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MODELING CONTAMINANT TRANSPORT OF METAL IONS THROUGH SOIL

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Abstract: **Managing the waste material unscientifically is causing a lot of direct and indirect environmental problems. Due to increase in the hydro-environmental pollution on the earth, the reactive- advective -dispersion phenomenon which describes the reactive solute transport in the medium has got significant attention world over. Various analytical and numerical methods are available to analyze this phenomenon under different initial boundary conditions. The objective of this study is to model the contaminant transport of the metal ions i.e. copper and zinc through the black cotton soil using finite layer and finite difference methods viz: Backward Time Centered Scheme (BTCS), Upwind and Crank-Nicolson implicit schemes. The column experiments were conducted with constant and decreasing concentrations from the contaminant sources. The experimental results were modeled with the finite layer method using POLLUTE software and the finite difference method with Excel spreadsheet solution. It was found that more accurate values of the transport parameters i.e. dispersion coefficient and the distribution coefficient were obtained with finite layer method and finite difference method using Crank-Nicolson scheme. A new Excel spreadsheet solution for the reactive-advective- dispersion phenomenon was developed by incorporating the retardation factor in the non-reactive method proposed by Karahan in 2006. The dispersion coefficient of copper ions was observed to be lower than that of zinc ions while the distribution coefficient of copper ions was found to be higher than that of zinc ions and the metal ion retention sequence was found to be Cu > Zn in the black cotton soil.**

Keywords – *Solute, Black cotton soil, Copper, Zinc, Concentration, POLLUTE software.*

I INTRODUCTION

With the increasing population growth and the industrial and agricultural development, the amounts of wastes generated are increasing and polluting the air, water and soil, thereby causing threat to the human health. The increasing solid wastes and their disposal sites like landfills are not only causing groundwater contamination and soil pollution but also leaving many productive lands as waste lands. Hence, there is a need to reduce and recycle the waste, design the secured landfill systems and innovate different remediation techniques to reuse the waste lands for productive purposes.

As the solid waste contains different types of wastes, the leachate generated from the wastes contains different types of harmful chemical, toxins and harmful metals. The leachate, if not properly regulated, may migrate through the landfill liner and contaminate the ground- water. Hence, the design of the liner system is a crucial task in solid waste management which requires knowledge of different types of wastes, chemical composition of the leachates, types of liner systems, compatibility of liner systems etc. The compatibility analysis of a particular liner system is carried out for each of the harmful chemical constituent present in the leachate for which knowledge of different contaminant transport processes is essential.

The commonly used and economical type of liner system is soil liner. The different contaminant transport processes through a soil liner are advection, dispersion, and loss or gain of the solute mass. These processes depend on the type of soil, type of soil and its characteristics in terms of density, porosity and permeability, type of chemicals, time, temperature, pH of the system, and can be assessed using two important transport parameters i.e. the dispersion coefficient and the distribution coefficient and are essential for modeling the contaminant transport and for the design of soil liner system. The transport parameters of different chemicals and metal ions can be determined by conducting column experiments for the liner material. The determination of transport parameters is a time consuming process as the column experiments take a long time to get the breakthrough. The analytical and numerical methods used to determine these parameters using the column test results need several trial calculations which are also time marching procedure. Hence, it is necessary to find a suitable technique to estimate the contaminant transport parameters which saves time and effort.

II OBJECTIVE

The objective of the study is to find the contaminant transport parameters of metal ions i.e. copper and zinc ions transported through the black cotton soil by performing column tests using finite layer and finite difference methods with different implicit schemes using constant concentration source and the decreasing concentration source.

III MATERIALS AND METHODS

Testing materials:

The black cotton soil used in this study was obtained from Belgaum District located in the state of Karnataka in India. The composition of the soil was found to be 63, 31 and 6% for clay, silt and sand, respectively. The soil type as per IS plasticity chart is "CH". The characteristics of the soil are given in Table 1.

Table 1 Characteristic of the Soil Samples Used in the Tests

Specific Gravity	Liquid Limit (%)	Plastic Limit (%)	Shrinkage Limit (%)	Max.dry density (g/cc)	Optimum water content (%)	Free swell Index	Modified Free swell Index
2.67	72.1	31.7	13.6	1.365	32.5	72.7	1.9

Source solutions:

The zinc solution of 100 ppm which was prepared using zinc dust and copper solution of 100 ppm prepared from pure copper sheet were used as source solutions.

Apparatus used:

To determine the seepage velocity, dispersion coefficient (D) and the distribution coefficient (K), a simple column test apparatus was designed to simulate one-dimensional contaminant migration through the soil by advection and dispersion processes. The schematic diagram and the photograph of the apparatus are shown in figures 1 & 2. The apparatus consists of an overhead tank which is mounted on a stand fixed to the wall and the soil column is connected to the overhead tank through a plastic pipe to allow seepage of solution through the soil sample. The effluent is collected in the effluent tank placed below the soil column.

Testing methods:

Column test

The oven-dried soil sample was mixed with known amount of water and was kept in the desiccators for about 24 hours to get uniform distribution of water content in the soil sample. The soil was then compacted in the column using small rammer in three layers. The water content was determined by oven-drying method and dry density and porosity of the soil were determined. The overhead tank was filled with water and connected to the soil column to saturate the soil sample. After the soil sample was completely saturated and when steady state flow was achieved, the permeability of soil sample was measured using variable head test method. The copper solution of 100 ppm was filled in the overhead tank and effluent coming out from the bottom of the column was collected at regular time intervals.

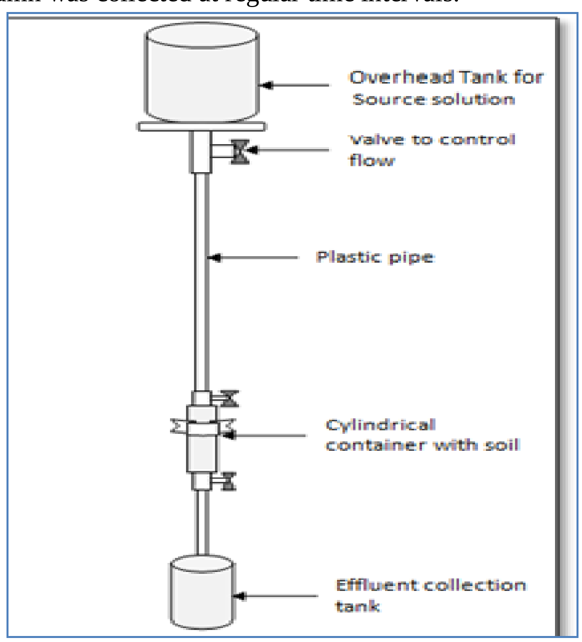

Figure 1 Schematic diagram of column test apparatus

Two types of tests were conducted to simulate the field conditions i.e. constant source concentration and the decreasing source concentration tests. For constant source concentration test, the hydraulic head was maintained constant by adding the same source solution and for variable source concentration test, the constant hydraulic gradient was maintained by adding distilled water to the source solution. The effluent volume was monitored at regular time intervals and the concentrations of the effluents were determined using atomic absorption spectrophotometer (AAS). By adjusting the dispersion coefficient (D) and the distribution coefficient (K), the theoretical curves were matched with the observed concentration profiles to give inferred values of both D and K. The values of D and K deduced in this way were checked by comparing the estimated and the observed variations of contaminant concentrations with time in the source leachate [1].

Figure 2 Photograph of the apparatus

As the time taken to obtain complete breakthrough curves is very large, the experiments were stopped and the soil section method was used to obtain the breakthrough curves. The soil samples were sectioned as per the procedure described by [2& 3] and pore water concentrations were determined at different depths. From this concentration profile, the transport parameters were determined by trial and error method.

Batch test

Batch test was conducted to find the distribution coefficient (K) as per ASTM D4646-03 Code. An oven-dried soil sample of weight 5g was taken and mixed with 100 ppm zinc solution in a ratio of 1:20 soil to solution ratio. The sample flask was then put on the then separated and filtered through a 0.45-µm pore size membrane filter. The concentration of solute remaining in solution was measured and the amount of solute adsorbed was calculated. The distribution coefficient was then calculated from the following equation.

$$K = \frac{(C_o - C_t)\,V}{M\,C_t} \qquad \text{--- (1)}$$

Where K is the distribution coefficient (L^3/M), C_o is the initial concentration of solution (M/L^3), V is the volume of the solution (L^3) and M is the mass of the soil (M).

IV MODELING CONTAMINANT TRANSPORT

The contaminant transport can be modeled using one-dimensional reactive-advection-dispersion equation [4] and described mathematically as under:

$$R\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2} - v_z\frac{\partial c}{\partial z} \qquad \text{--- (2)}$$

Where R is the retardation factor which is equal to $1 + \rho_d K/n$ (If there is no adsorption i.e. distribution coefficient K is equal to 0, then R is equal to 1), ρ_d is the dry density of the medium, n is the porosity of the transport medium, C is the concentration of the solute (M/L^3), t is the time (T), z is the vertical distance/ depth (L), v_z is the seepage velocity (L/T) and D is the dispersion coefficient (L^2/T).

The most commonly used methods for obtaining the solution for Eq. [2] can be categorized [1] viz: analytical methods and numerical methods using finite-layer, boundary element, finite element and finite difference methods. The finite difference methods with explicit schemes have certain limitations in terms of convergence and stability, so in this study the implicit schemes were employed which are unconditionally convergent and stable and truncation errors are less.

In this study, two methods i.e. finite-layer and finite difference methods were used and the observed results were compared with the simulated results obtained using these methods. These numerical methods are described briefly as under:

Finite layer method:

In situations where soil properties are taken same at any horizontal grid (location) within the barrier layer, the Eq. [2] can be transformed by introducing the Laplace transform (in case of one-dimensional problems) and the Fourier transform (in case of two and three- dimensional problems) and can be solved [4]. POLLUTE v7 software was used to find the transport parameters using finite layer method. Using this method the thickness of the soil sample was divided into number of layers and the concentrations at different depths and at different times were simulated simultaneously without any dependence on the concentrations of the previous times.

Finite difference method:

The one–dimensional reactive-advective–dispersion equation can be solved with finite difference method (FDM) using Excel spreadsheet. The unknown concentrations at any node in the new time level in the space-grid time depends on the concentrations at the adjacent nodes at the new time level, which are also unknown and can be found using implicit schemes. Three implicit schemes viz: backward time centered scheme (BTCS), Upwind scheme and Crank- Nicolson scheme were used to find the transport parameters using the trail values of R and D coefficients in the beginning and the iterations were made till the theoretical curves fit the experimental data.

In this study, the method described by Karahan [5] which is for non-reactive case (R=1) was modified to incorporate the retardation factor R and the modified finite difference equations are written as:

$$C_i^{n+1} = [f(i,n) - AC_{i-1}^{n+1} - C\, C_{i+1}^{n+1}]/B \quad ---(3)$$

Where C_{i-1}^{n+1}, C_i^{n+1} and C_{i+1}^{n+1} are the concentrations at i-1, i and i+1 nodes at time n+1.

The equations given by Karahan [5] for non-reactive solute are as given below:

$$A = \emptyset\left(\frac{Cr}{Pe}\right) + \emptyset E Cr,$$

$$B = -2\emptyset\left(\frac{Cr}{Pe}\right) - \emptyset(1-2\theta)Cr,$$

$$C = \emptyset\left(\frac{Cr}{Pe}\right) - \emptyset\theta Cr$$

$$f(i,n) = D\left(\frac{Cr}{Pe}\right)[C_{i-1}^n - 2C_i^n + C_{i+1}^n] + DCr[EC_i^n + \theta C_{i+1}^n - EC_{i-1}^n - \theta C_i^n])$$

$D = 1 - \emptyset$ And $E = 1 - \theta$

The equations for B and f(i,n) are slightly modified as given below

$$B = -2\emptyset\left(\frac{Cr}{Pe}\right) - \emptyset(1-2\theta)Cr - R,$$

$$f(i,n) = -RC_i^n - D\left(\frac{Cr}{Pe}\right)[C_{i-1}^n - 2C_i^n + C_{i+1}^n] + DCr[EC_i^n + \theta C_{i+1}^n - EC_{i-1}^n - \theta C_i^n]$$

A, B, C, D and E are the constants. The constant D here as given by Karahan is different from the dispersion coefficient D in the reactive-advective-dispersion equation. Ø and θ are time and spatial weighting factors, respectively and their values for different schemes [5] are under:

For BTCS (Backward Time Centered Space) scheme, Ø = 1 and θ = 1/2; for Upwind scheme, Ø = 1 and θ = 0 and for Crank-Nicolson scheme, Ø = 1/2 and θ = 1/2.

Courant number (Cr) for one-dimensional analysis can be written as $u\,\Delta t/\Delta z$ and Pelect number (Pe) which is the ratio of the advection rate of mass transfer by flow to the mass diffusion rate can be written as $u\,\Delta z/D$, where u is the local flow velocity, Δt is the time step and Δz is the grid size in the numerical scheme and D is the diffusion coefficient.

The finite difference equations for different implicit schemes are given as under:

BTCS Scheme: In this scheme, the backward difference scheme is used for time derivative and the central differences are taken for space derivatives at the next time step n+1 and the reactive-advective- dispersion equation is written in the finite difference form as:

$$R\frac{C_i^{n+1} - C_i^n}{\Delta t} = D\,\frac{C_{i-1}^{n+1} - 2C_i^{n+1} + C_{i+1}^{n+1}}{\Delta z^2} - v_z\,\frac{C_{i+1}^{n+1} - C_{i-1}^{n+1}}{2\Delta z}$$

Upwind Scheme: The backward difference scheme is applied for the time derivative while the 1st order space derivative and central difference for 2nd order space derivatives at the next time step n+1 are taken. The finite difference form of the reactive-advective- dispersion equation is written as:

$$R\frac{C_i^{n+1} - C_i^n}{\Delta t} = D\,\frac{C_{i-1}^{n+1} - 2C_i^{n+1} + C_{i+1}^{n+1}}{\Delta z^2} - v_z\,\frac{C_i^{n+1} - C_{i-1}^{n+1}}{2\Delta z}$$

Crank-Nicolson scheme: In this scheme, the backward difference is taken for the time derivative and the central differences are taken for the space derivatives at the time step n+1/2.

$$R\frac{C_i^{n+1} - C_i^n}{\Delta t} = \frac{D}{2}\left(\frac{C_{i-1}^n - 2C_i^n + C_{i+1}^n}{\Delta z^2} + \frac{C_{i-1}^{n+1} - 2C_i^{n+1} + C_{i+1}^{n+1}}{\Delta z^2}\right)$$

$$-\frac{v_z}{2}\left(\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta z} + \frac{C_{i+1}^{n+1} - C_{i-1}^{n+1}}{2\Delta z}\right)$$

In all these three finite difference equations stated above appropriate initial and boundary conditions were used and the assumed values of R and D were given and iterations were made till the theoretical curves matches with the experimental data and at that stage the R and D values were taken as optimal values.

V RESULTS AND DISCUSSION

Twelve remolded black cotton (BC) soil samples were tested with 2 source solutions with 6 samples for each solution. The diameter and height of the test samples were 4 and 10 cm, respectively. The physical properties of the test samples are reported in Tables 2 & 3.

The effluent with different concentrations coming out through the bottom of different samples during different time periods were measured using AAS. The effluent concentrations were observed to be very low even after longer time periods and hence the soil samples were sectioned as per the procedure described [1] and pore water concentrations were determined at different depths for each soil sample. From these data, the concentration profiles were developed and from these concentration profiles, the transport parameters were determined by trial and error method using POLLUTE v7.

Table 2 Physical properties of test samples with zinc as source solution

Sample Code	Type of test	Dry Density (g/cc)	Porosity n	Coefficient of permeability (cm/s)	Darcy velocity v (cm/s)	Seepage velocity v_z (cm/s)
BC/ZN/C-1	Constant source concentration test	1.042	0.61	$1.08x10^{-5}$	$1.30x10^{-4}$	$2.13x10^{-4}$
BC/ZN/C-2		1.163	0.56	$0.67x10^{-5}$	$0.80x10^{-4}$	$1.42x10^{-4}$
BC/ZN/C-3		1.217	0.54	$0.58x10^{-5}$	$0.70x10^{-4}$	$1.28x10^{-4}$
BC/ZN/V-1	Decreasing source concentration test	1.142	0.57	$0.73x10^{-5}$	$0.87x10^{-4}$	$1.53x10^{-4}$
BC/ZN/V-2		1.181	0.56	$0.61x10^{-5}$	$0.73x10^{-4}$	$1.31x10^{-4}$
BC/ZN/V-3		1.234	0.54	$0.52x10^{-5}$	$0.62x10^{-4}$	$1.16x10^{-4}$

Table 3 Physical properties of test samples with copper as source solution

Sample Code	Type of test	Dry Density (g/cc)	Porosity n	Coefficient of permeability (cm/s)	Darcy velocity v (cm/s)	Seepage velocity v_z (cm/s)
BC/CU/C-1	Constant source concentration test	1.221	0.54	$0.57x10^{-5}$	$0.45x10^{-4}$	$8.40x10^{-5}$
BC/CU/C-2		1.282	0.52	$0.47x10^{-5}$	$3.77x10^{-5}$	$7.25x10^{-5}$
BC/CU/C-3		1.314	0.51	$0.39x10^{-5}$	$3.13x10^{-5}$	$6.16x10^{-5}$
BC/CU/V-1	Decreasing source concentration test	1.245	0.53	$4.98x10^{-6}$	$3.98x10^{-5}$	$7.46x10^{-5}$
BC/CU/V-2		1.292	0.52	$4.42x10^{-6}$	$3.54x10^{-5}$	$6.85x10^{-5}$
BC/CU/V-3		1.323	0.50	$3.75x10^{-6}$	$3.00x10^{-5}$	$5.95x10^{-5}$

Note: Sample Code BC/ZN/C-1 represents black cotton soil/ with zinc as source solution/ using constant test - for density-1 and Code BC/ZN/V-1 represents black cotton soil/ with zinc as source solution/ using variable concentration test - for density-1 and like-wise for others. Seepage velocity was taken as Darcy velocity divided by porosity.

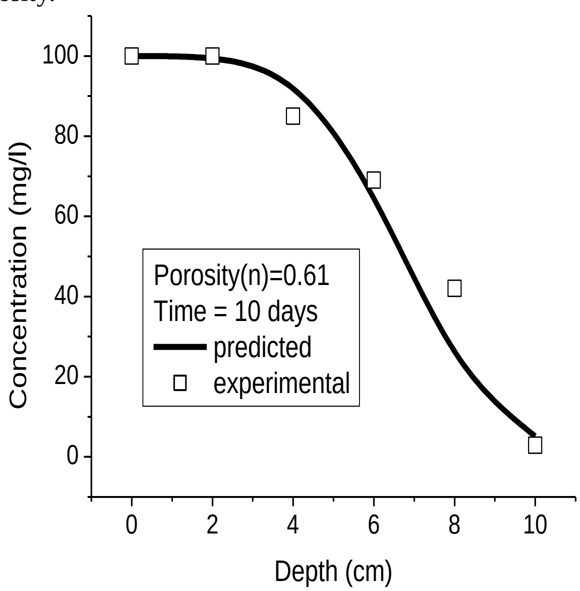

Figure 3 Variation of concentration with depth for sample BC/ZN/C-1

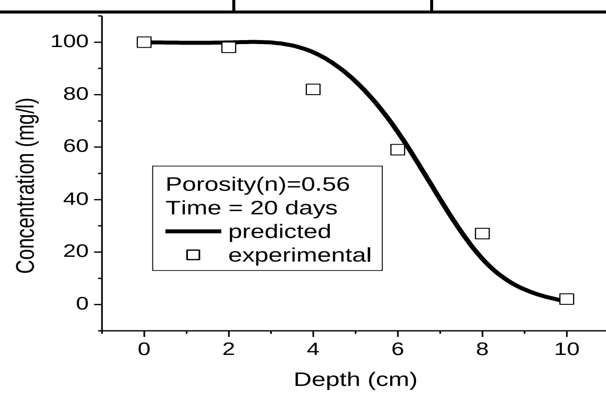

Figure 4 Variation of concentration with depth for sample BC/ZN/C-2

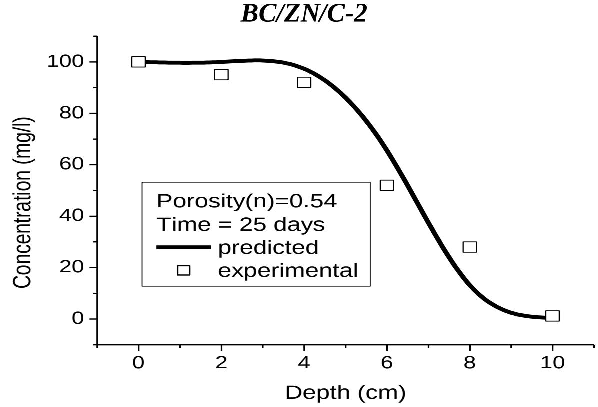

Figure 5 Variation of concentration with depth for sample BC/ZN/C-3

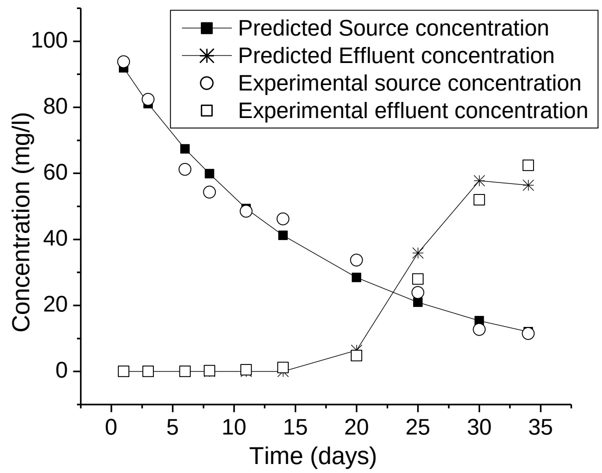

Figure 6 Variation of concentration with time for sample BC/ZN/V-1

Constant and decreasing source concentration tests with zinc as source solution:

Six BC soil samples of different densities were tested by constant and decreasing source concentration methods with zinc as source solution. The transport parameters were determined by matching the theoretical curves with the experimentally determined concentrations at different times and depths (Figures 3-8) using **POLLUTE v7** software.

For constant source concentration test, the contaminant transport parameters can also be determined by FDM using Excel spreadsheet calculation by matching the experimental concentrations to theoretical values. Three implicit schemes (BTCS, Upwind and Crank-Nicolson) were employed for prediction of transport parameters and these were compared with the transport parameters obtained using POLLUTE model. From these comparisons, the Crank-Nicolson scheme was found to be the most accurate method among these three schemes (Figures 9-11) for the sample BC/ZN/C-1) which are shown here. The same results were obtained from other soil samples not shown here.

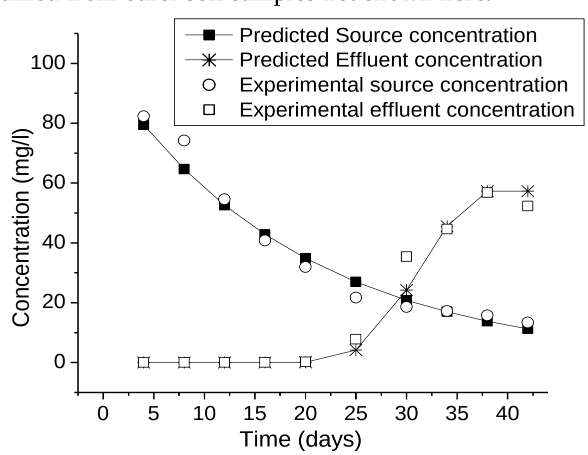

Figure 7 Variation of concentration with time for sample BC/ZN/V-2

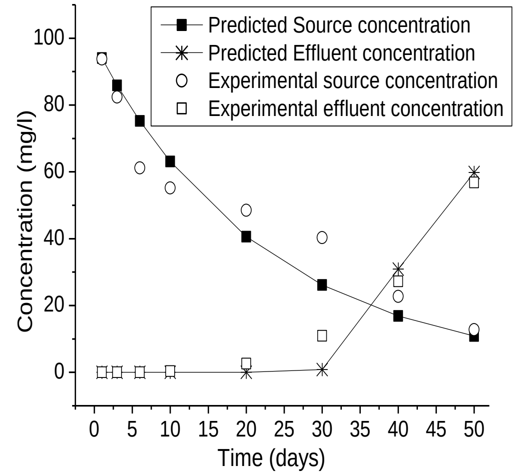

Figure 8 Variation of concentration with time for sample BC/ZN/V-3

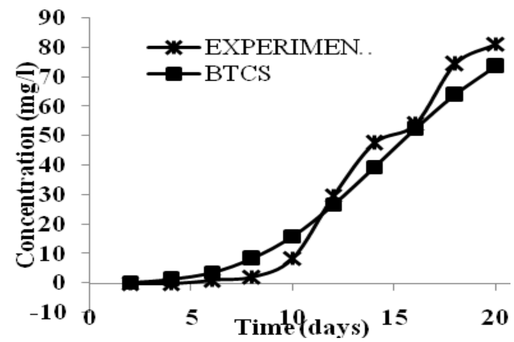

Figure 9 Variation of concentration with time for sample BC/ZN/C-1 (FDM-BTCS)

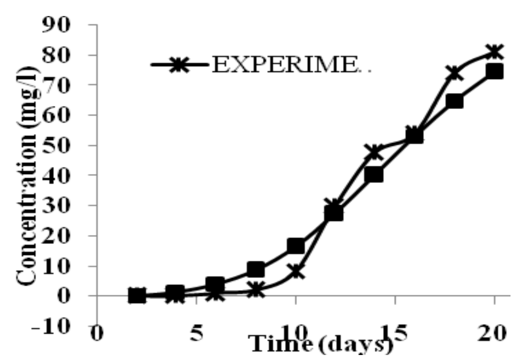

Figure 10 Variation of concentration with time for sample BC/ZN/C-1(FDM-Upwind)

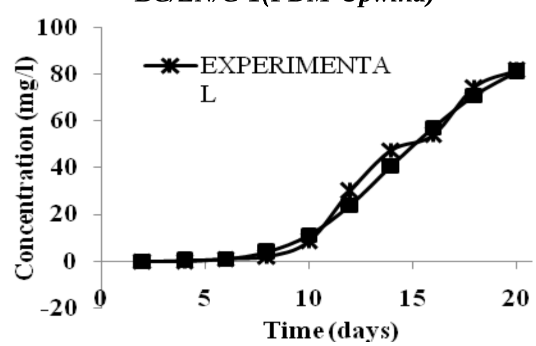

Figure 11 Variation of concentration with time for sample BC/ZN/C-1 (FDM-Crank-Nicolson)

Constant and decreasing source concentration tests with copper as source solution:

Six soil samples were tested using constant and decreasing source solutions and were modeled using POLLUTE v7. The experimental and simulated results are shown in Figures 12-17 and were also compared using FDM as shown in Figures 18-20.

It was observed that the simulated concentrations using BTCS and Upwind schemes were comparatively less than the experimental values and the concentrations simulated using Crank-Nicolson scheme were observed to be almost same as experimental data.

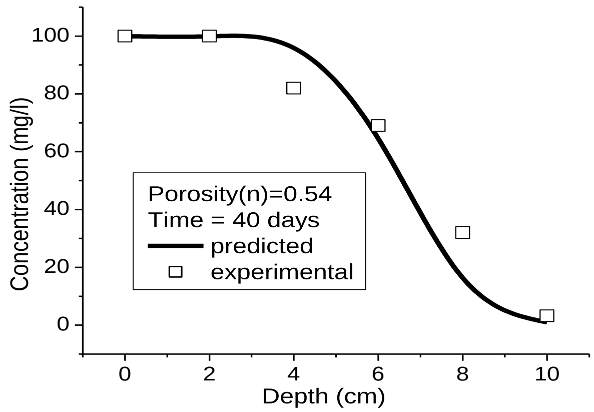

Figure 12 Variation of concentration with BC/CU/C-1

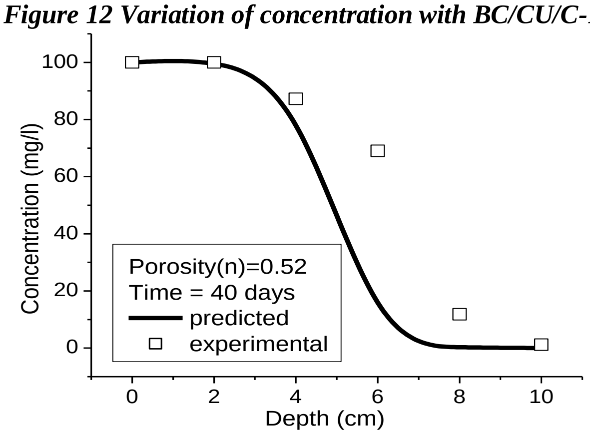

Figure 13 Variation of concentration with depth for sample depth for sample BC/CU/C-2

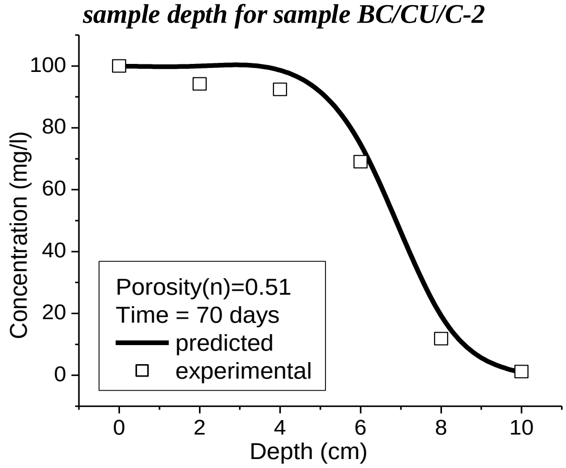

Figure 14 Variation of concentration with BC/CU/C-3

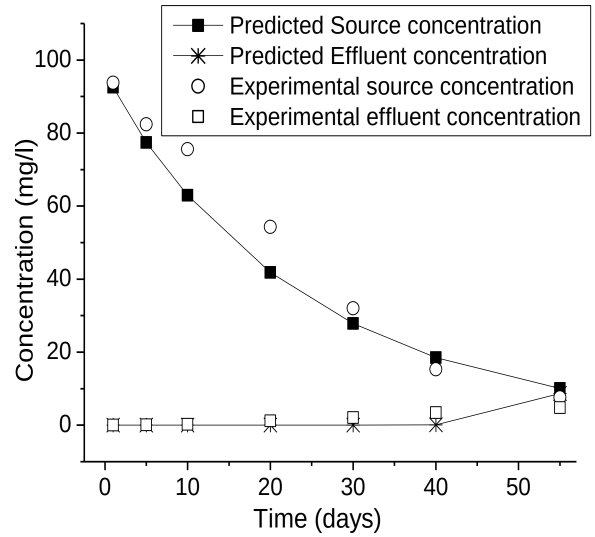

Figure 15 Variation of concentration with depth for sample time for sample BC/CU/V-1

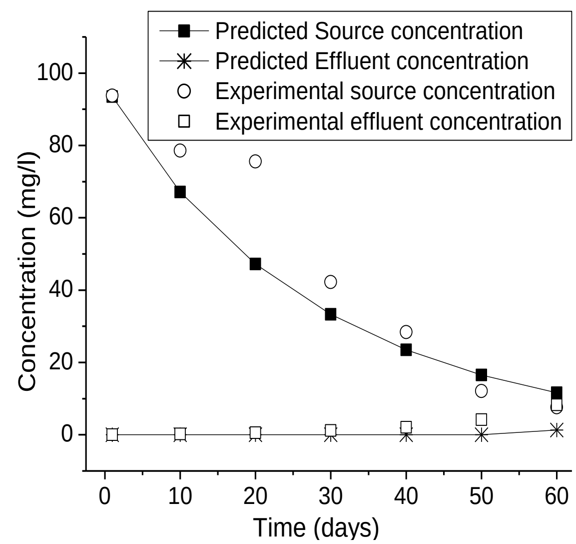

Figure 16 Variation of concentration with BC/CU/V-2

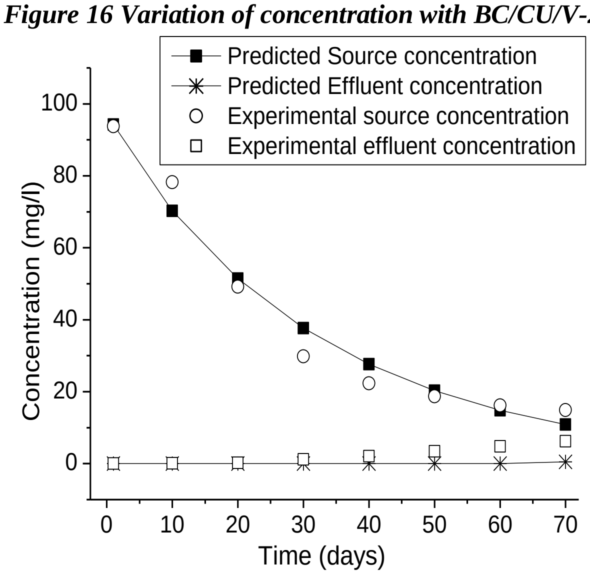

Figure 17 Variation of concentration with time for sample time for sample BC/CU/V-3

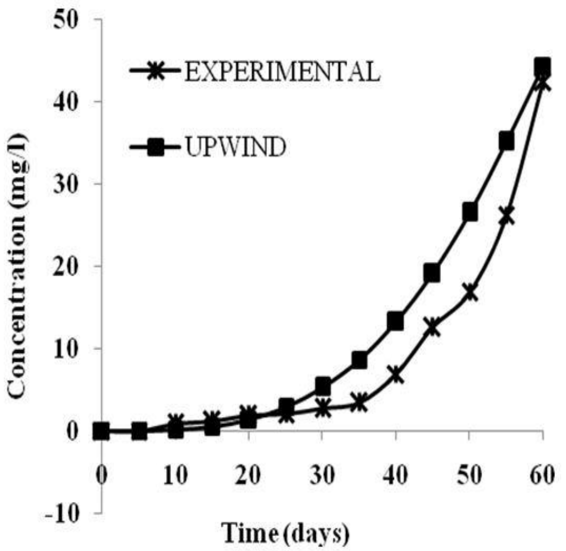

Figure 18 Variation of concentration with time for sample BC/CU/C-1 (FDM-UPWIND)

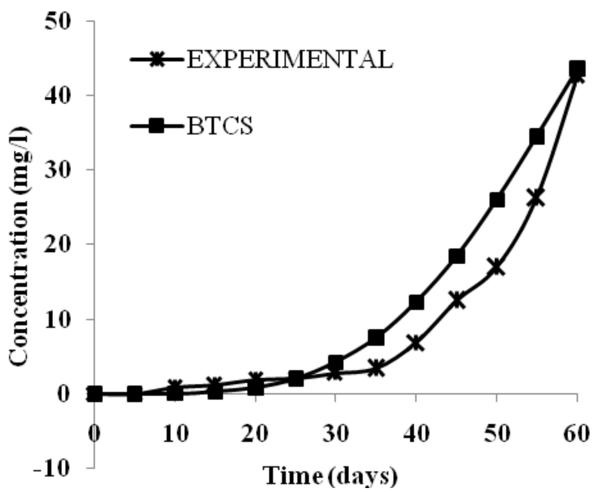

Figure 19 Variation of concentration with time for sample BC/CU/C-1 (FDM-BTCS)

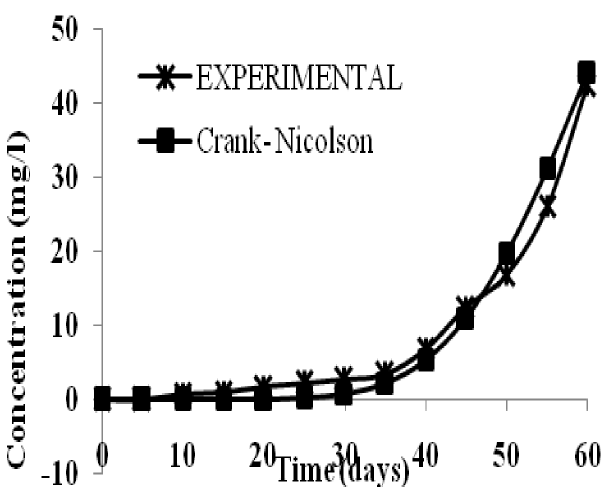

Figure 20 Variation of concentration with time for sample BC/CU/C-1 (FDM-Crank-Nicolson)

Contaminant transport parameters:

The contaminant transport parameters as with obtained using most accurate method i.e. FDM Crank-Nicolson Scheme are given in Table 4. The effect of soil physical characteristic in terms of dry density, the flow characteristics in terms of advective velocity, the effect of the type of metal ions and the effect of test on different contaminant transport parameters are discussed in this paper.

The effect of soil physical characteristic in term of dry density, the flow characteristic in term of advective velocity, effect of the type of metal ion and the effect of the type of the test on different contaminant transport parameters are discussed as under:

Effect of soil density: It was observed that as the density of the soil increases the dispersion coefficient decreases and the distribution coefficient increases as shown in Figures 21 and 22, respectively for Zn ions with constant concentration as applied from the source. This effect may be due to the reduction in the mechanical dispersion and the decrease in the pore water velocity caused by the decrease in the porosity of the soil.

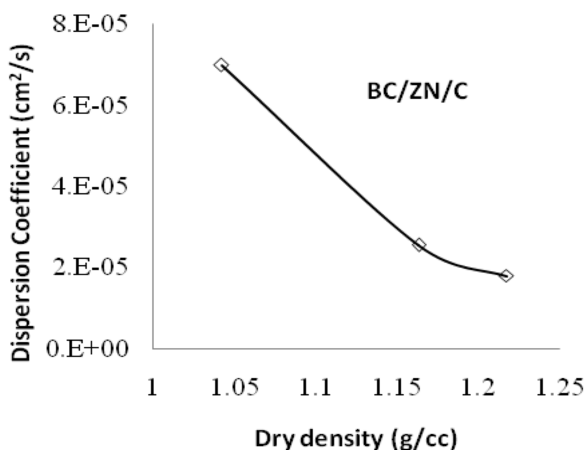

Figure 21 Variation of Dispersion coefficient with dry density

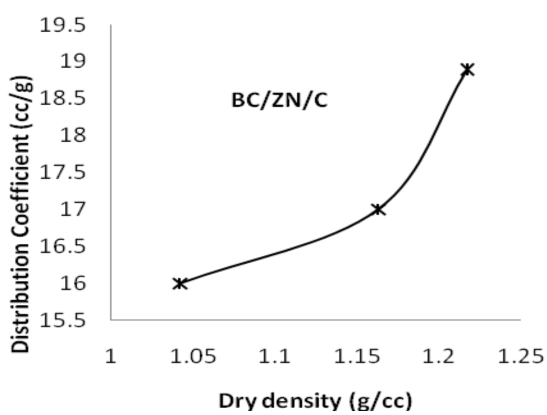

Figure 22 Variation of Distribution coefficient with dry density

Table 4 Contaminant transport parameters

Sample Code	Type of test	Dry Density (g/cc)	Porosity n	Dispersion Coefficient D (cm^2/s)	Distribution Coefficient K (cm^3/g)	Retardation factor R
BC/ZN/C-1	Constant source concentration test	1.042	0.61	7.00×10^{-5}	16.0	28.67
BC/ZN/C-2		1.163	0.56	2.56x10-5	17.0	38.54
BC/ZN/C-3		1.217	0.54	1.80×10^{-5}	18.9	43.64
BC/ZN/V-1	Decreasing source concentration test	1.142	0.57	2.30×10^{-5}	16.5	34.65
BC/ZN/V-2		1.181	0.55	1.77×10^{-5}	17.0	38.36
BC/ZN/V-3		1.230	0.54	1.20×10^{-5}	18.1	42.20
BC/CU/C-1	Constant source concentration test	1.22	0.54	1.50×10^{-5}	19.8	45.73
BC/CU/C-2		1.28	0.52	1.00×10^{-5}	20.70	51.95
BC/CU/C-3		1.31	0.51	0.80×10^{-5}	21.00	54.94
BC/CU/V-1	Decreasing source concentration test	1.24	0.53	1.30×10^{-5}	19.00	45.45
BC/CU/V-2		1.29	0.52	0.94×10^{-5}	19.70	49.87
BC/CU/V-3		1.32	0.50	0.72×10^{-5}	20.20	54.33

Effect of advective velocity: It was observed that the dispersion coefficient increases with the increase in the advective velocity which may be due to increased mechanical dispersion being dependent on advective velocity as shown in Figure 23. Also it was also observed that the distribution coefficient decreases as the advective velocity increases (Figure 24). This effect may be related to the less interaction of ions with the soil particles due to the more pore water velocity which causes less adsorption due to the faster movement of ions.

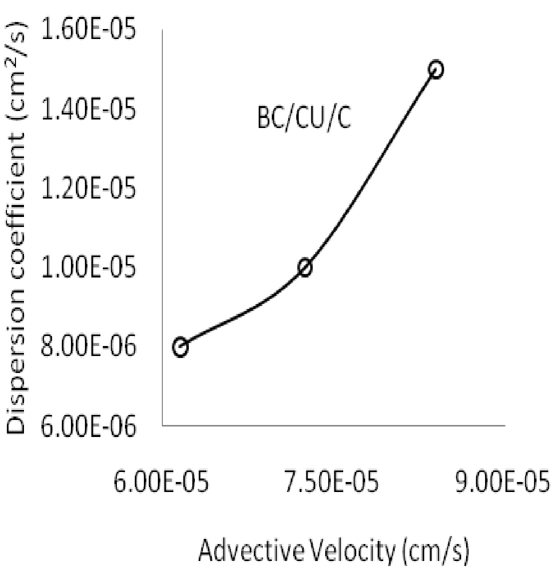

Figure 23 Variation of Dispersion coefficient with advective velocity

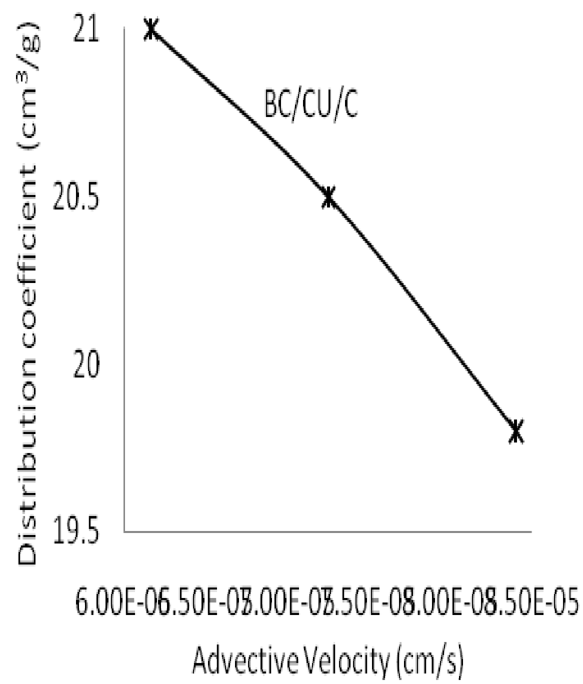

Figure 24 Variation of Distribution coefficient with advective velocity

Effect of type of ion: The test results revealed that the dispersion coefficient of copper is less than that of Cu and Zn is similar to that obtained in the study conducted by Korf et al. [6] Whereas in their study it was reported that the Cu metal ions were found to be less mobile in the soil as compared to Zn, Ni and Cd metal ions.

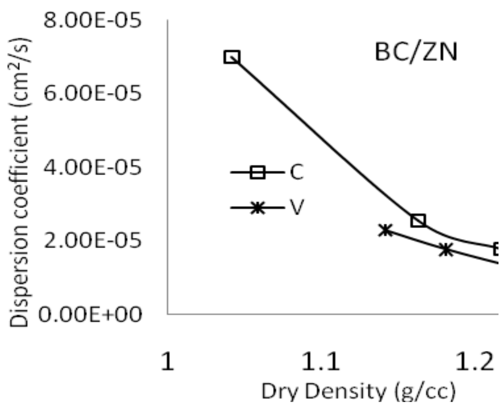

Figure 25 Variation of Dispersion coefficient for constant and decreasing source methods

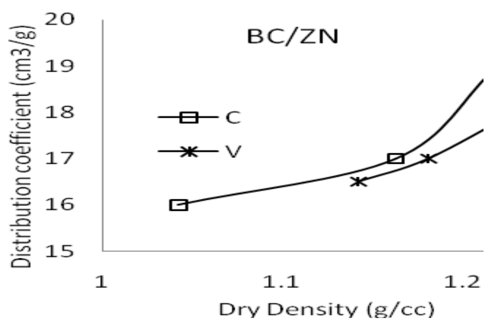

Figure 26 Variation of Distribution coefficient for constant and decreasing source methods

Effect of type of test: From this study, the transport parameters (D and K) obtained using of zinc whereas the distribution coefficient of copper is more than that of zinc. This affinity order constant concentration test were observed to be slightly higher than those obtained using decreasing concentration test. This variation may be due to the decrease in source concentration with time which reduces the amount of contaminant transported and retarded by the soil.

VI CONCLUSIONS

Soil column test by sectioning to obtain the experimental breakthrough curves for determination of dispersion coefficient and retardation factor for soils with low hydraulic conductivity and with more adsorption capacity such as black cotton soils was found to be beneficial as it reduces the time and effort asunder such situations the effluent concentrations are increasing at very slow rate. Transport parameters for copper and zinc ions migrated through black cotton soil were obtained by matching the experimental breakthrough curves with the theoretical curves developed using different implicit finite difference schemes employing Excel spread sheet and the finite layer method using Pollute v7 software. Out of the three finite difference implicit schemes i.e. Backward Time Centered Scheme (BTCS), Upwind and Crank- Nicolson schemes , the finite difference method using Crank-Nicolson scheme was found to be the most accurate method for estimating the contaminant transport parameters. A new Excel spreadsheet solution for the reactive- advective- dispersion phenomenon was developed by incorporating the retardation factor in the non-reactive method proposed by Karahan in 2006. Density of the black cotton soil was found to have significant effect on the contaminant transport parameters i.e. with the increase in the soil density, the dispersion coefficient decreases while the distribution coefficient increases. The dispersion coefficient of copper ions was observed to be lower than that of zinc ions while the distribution coefficient of copper ions was found to be higher than that of zinc ions and the metal ion retention sequence was found to be Cu > Zn in the black cotton soil.

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