad (13)$$

$$S_i = \frac{D_T}{(\Delta Y)^2} C_{i,j-1}^{n+1} - \left(\frac{2D_T}{(\Delta Y)^2} - \frac{R}{\Delta T}\right) C_{i,j}^{n+1} + \frac{D_T}{(\Delta Y)^2} C_{i,j+1}^{n+1} \quad (14)$$

The finite difference analogues of the entry and boundary conditions are also discussed accordingly. I order to solve equations (6) and (10), tridiagonal solver has been used. This ADI method applied here gives rise to an unconditional stable difference scheme with second order accuracy.

RESULT AND DISCUSSION:

Due to non-dimensional analysis, aquifer concentration is made to vary between 0 and 1. The transport process is subjected to the study under two scenarios of input. The numerical simultaneous were carried out it for a maximum period of six years with three values of second order decay parameter ($\mu = 0.1, 10, 20$). The results are stidied for the evolution of the zone of contaminanats in two years, four years and six years if simulations.

Scenario I:

In the first scenario, constant concentration of 10% strength with respect to maximum concentration has been considered for 1000 days of input. Assuming the dilution strength of 1% with respect to maximum concertation as potentially harmful, the monitoring concentration has been chosen as 0.01. It has been observed from the Fig. 2(a) that after two years of simulation, the concertation plume progresses up to 40% distance in the longitudinal direction and 70% distance along the depth of the aquifer Figs 2(a)-2(c) shows the significant influence of decay parameter for two years of simulation, At the end of four years of simulation, concentration plume moves up to a distance (non-dimensional) 3.2 for $\mu = 0.1, 3.1$ for $\mu = 10$ and 2.9 for $\mu = 20$. Similarly, along the vertical direction of the aquifer ot spread up to 90% of the depth for $\mu = 0.1$, 80% depth for $\mu = 10$ and 70% depth for $\mu = 20$. This evident from figs 3(a)-3(c). The effect of decay parameter on the spread of contaminant is found to be very significant for six years of simulation Fig 4(a)-4(c). In all the cases the plume advances towards the right boundary in comparison with the four years of simulation. For small decay parameter ($\mu = 0.1$), the plume spread out by 5 grids in the longitudinal direction in comparison with four years of simulation and also touches the bottom boundary. When decay parameter is moderate ($\mu = 10$), the concentration of the plume reduces significantly. For higher decay rate ($\mu = 20$), contour lines with only 0.01 concentration are noticed showing significant reduction in the area of spreading. In this case it spreads six along vertical direction and 24 grids along the longitudinal direction. As the period of simulation increases, contour lines attain near symmetric profile.

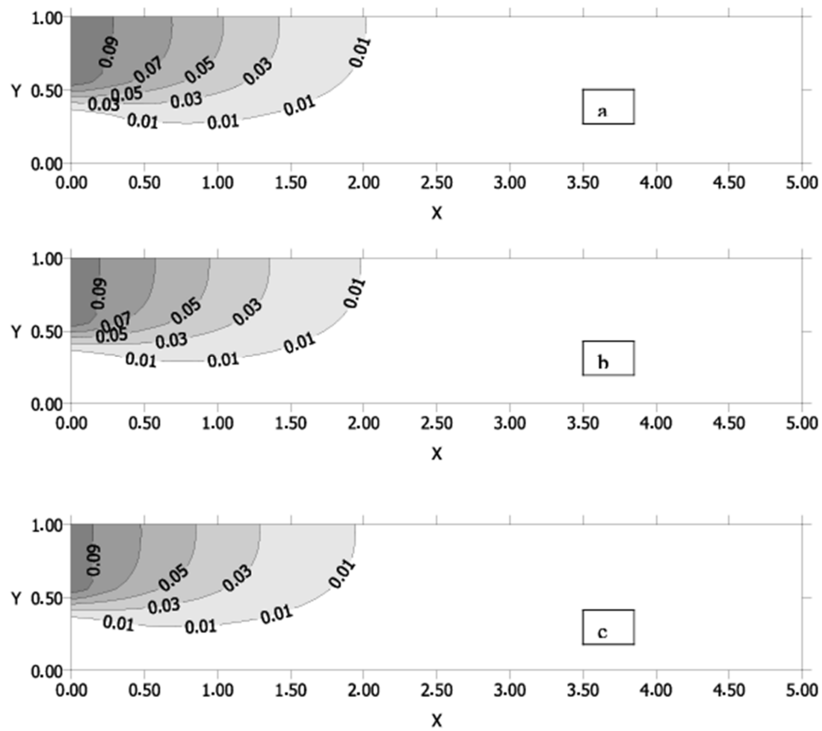

Fig 2: Evolution of the zone of contaminant concentration in two years simulation with second order decay for $\mu = 0.1, 10$ and 20 (Scenario I)

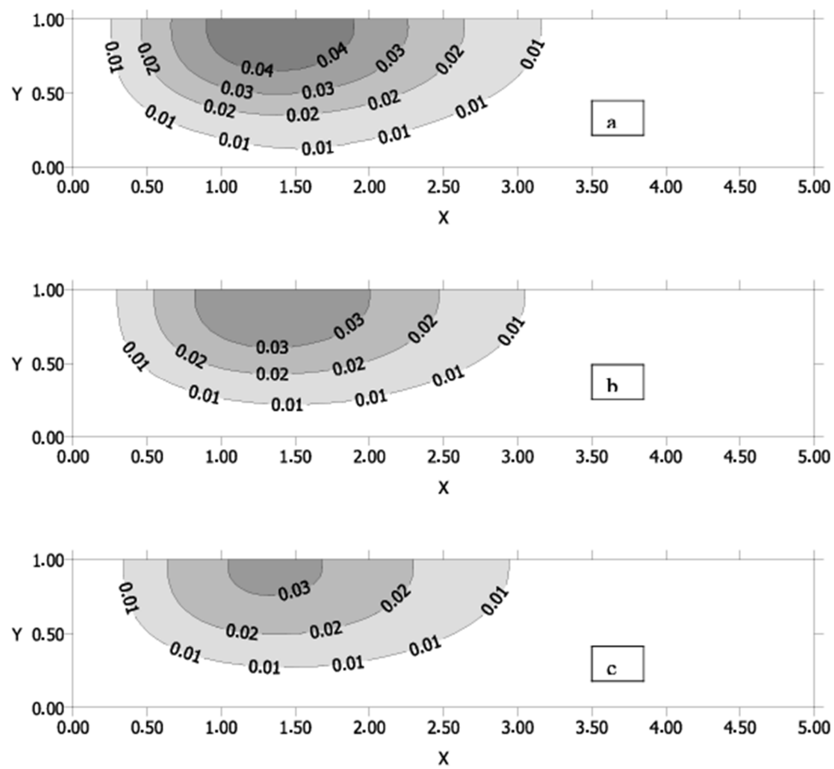

Fig 3: Evolution of the zone of contaminant concentration in four years simulation with second order decay for $\mu = 0.1, 10$ and 20 (Scenario I)

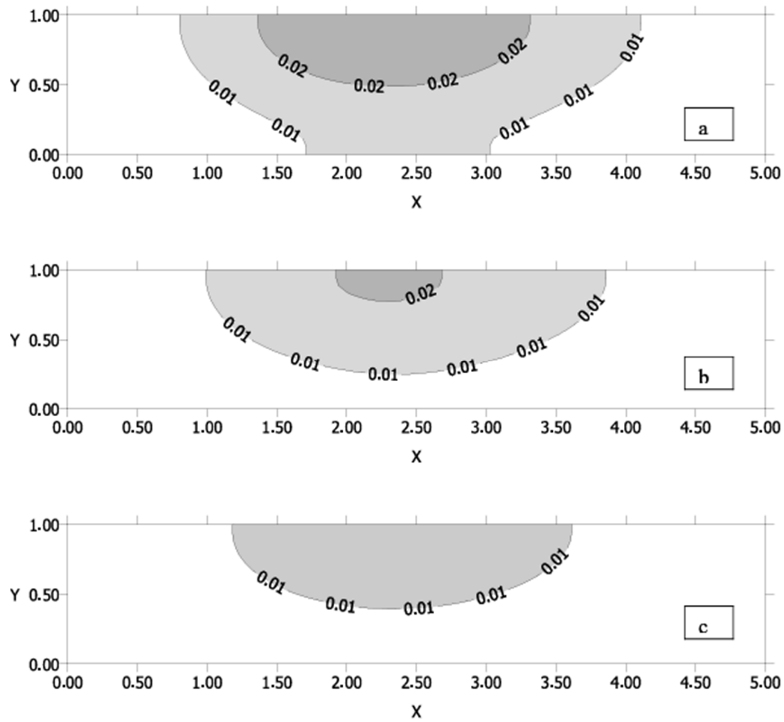

Fig 4: Evolution of the zone of contaminant concentration in six years simulation with second order decay for $\mu = 0.1, 10$ and 20 (Scenario I)

Scenario II:

In the second scenario, full concentration (100%, normalized to unity) has been considered for 100 days of input. As the entire source is being discharged within 100 days, two years of simulation shows closed contour lines. It has been observed from Fig. 5(a) that during two years period of simulation, the concentration plume spreads up to 25 grids along the length and 8 grids along the depth of aquifer for $\mu = 0.1$. For $\mu = 10$, the plume size is reduced by two grids along the length one grid along the depth while comparing it with the result for $\mu = 0.1$ Fig.5(b). The plume size is further reduced for higher decay parameter ($\mu = 20$). One grid reduction each along the length and depth of the aquifer is observed Fig.5(c). Fig. 6(a), (b) and (c) show that the depletion of the zone of contaminant concentration due to decay parameter for four years of simulation, for $\mu = 0.1$, $\mu = 10$ and $\mu = 20$ respectively. For $\mu = 0.1$ the plume moves between 7 and 38 grids along the length and touches to the bottom boundary Fig. 6(a). Fig 6(b) shows the depletion of 0.03 contour lines with plume length lies between 9 to 34 grids and 7 grids along the direction. Further reduction in spreading of concentration has been observed in Fig. 6(c), with the depletion 0.03 and 0.02 contour lines for $\mu = 20$. As the simulation were carried under constant seepage velocity in the longitudinal direction, Fig. 7(a), (b) and (c) show the advancement of contaminant plume towards right boundary and simultaneous reduction in strength due to second order parameter. Although the spreading takes place between 14 grids to 47 grids Fig. 7(a), 0.03 concentration core is absent for $\mu = 0.1$. For $\mu = 10$ and 20, only 1% of its input concentration strength exits, showing significant reduction in contaminant spread due to decay. However, the decay parameter $\mu = 20$ controls the spreading most significantly.

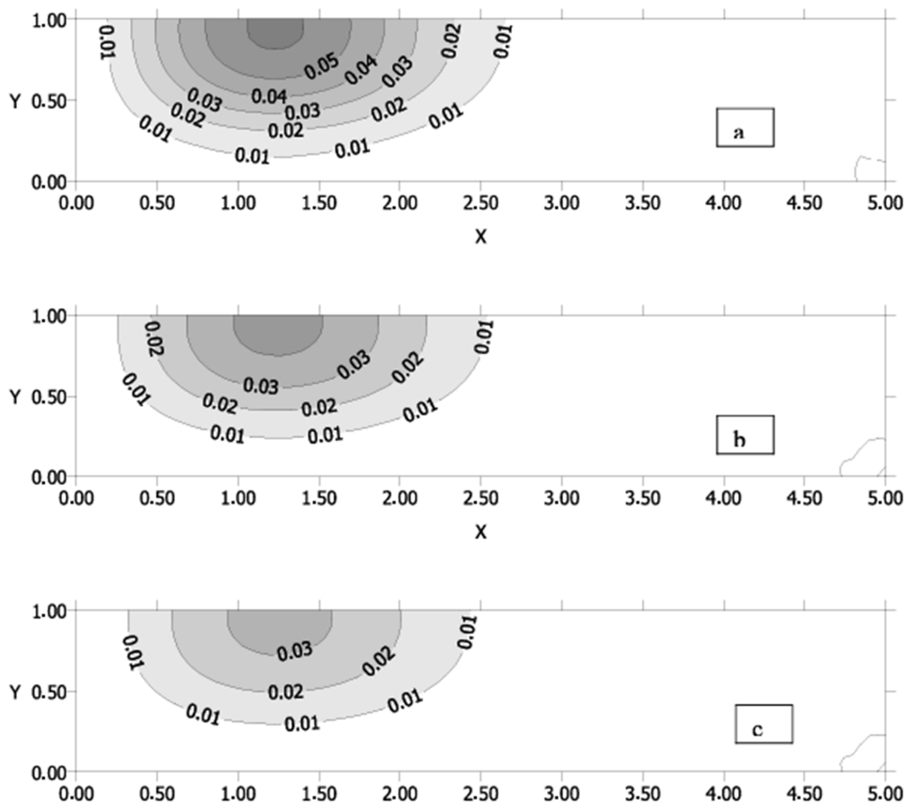

Fig 5: Evolution of the zone of contaminant concentration in two years simulation with second order decay for $\mu = 0.1, 10$ and 20 (Scenario II)

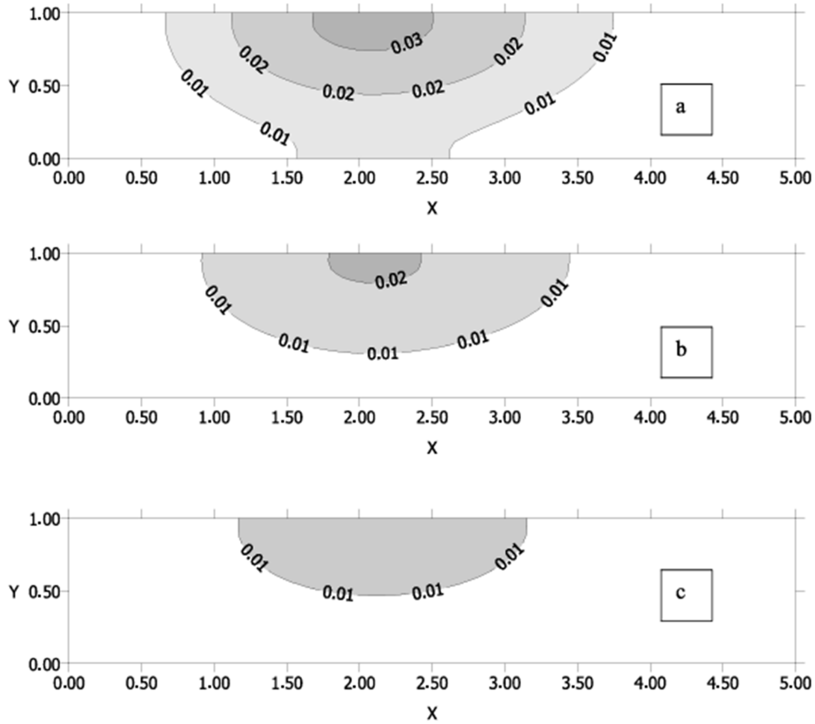

Fig 6: Evolution of the zone of contaminant concentration in four years simulation with second order decay for $\mu = 0.1, 10$ and 20 (Scenario II)

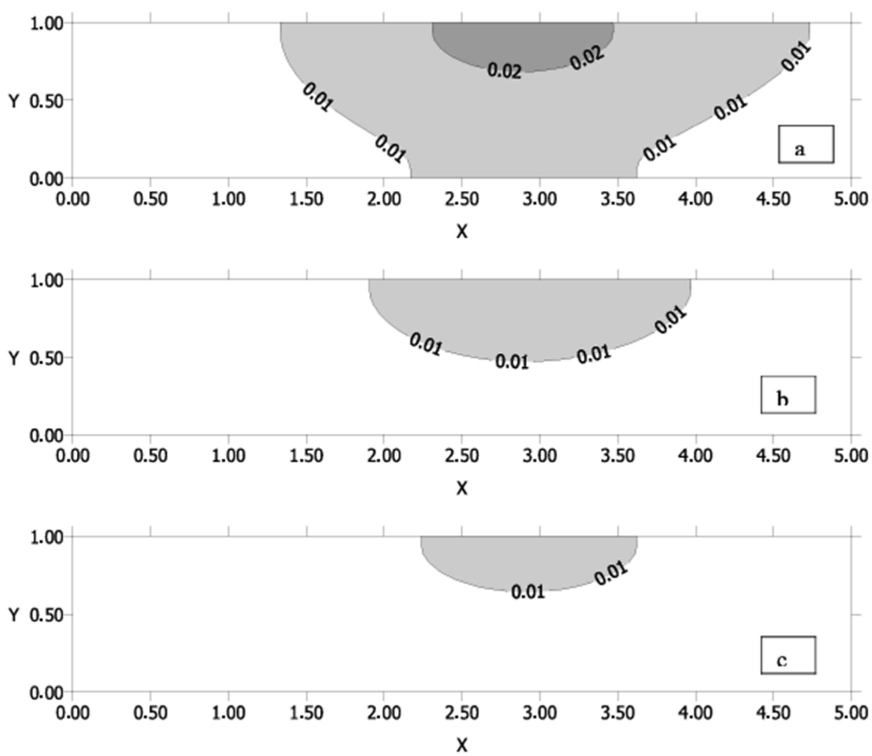

Fig 7: Evolution of the zone of contaminant concentration in six years simulation with second order decay for $\mu = 0.1, 10$ and 20 (Scenario II)

CONCLUSION:

Above study indicates that the higher values of second decay parameter controls the spread of contaminant significantly. Depending upon the requirement, the discharge schedule indicated by scenario I and II can be adopted. This paper shows the model result qualitatively and can be applied in the absence of in-situ information.

REFERENCES:

Martinus, Van Genuchten, 1981. Analytical solutions for chemical transport with simultaneous adsorption, zero-order production and first-order decay, Journal of Hydrology, Volume 49, Issues 3–4, 1981, Pages 213-233, ISSN 0022-1694, https://doi.org/10.1016/0022-1694(81)90214-6.

Sharma, P. K., Sawant, V. A., Shukla, S. K., & Khan, Z. 2014. Experimental and numerical simulation of contaminant transport through layered soil. International Journal of Geotechnical Engineering, 8(4), 345–351. https://doi.org/10.1179/1939787913Y.0000000014

L. Li, W. Zhao, Y. Wang, F. Meng, H. Ao and C. Wang, 2010. "Numerical Simulation of Contaminant Transport in Porous Soil," 4th International Conference on Bioinformatics and Biomedical Engineering, pp. 1-4, doi: 10.1109/ICBBE.2010.5517308.

Bincy, B., Devatha, C.P., Thalla, A.K. 2023. Numerical Simulation of Contaminant Transport in Subsurface Soil Using MODFLOW Software. In: Chenchouni, H., et al. Recent Research on Hydrogeology, Geoecology and Atmospheric Sciences. MedGU 2021. Advances in Science, Technology & Innovation. Springer, Cham. https://doi.org/10.1007/978-3-031-43169-2_17

Usoh, G.A., Ahaneku, I.E., Ugwu, E.C. et al. Mathematical modeling and numerical simulation technique for selected heavy metal transport in MSW dumpsite. Sci Rep 13, 5674 (2023). https://doi.org/10.1038/s41598-023-32984-9