NUMERICAL MODELLING OF CONTAMINANT TRANSPORT IN SOIL

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Abstract: The study of migration or the fate of the contaminant miscible in ground water from waste site, dumping yards or landfills is essential for preparation of ground water contamination models. Numerical methods are generally adopted to measure the key parameters at a small scale as it is time consuming and costly to determine them in the field and used for quantifying flow and transport in large scales in in-situ conditions applied to simulate real contaminant transport models. These methods need a number of key parameters such as porosity, hydrodynamic dispersion, velocity of contaminant flow and Temperatures. The main aim of this research is to evaluate the nonlinear variation of the Distribution coefficient with parameters like porosity, power factor and bulk density based on detailed experimentation carried out on physical models in the laboratory and development of a suitable and appropriate numerical model. The batch and column tests were conducted to evaluate the distribution coefficient and sorption capacity.

Keywords: Contamination, Distribution Coefficient, Dispersion Coefficient.

I. INTRODUCTION

Soil is a vibrant system in which numerous chemical, physical, and biological reactions occur singly or simultaneously. Evaluation of fluid flows is essential part to understand subsurface phenomena including contaminant transport and waste contaminant. Subsurface contamination is the acute problem faced by mankind. Understanding the long- term behavior of contaminants in the subsurface is essential to avoid ground water contamination. Once groundwater is contaminated, it is important to understand how the contaminant moves in the subsurface environment. Proper understanding of the contaminant fate and transport is necessary in order to characterize the risks associated with the contamination. The parameters known as the Distribution coefficient (K_d) and Retardation factor (R) are the most important parameters used in estimating the migration potential of contaminants present in aqueous solutions in contact with surface, subsurface and suspended solids. Hence evaluating these parameters is very important to predict the extent of contamination at a particular site. Numerical methods are in general superior to analytical methods in terms of being able to solve much more practical problems. Numerical methods usually subdivide the time and spatial coordinates into smaller pieces, such as finite differences, finite elements, and finite volumes, and reformulate the continuous form of governing partial differential equations in terms of a system of algebraic equations. To obtain solutions at certain times, numerical methods generally require intermediate simulations (time-stepping) between the initial condition and the points in time for which the solution is needed. The object of the present work is to develop a method of analysis to determine the Linear and Nonlinear variation of the Distribution Coefficient with different physical parameters. Laboratory studies were conducted on soil columns of 15 to 95cm length. Analytical solution (Fried, 1975) was used for obtaining the Distribution coefficient from the Break-through curves. A numerical method introducing constant dispersion coefficient was developed.

II. LITERATURE REVIEW

Wu et al. (1997) proposed a stochastic model for modelling solute transport for heterogeneous soils. In this approach, a hydrologic environment is divided into sub-environments based on the knowledge of the omains deterministic spatial variability. The sub environments are assumed to form statistically independent soil columns within which vertical flow occurs. Each sub-environment is discredited based on morphological horizon information as many layers with varying thickness to form modelling units that are statistically independent. Selected soil properties in each sub environment are described with a multivariate normal random vector. Several realisations of the soil properties are then generated for each of the modelling units. Monte-Carlo runs of the model are then carried out to provide statistical information of the output variables of the column.

Srinivas and Krishna Reddy (1996) presented the adsorption tests results for hexavalent chromium, Cr (VI) The break-through time due to combined advection, diffusion and nonlinear adsorption will be greater than that of advection and diffusion but lower than that of advection, diffusion and linear sorption. Further different contaminants get absorbed in different amounts to the same adsorbate. For example, the adsorption of inorganic contaminants is primarily dependent on the cation or anion exchange capacity of the clay, and different clays have different adsorption mechanisms Therefore even in linear adsorption different distribution coefficient values are possible leading to different break-through times for different contaminants.

III. DEVELOPMENT OF NUMERICAL MODEL

The theoretical basis for the equation describing solute transport has been well documented in literature (Bear, 1997). Changes in chemical; concentration occur in a dynamic soil system due to the different processes of transport involved, such as advective transport, dispersion, sorption, biodegradation etc. In the present study, advective and dispersive transport along with sorption for reactive contaminant has been considered for deriving the governing equations. These governing partial differential equations can be solved

numerically. The continuous differential equation, which defines solute concentration every-where in the system, is replaced by a finite number of algebraic equations that defines concentrations at different time periods.

The various steps involved in development of numerical model are as follows:

a) Conceptualization of the model.
b) Mathematical model expressing the set of assumptions into a set of differential equations associated with a set of auxiliary boundary conditions.
c) Convective dispersive equation with sorption
d) Finite difference method of solution of the partial differential equation.

Conceptualization of the model

The contaminant disperses through the low permeable layer into the next layer. the flow through the low permeable layer is considered as one – dimensional. For conceptualization of the model the assumptions made are

a) The flow is considered to be one –Dimensional.
b) The source of contamination is continuous with the same concentration of C_o.
c) The depth of the porous medium under consideration is finite.
d) The porous medium is saturated.
e) The concentration of the contaminant initially is zero in the porous medium.

Mathematical modeling

The second step of modeling process involves the translation of conceptual model in to the mathematical terms by a set of partial differential equations with an associated set of auxiliary boundary conditions. Based on the assumptions made, the governing equations is as follows

a) Convective- Advective Equation for a reactive contaminant is given by

$$D_x \frac{\partial^2 C}{\partial x^2} - V_x = R \tag{1}$$

Where

D_x: Hydrodynamic dispersion coefficient
V_x: Contaminant flow velocity
R: Retardation coefficient.

b) The Initial boundary conditions are

$$C(x, 0) = 0 \quad \text{at} \quad t=0$$

In many practical situations the most hazardous pollutant has a maximum concentration, c_0 initially (zero time). This concentration will then decrease with time as leachate is transmitted through the soil. Though this assumption of constant concentration is extremely conservative still, it is used because it covers many important aspects of the problem of pollutant migration through a finite layer. Therefore, it is assumed that

$$C(0, t) = C_0 \quad \text{for } t > 0$$

It is assumed that the concentration in the underlying permeable stratum does not vary with vertical or horizontal position. Therefore

$$C(L_1, t) = C(L, t) \; L_1 > L$$

L: the total depth or thickness of the stratum.

Convective - dispersive equation with sorption

Convective-dispersive equation with retardation factor to include the sorption effect of the soil was considered in framing the governing equation as given above

IV. NON - LINEAR SORPTION

The solute Retardation factor for nonlinear adsorption is not constant, as is the case for linear adsorption, but changes as a function of concentration. Many models have been used in the past to describe nonlinear sorption. The most commonly used nonlinear sorption models are those by Freundlich (1909) is

$$S = K_d C^N \tag{2}$$

Non - linear variation of distribution coefficient .Taking into consideration nonlinear variation of the distribution coefficient, and differentiating

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - V_s \frac{\partial C}{\partial x} - \frac{\rho_d}{n} \frac{\partial S}{\partial t} \tag{3}$$

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - V_s \frac{\partial C}{\partial x} - \frac{\rho_d}{n} \frac{\partial S}{\partial C} \tag{4}$$

$$S = K C^N \tag{5}$$

By differentiating above equation we get

$$\frac{\partial S}{\partial C} = K\,N\,C^{N-1} \tag{6}$$

Substituting Eq 6 in Eq 4 one gets

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - V_s \frac{\partial C}{\partial x} - \frac{\rho_d}{n} \, K\,NC^{N-1}\,\frac{\partial C}{\partial t}$$

On simplification the equation reduces to

$$D_x \frac{\partial^2 C}{\partial x^2} - V_s \frac{\partial C}{\partial x} = \frac{\rho_d}{n}\,K\,NC^{N-1}\,\frac{\partial C}{\partial t} + \frac{\partial C}{\partial t}$$

$$\frac{\partial^2 C}{\partial x^2} - V_s \frac{\partial C}{\partial x} = \left(1 + \frac{\rho_d}{n}K\,NC^{N-1}\right)\frac{\partial C}{\partial t} \tag{7}$$

Normalizing Equation with $\quad X = \frac{x}{L} \quad$ and $\quad T = t/t_o$

$$\partial X = \frac{1}{L}\partial x \qquad\qquad \partial T = \frac{1}{t_o}\,\partial t$$

$$\partial^2 X = \frac{1}{L^2}\partial x^2 \qquad\qquad \partial t = t_o\,\partial T$$

$$D_x \frac{\partial^2 C}{L^2\,\partial X^2} - V_s \frac{\partial C}{L\,\partial X} = \left(1 + \frac{\rho_d}{n}K\,NC^{N-1}\right)\frac{\partial C}{t_o\,\partial T}$$

$$D_x \frac{\partial^2 C}{L^2\,\partial X^2}\frac{\partial T\,t_o}{} - V_s \frac{\partial C\,t_o}{L\,\partial X} = \left(1 + \frac{\rho_d}{n}K\,NC^{N-1}\right)\frac{\partial C}{\partial T} \tag{8}$$

Substituting $t_0 = L/V_x$ in Eq. (8) the following expression was obtained

$$\left(\frac{D_x}{V_x L}\right)\frac{\partial^2 C}{\partial X^2} - \left(\frac{V_S}{V_x}\right)\frac{\partial C}{\partial x} = \left(1 + \frac{\rho_d}{n}\,K\,NC^{N-1}\right)\frac{\partial C}{\partial T}$$

If $\quad R = \left(1 + \frac{\rho_d}{n}K\,NC^{N-1}\right)$ the above Eq. Reduces to

$$\left(\frac{D_x}{V_x L}\right)\frac{\partial^2 C}{\partial X^2} - \left(\frac{V_S}{V_x}\right)\frac{\partial C}{\partial x} = (R)\frac{\partial C}{\partial T} \tag{9}$$

From finite difference method   the Eq. (14) one obtained as

$$\left(\frac{D_x}{RV_x L\Delta x^2}\right)(C_{i+1,t} - 2C_{i,t} + C_{i+1,t}) - \left(\frac{1}{\Delta X}\right)C_{i+1,t} - C_{i-1,t} = \frac{C_{i,t+\Delta t} - C_{i,t}}{\Delta t}$$

$$\left(\frac{D_x\,\Delta t}{RV_x L\Delta x^2}\right)(C_{i+1,t} - 2C_{i,t} + C_{i+1,t}) - \left(\frac{1\,\Delta t}{R\,2\,\Delta X}\right)C_{i+1,t} - C_{i-1,t} = C_{i,t+\Delta t} - C_{i,t}$$

Let $\quad \alpha = \left(\frac{D_x\,\Delta t}{R\,V_x\,L\,\Delta x^2}\right) \qquad \beta = \frac{\Delta t}{R\,2\,\Delta X}$

Then above Equation in terms of α and β is given by

$$\alpha\,(C_{i+1,t} - 2C_{i,t} + C_{i+1,t}) - \beta\,(C_{i+1,t} - C_{i-1,t}) = C_{i,t+\Delta t} - C_{i,t}$$

On further simplification

$$(\alpha - \beta)\,C_{i+1,t} + (1 - 2\alpha)C_{i,t} + (\alpha + \beta)C_{i-1,t} = C_{i,t+\Delta t} \tag{10}$$

Checking the convergence and stability of the cdm with sorption for nonlinear variation. For a reactive contaminant with nonlinear variation of the distributive coefficient, with distance

$$\alpha = \left(\frac{D_x\,\Delta t}{R\,V_x\,L\,\Delta x^2}\right) \qquad \beta = \frac{\Delta t}{R\,2\Delta X}$$

Table 1 Input Parameters to Check Stability of the Model for Nonlinear Variation of Distributive Coefficient for Reactive Contaminant

L	15	15
ρ_d	0.0016	0.0016
N	0.6	0.6
K	100	100
N	5	5
C	1	1
N-1	4	4
$\rho_d/nx(KxNx\,C^{N-1})$	1.333333	1.333333
R	2.333333	2.333333
A	0.111561	0.200809
B	0.054665	0.098397

α-β	0.056896	0.102413
1- 2α	0.776879	0.598382
α+ß	0.166225	0.299206

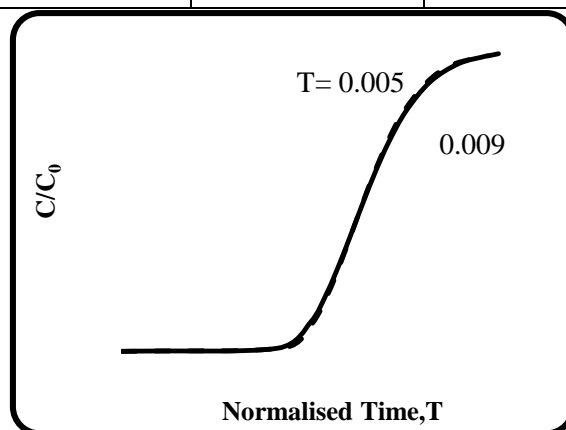*Fig 1 Breakthrough Curves for Different ΔT Values to Check the Convergence and Stability of the Model*

The equation for unknown concentration is $(\alpha - \beta)\, C_{i+1,t} + (1 - 2\alpha)C_{i,t} + (\alpha + \beta)C_{i-1,t} = C_{i,t+\Delta t}$

Using this expression, the concentrations were calculated at each node of the column using the input parameters shown in the table 3 The Break-through curves are furnished in Fig 3.

Fig 1 shows the Break-Through curves for $D_x = 3\times10^{-6} cm^2/sec$, $V_x = 1\times10^{-5} cm/sec$, and for Δ T values of 5×10^{-2} and 9×10^{-2} minutes. It is observed that the curves corresponding to Δ T $=5\times10^{-2}$ and Δ T $=9\times10^{-2}$ converge to the same breakthrough curve. for these values of Δ T, for Δ X=0.0196 the values α+ß, α-β and 1- 2α are positive. For Δ T $=2\times10^{-2}$ the value of 1- 2α is negative. While the other two are positive, therefore these values do not yield proper solution. Hence to obtain convergence of the curves, the size of time step, Δ T should not exceed 2×10^{-2} for values of Δ X=0.0196. It is also observed that the initial normalized time is at about 1.4 and attained the maximum point at a normalized time of about 3.4.the range of the curve remains constant for different normalized time (Δ T) values.

V.PARAMATRIC STUDY FOR NON - LINEAR VARIATION

The governing equation for nonlinear variation of distributive coefficient and retardation is given by a equation This CDM with sorption considers the nonlinear variation of distributive coefficient with length of the column. The sensitivity of the model was carried out by studying the effect of these key parameters Distribution coefficient (K), Power factor(N), Bulk density (ρ_d), Porosity (n), and contaminant flow velocity (V_x) on the Break-Through curves.

The range of Distribution Coefficient K for this study ranges from 10 to 1000, Power factor(N)from 1 to 10 Bulk density (ρ_d) from 0.0013 to 0.0018 and Porosity (n) from 0.4 to 0.9 contaminant flow velocity (V_x) for $1\times10^{-5}cm/sec$ and $1\times10^{-6}cm/sec$. The resulted breaks through curves are presented in Figures below.

Effect of power factor 'n' on break through curves

The sensitivity of parameter power factor(N) on break-through curves was studied by varying N values from 1 to 10 for values of bulk density (ρ_d) =0.0016 and porosity(n)=0.6, Distribution coefficient K=10.

Table2 Input Parameters for Different Power Factor Values for K=10

L	15	15	15	15
ρ_d	0.0016	0.0016	0.0016	0.0016
n	0.6	0.6	0.6	0.6
K	10	10	10	10
N	2	5	7	10
C	1	1	1	1
N-1	1	4	6	9
$\rho_d/nx(KxNxC^{N-1})$	0.053333	0.133333	0.186667	0.266667
R	1.053333	1.133333	1.186667	1.266667
α	0.247128	0.229684	0.219361	0.205506
β	0.121093	0.112545	0.107487	0.100698
α-β	0.126035	0.117139	0.111874	0.104808
1- 2α	0.505744	0.540633	0.561278	0.588987
α+ß	0.368221	`0.342229	0.326848	0.306205

From the Fig 2 it is observed that initial time for N=2 is 0.6 and final normalized time is around1.5.for N=5 the initial normalized time is 0.6 and final is around1.8.for N=7 and N=10 it is observed that the initial normalized time is slightly increasing with increasing Power factor (N), whereas the final normalized break-through curves are almost coinciding at 1.8

From these plots it is observed that as Power factor (N) value increases the Normalized time (T) increases for any given value of C/C$_0$

Effect of distribution coefficient 'k' on break through curves
The sensitivity of parameter K on break-through curves was studied by varying K values for Power Factor N=1, bulk density(ρ_d)   =0.0016 and porosity(n)=0.6

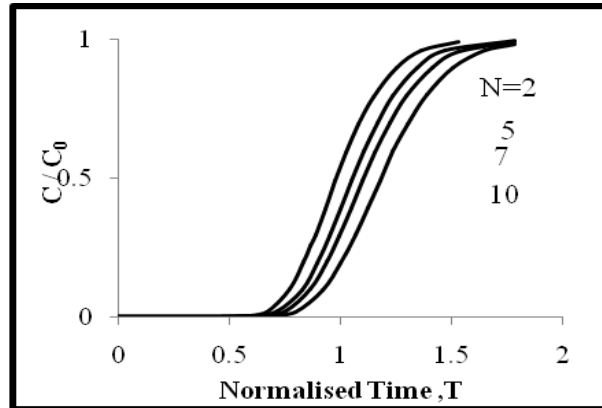*Fig :2 Breakthrough Curves for Different N Values for K=10*

Table 3 Input Parameters for Varying Distribution Coefficient Values for N=1

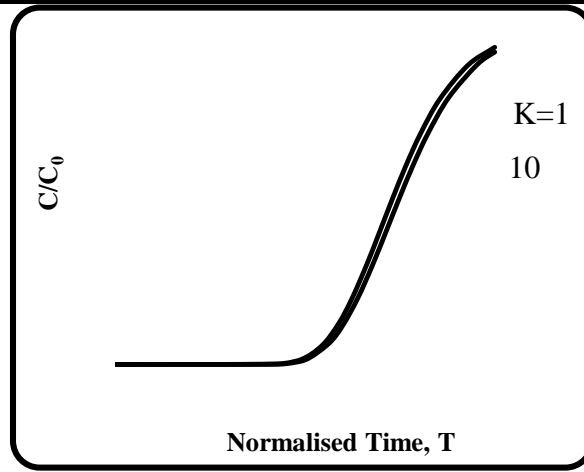|	15	15
L		
D_x	0.000003	0.000003
V_x	0.00001	0.00001
ΔT	0.005	0.005
ΔX	0.0196	0.0196
ΔX^2	0.000384	0.000384
ρ_d	0.0016	0.0016
n	0.6	0.6
K	1	10
N	1	1
C	1	1
N-1	0	0
$\rho_d/nx(KxNxC^{N-1})$	0.002667	0.026667
R	1.002667	1.026667
α	0.259616	0.253547
β	0.127212	0.124238
$\alpha-\beta$	0.132404	0.129309
1- 2α	0.480768	0.492906
$\alpha+\beta$	0.386828	0.377785

Fig 3 Breakthrough Curves for Different K Values for N=1

From Fig 3 it is observed that the break through curves for K=1 and K=10 are almost coinciding. The initial normalized time for both the break-through curves is 0.6 and final normalized time interval is 1.5. The sensitivity of parameter K on break-through curves was studied by varying K values for Power Factor N=5, ρ_d=0.0016 and n=0.9

Table 4 Input Parameters for Different Distribution Coefficient Values for N=5

| L	15	15	15	15
D_x	0.000003	0.000003	0.000003	0.000003
ΔT	0.005	0.005	0.005	0.005
ΔX	0.0196	0.0196	0.0196	0.019
ΔX^2	0.000384	0.000384	0.000384	0.000384
ρ_d	0.0016	0.0016	0.0016	0.0016
n	0.6	0.6	0.6	0.6
K	10	100	500	1000
N	5	5	5	5
C	1	1	1	1
N-1	4	4	4	4
$\rho_d/nx(KxNxC^{N-1})$	0.133333	1.333333	6.666667	13.33333
R	1.133333	2.333333	7.666667	14.33333
α	0.229684	0.111561	0.033953	0.018161
β	0.112545	0.054665	0.016637	0.008899
$\alpha-\beta$	0.117139	0.056896	0.017316	0.009262
1- 2α	0.540633	0.776879	0.932094	0.963678
$\alpha+\beta$	0.342229	0.166225	0.05059	0.02706
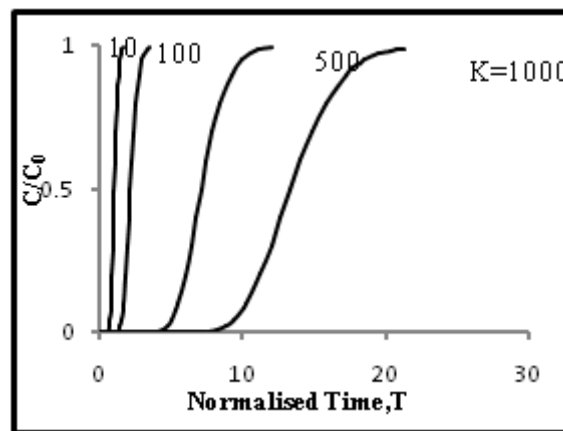
Fig 4 Break through Curves for Different K Values and N=10

From Fig 4 it could be observed that as Distribution coefficient increases normalized time also increases for any given value of C/C$_0$. By comparing Fig 4 and Fig 5 it could be observed that the initial normalized time attained by the break-through curves for K<500 has almost remained same, whereas for K=1000 it is observed that the initial and final normalized time has increased with increased porosity and power factor.

The initial normalized time for K=1000 is around 9.5, whereas in Fig 5 the initial normalized time has increased to 11 and the final normalized time has also increased from 18 to 29. From these plots it is observed that as Distribution coefficient (K) value increases the Normalized time (T) increases for any given value of C/C_0.

Effect of different bulk density ρ_d on break through curves

The sensitivity of the parameter ρ_d on break–through curves was studied by varying ρ_d values from 0.0013 to 0.0018 for n = 0.6 and K=10 and Power Factor N =2.

Table 5 Input Parameters for Different Bulk Density (ρ_d) Values for K=10, N=2

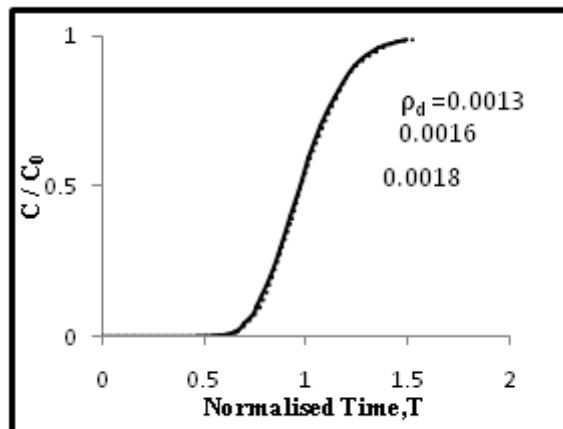| L	15	15	15
ρ_d	0.0013	0.0016	0.0018
n	0.6	0.6	0.6
K	10	10	10
N	2	2	2
C	1	1	1
N-1	1	1	1
$\rho_d/nx(KxNxC^{N-1})$	0.043333	0.053333	0.06
R	1.043333	1.053333	1.06
α	0.249497	0.247128	0.245574
β	0.122253	0.121093	0.120331
$\alpha-\beta$	0.127243	0.126035	0.125243
$1-2\alpha$	0.501007	0.505744	0.508852
$\alpha+\beta$	0.37175	0.368221	0.365905

Fig 5 Breakthrough Curves for Different ρ_d Values for Input Parameters K=10, N=2

From Fig 5 it is observed that the normalized time attained for different values of bulk density ρ_d is constant. The initial normalized time is 0.5 and attains final normalized time at 1.6 Distribution coefficient (K) and Power factor (N) values are increased from K=10 and N=2 to K=1000 and N=10.variation of the break-through curves is observed in Fig 7

Table 6 Input Parameters for Different Bulk Density Values for K=1000, N=10

L	15	15	15
ρ_d	0.0013	0.0016	0.0018
n	0.4	0.4	0.4
K	1000	1000	1000
N	10	10	10
C	1	1	1
N-1	9	9	9
$\rho_d/nx(KxNxC^{N-1})$	32.5	40	45

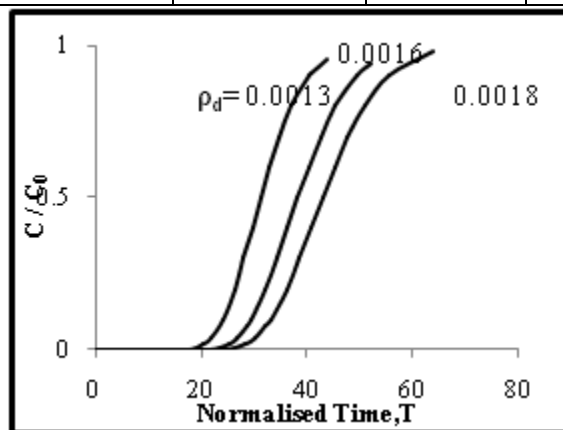| R	33.5	41	46
α	0.00777	0.006349	0.005659
β	0.003807	0.003111	0.002773
α-β	0.003963	0.003238	0.002886
1- 2α	0.984459	0.987302	0.988682
α+ß	0.011578	0.00946	0.008432

Fig 6 Breakthrough Curves for Different ρ_d Values for Input Parameters K=10, N=2

From Fig 6 it could be observed that for bulk density $\rho_d < 0.0018$ the normalized time for any given value of C/C_0 decreases with decrease in bulk density. It is also observed that when Distribution coefficient (K) and power factor (N) values are increased from K=10 and N=2 to K=1000 and N=10 for varying bulk density values, the normalized time increases almost 40 times the initial values.

VI. CONCLUSION

Based on the Numerical Modeling and the analytical results obtained, the following conclusions are obtained

- Variation of Distribution coefficient depends on the parameters Porosity, Bulk density and Power factor.
- For reactive contaminant in nonlinear variation, bulk density, Power factor are directly proportional to Distribution coefficient. Whereas Porosity is inversely proportional to Distribution coefficient.
- When Retardation factor is high nonlinear variation of Distribution coefficient is observed.
- Break-through curves coincide for low Retardation factor. But as Retardation factor increases range of the Break-through curve increases.

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