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Solute Transport with Time-dependent Periodic Source Concentration in Aquifer

Sultana Begam[1], Premlata Singh[2] and Mritunjay Kumar Singh[3]
[1,3]Department of Mathematics and Computing, Indian Institute of Technology (Indian School of Mines), Dhanbad
[1,3]Emails: sultanabegam26@gmail.com, drmks29@iitism.ac.in
[2]Department of Mathematics, Birla Institute of Technology, Patna Campus, Patna
[2]Email: psingh@bitmesra.ac.in

Abstract

A mathematical model is presented for describing the solute transport with periodic time-dependent source concentration in a homogeneous semi-infinite aquifer. An extra source term is imposed on solute transport equation to discuss the nature of contaminant concentration. Initially the aquifer contains space-dependent concentration. Time-dependent periodic boundary condition is considered at the inlet boundary, and a flux type boundary condition is taken at the outlet boundary. The concept of dispersion theory is employed in which the impact of diffusion coefficient is also considered in this study. The Laplace transform and explicit finite difference techniques are adopted to obtain the analytical and numerical solutions respectively. An error analysis is also made and discussed RMS, Relative and Percentage errors for accuracy of the solutions obtained.

1. Introduction

One-, two- or three-dimensional groundwater flow or transport equations popularly known as advection-dispersion equations with uniform, non-uniform flows have been discussed since last two-three decades. Analytical solutions and Methods of solution with classical references were available in the hydrological literature (Barry and Sposito, 1989; Aral and Liao, 1996; Runkel, 1996; Kumar, 1983; Pistiner and Shapiro, 1998). Fry et al. (1993) proposed an analytical solution for solute transport equation with rate limited desorption and decay. Toride et al. (1993) proposed a comprehensive set of analytical solutions for non-equilibrium solute transport with first-order decay and zero order production. Flury et al. (1998) derived the analytical solution of the one-dimensional convection-dispersion equation (CDE) with depth-dependent degradation or adsorption coefficients, expressed as sigmoidal function of depth. Flury et al. (1998) considered adsorption and degradation separately in CDE. However, these two always occurs simultaneously with contaminant transport in soil. Furthermore, they only studied the case of solute transport in a semi-infinite system with short pulse input at the inlet. Gao et al. (2013) extended the work of Flury et al. (1998) and tried to cover the shortcomings to provide an analytical solution for contaminant transport in soil with depth-dependent reaction coefficients and time-dependent inlet boundary conditions. The solute adsorption described with a linear isotherm, and solute degradation assumed to be a first-order process. But they considered a constant velocity and dispersion coefficients but not time or space dependent. Park and Zhan (2001) provided analytical solutions of contaminant transport from one-, two-, and three-dimensional finite sources in a finite-thickness aquifer using Green's function method. Bauer et al. (2001) presented an analytical solution to discuss the solute transport of a decay chain in homogenous porous media. Guerrero et al. (2010) explored an analytical solution of a multi-species advection-dispersion transport equation featuring sequential first-order decay reactions, distinct linear sorption reactions for each species with constant boundary conditions in a finite domain. Vanderborght et al. (2005) provided a set of analytical benchmarks to test numerical models of flow and transport in soils. Chen et al. (2012) presented a novel method for analytical solution of multi-species advective-dispersive transport equations sequentially coupled with first-order decay reactions. Jaiswal et al. (2011) obtained an analytical solution for one-dimensional temporally dependent advection-dispersion equation in finite

homogeneous porous media in which the retardation coefficient and the first order decay term were included. But simple constant boundary conditions were taken to avoid the complexity of the problem. Mazumder and Bandyopadhyay (2000) examined the streamwise dispersion of contaminant molecules due to a turbulent shear flow over a gravel-bed surface subject to the solute is released from an elevated line source. Singh et al. (2015) obtained analytical and numerical solutions to the advection-dispersion-reaction equation in a semi-infinite geological formation with variable porosity values. An effect of retardation factor, zero-order production and first-order decay constant were discussed in their work. Singh et al. (2016a,b) discussed about the transform techniques for solute transport in groundwater and explored mathematical modelling for solute transport in aquifer as well. In most of the available hydrological literature, the boundary conditions were taken constant or time-dependent algebraic and exponential functions but not the periodic one. Logan (1996) proposed a solute transport model in porous media with scale-dependent dispersion with periodic boundary conditions. Ferris (1963) derived a solution for the steady periodic response of the piezometric heads in a semi-infinite aquifer subject to a sinusoidal variation of the stream water level.
The objective of this study are- (i) to derive an analytical solution for contaminant transport in semi-infinite homogeneous porous media with time-dependent periodic boundary conditions; (ii) to investigate the impact of first order decay and elemental recharge rate of aquifer; (iii) to validate the analytical solution with the numerical solution obtained by using explicit finite difference method; and (iv) to obtained the accuracy of the solution. To achieve the aforesaid objective, analytical and numerical approaches are taken into consideration and their application in the field hydrological study exclusively in vazose zone hydrology. The geometry of the problem is shown in Fig.1.

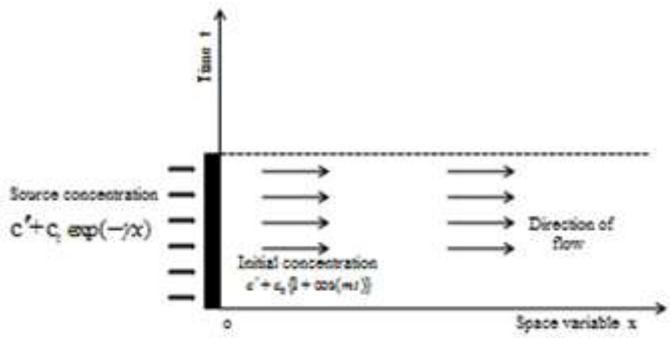

Fig-1: Geometry of the model

2. Mathematical Formulation

The solute transport in aquifer system is usually dealt with advective-dispersive equation with and/or without impact of various parameters i.e., advection, dispersion, retardation factor, zero-order production and first order decay terms etc. In the present work, a one-dimensional contaminant transport with advection, dispersion, and first-order contaminant decay, is presented mathematically as follows:

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left[D(x,t)\frac{\partial C}{\partial x}-u(x,t)C\right]-\mu C \tag{1}$$

Sometimes, source of contamination such as ash pond, dump site or industrial disposal site lies above the aquifer through which there is a possibility of pollution reaching the underlying aquifer (Rastogi, 2007). For this physical situation, an extra term $\frac{c'w}{\theta}$ is included in the equation (1). The advection-dispersion reaction (ADR) equation can be written as:

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left[D(x,t)\frac{\partial C}{\partial x}-u(x,t)C\right]-\mu C+\frac{c'w}{\theta} \tag{2}$$

where, $C(x,t)[ML^{-3}]$ is the Contaminant concentration, $u(x,t)[LT^{-1}]$ is the groundwater velocity or seepage velocity, $D(x,t)[L^2T^{-1}]$ is the dispersion coefficient, $\mu\ [T^{-1}]$ is first-order decay term, $t\ [T]$ is time and $x\ [L]$ is distance variable, w is elemental recharge rate with solute concentration $c'\ [ML^{-3}]$ and θ is effective porosity of the aquifer.

The initial and boundary conditions are considered as follows:

$$C(x,t) = c' + c_i \exp(-\gamma x); \quad x \geq 0, t = 0 \tag{3}$$

where, c_i is initial background solute concentration, γ is a constant coefficient parameter whose dimension is the inverse of the space variable.

$$C(x,t) = c' + c_0\{1 + \cos(mt)\}; \quad x = 0, t > 0 \tag{4}$$

The periodic source boundary is considered reaching to the groundwater table at a point $x = 0$ and the solute dispersion is along with flow of water. Only longitudinal dispersion is taken into consideration neglecting transverse dispersion in one-dimensional advection-dispersion equation with an elemental recharge rate with solute concentration. Flux concentration is assumed zero at an infinite extent of the aquifer.

$$\frac{\partial C}{\partial x} = 0; \quad x \to \infty, t > 0 \tag{5}$$

2.1 Analytical Solution with Dirichlet-type Boundary Condition

Sinusoidally varying seepage velocity is considered for the purposes of studying seasonal variation occurring into the system. The dispersion theory is employed which was proposed and followed by many researchers (Freeze and Cherry, 1979; Kumar,1983; Singh, 2009). We considered as

$$u(x,t) = u_0|\sin(mt)|; \quad D(x,t) = D_0|\sin(mt)|; \quad \mu(x,t) = \mu_0|\sin(mt)| \tag{6a}$$

where, u_0, D_0 and μ_0 are the initial seepage velocity, dispersion coefficient and first-order decay respectively.

The initial dispersion coefficient is expressed as a combination of hydrodynamic dispersion and diffusion as

$$D_0 = qxu_0 + D^* \tag{6b}$$

where, q is the non-dimensional parameter expressing the growth rate of dispersivity with respect to distance. Here $\alpha_0 = qx$ is the asymptotic dispersivity [L] and $D^*\left[L^2T^{-1}\right]$ is the molecular diffusion coefficient. The impact of diffusion has not been considered by most of the researchers, because it does not vary significantly for different geological formations and ranges from 1×10^{9} to $2\times10^{-9} m^2/sec$ (Mitchell, 1976). However, it was found that even a small value of diffusion coefficient may have a significant impact on solute transport in fine-grained geologic materials (Gillham and Cherry, 1982).

Applying equations (6a) in equation (2) we get as follows:

$$\frac{\partial C}{\partial t} = D_0|\sin(mt)|\frac{\partial^2 C}{\partial x^2} - u_0|\sin(mt)|\frac{\partial C}{\partial x} - \mu_0|\sin(mt)|C + \frac{c'w}{\theta} \tag{7}$$

A new variable T is introduced as

$$T = \int_0^t |\sin(mt)|\, dt \tag{8}$$

and it can be written as

$$T = \frac{1}{m}\{1 - \cos(mt)\} \tag{9}$$

Using the above transformation (8), the solute transport equation (7) becomes as follows:

$$\frac{\partial C}{\partial T} = D_0\frac{\partial^2 C}{\partial x^2} - u_0\frac{\partial C}{\partial x} - \mu_0 C + \frac{c'w}{\theta|\sin(mt)|} \tag{10}$$

Corresponding initial and boundary conditions transformed as follows:

$$C(x,T)=c^{'}+c_i\,exp(-\gamma x);\quad x\geq 0, T=0 \tag{11}$$

$$C(x,T)=c^{'}+c_0(2-mT);\quad x=0, T>0 \tag{12}$$

$$\frac{\partial C}{\partial x}=0;\quad x\rightarrow\infty, T>0 \tag{13}$$

Laplace transform technique is used to solve the problem analytically. To remove the convective term from equation (10) we use the following transformation:

$$C(x,T)=K(x,T)\,exp\left\{\frac{u_0 x}{2D_0}-\left(\frac{u_0^2}{4D_0}+\mu_0\right)T\right\}+\frac{c^{'}w}{\mu_0\theta\,|\,sin(mt)|} \tag{14}$$

The transformed AD equation can be written as follows:

$$\frac{\partial K}{\partial T}=D_0\frac{\partial^2 K}{\partial x^2} \tag{15}$$

The corresponding initial and boundary conditions can be written as,

$$K(x,T)=c^{'}\,exp\left(-\frac{u_0 x}{2D_0}\right)+c_i\,exp\left[-\left(\gamma+\frac{u_0}{2D_0}\right)x\right];\quad x\geq 0,\quad T=0 \tag{16}$$

$$K(x,T)=c^{'}\,exp\left\{\left(\frac{u_0^2}{4D_0}+\mu_0\right)T\right\}+c_0(2-mT)\,exp\left\{\left(\frac{u_0^2}{4D_0}+\mu_0\right)T\right\};\quad x=0,\quad T>0 \tag{17}$$

$$\frac{\partial K}{\partial x}+\frac{u_0}{2D_0}K=0;\quad x\rightarrow\infty,\quad T>0 \tag{18}$$

Using Laplace transform technique one can obtain the analytical solution with Dirichlet-type boundary condition as,

$$C(x,T)=\left[\frac{c^{'}+2c_0}{2}E(x,T)-mc_0F(x,T)-\frac{c^{'}}{2}G(x,T)-\frac{c_i}{2}H(x,T)+J(x,T)\right] \tag{19}$$

where, $E(x,T), F(x,T), G(x,T), H(x,T)$ and $J(x,T)$ are expressed as follows:

$$E(x,T)=exp\left(\frac{u_0 x}{2D0}-\frac{\beta x}{\sqrt{D_0}}\right)erfc\left(\frac{x}{2\sqrt{D_0T}}-\beta\sqrt{T}\right)+exp\left(\frac{u_0 x}{2D0}+\frac{\beta x}{\sqrt{D_0}}\right)erfc\left(\frac{x}{2\sqrt{D_0T}}+\beta\sqrt{T}\right) \tag{20a}$$

$$F(x,T)=\frac{1}{4\beta}\left[\left(2\beta T-\frac{x}{\sqrt{D_0}}\right)exp\left(\frac{u_0 x}{2D_0}-\frac{\beta x}{\sqrt{D_0}}\right)erfc\left(\frac{x}{2\sqrt{D_0T}}-\beta\sqrt{T}\right)\right.$$
$$\left.+\left(2\beta T+\frac{x}{\sqrt{D_0}}\right)exp\left(\frac{u_0 x}{2D_0}+\frac{\beta x}{\sqrt{D_0}}\right)erfc\left(\frac{x}{2\sqrt{D_0T}}+\beta\sqrt{T}\right)\right] \tag{20b}$$

$$G(x,T)=exp(-\mu_0T)\,erfc\left(\frac{x}{2\sqrt{D_0T}}-\frac{u_0}{2}\sqrt{\frac{T}{D_0}}\right)+exp\left(\frac{u_0 x}{D_0}-\mu_0T\right)erfc\left(\frac{x}{2\sqrt{D_0T}}+\frac{u_0}{2}\sqrt{\frac{T}{D_0}}\right) \tag{20c}$$

$$H(x,T)=\left[exp(D_0\alpha^2T-\gamma x-\beta^2T)\,erfc\left(\frac{x}{2\sqrt{(D_0T)}}-\alpha\sqrt{D_0T}\right)\right.$$
$$\left.+exp\left(\frac{u_0 x}{2D_0}+\alpha x+D_0\alpha^2T-\beta^2T\right)erfc\left(\frac{x}{2\sqrt{(D_0T)}}+\alpha\sqrt{D_0T}\right)\right] \tag{20d}$$

$$J(x,T)=c^{'}\,exp(-\mu_0T)+c_i\,exp(D_0\alpha^2T-\beta^2T-\gamma x)+\frac{c^{'}w}{\theta\mu_0\,|\,sin(mt)|} \tag{20e}$$

where, $\alpha = \gamma + \frac{u_0}{2D_0}$ and $\beta^2 = \frac{u_0^2}{4D_0} + \mu_0$

2.2 Analytical Solution with Cauchy-type Boundary Condition

$$-D(x,t)\frac{\partial C}{\partial x} + uC = u[c' + c_0\{1+\cos(mt)\}]; \quad x=0, \quad t>0 \tag{21}$$

In a similar manner, an analytical solution with Cauchy-type boundary condition can be obtained as,

$$C(x,T) = \frac{(u_0c' + 2c_0 - u_1)}{\sqrt{D_0}}E'(x,T) - \frac{2mc_0}{u_0}F'(x,T) - \frac{c'u_0}{\sqrt{D_0}}G'(x,T) - \frac{c_i(\alpha D_0 + 1)}{\sqrt{D_0}}H'(x,T) + J'(x,T) \tag{22}$$

where, $E'(x,T), F'(x,T), G'(x,T), H'(x,T)$ and $J'(x,T)$ are expressed as follows:

$$E'(x,T) = \left[\frac{1}{2(\beta + \frac{u_0}{2\sqrt{D_0}})}\exp\left\{\left(\beta^2 - \frac{u_0^2}{4D_0}\right)T - \left(\frac{\beta}{\sqrt{D_0}} - \frac{u_0}{2D_0}\right)x\right\}\operatorname{erfc}\left(\frac{x}{2\sqrt{D_0T}} - \beta\sqrt{T}\right)\right.$$
$$- \frac{1}{2(\beta - \frac{u_0}{2\sqrt{D_0}})}\exp\left\{\left(\beta^2 - \frac{u_0^2}{4D_0}\right)T + \left(\frac{\beta}{\sqrt{D_0}} + \frac{u_0}{2D_0}\right)x\right\}\operatorname{erfc}\left(\frac{x}{2\sqrt{D_0T}} + \beta\sqrt{T}\right) \tag{23a}$$
$$\left. + \frac{u_0}{2\sqrt{D_0}\left(\beta^2 - \frac{u_0^2}{4D_0}\right)}\exp\left(\frac{u_0x}{D_0}\right)\operatorname{erfc}\left(\frac{x}{2\sqrt{D_0T}} + \frac{u_0}{2}\sqrt{\frac{T}{D_0}}\right)\right]$$

$$F'(x,T) = \left[\frac{1}{4\beta}\left(2\beta T - \frac{x}{\sqrt{D_0}}\right)\exp\left\{\left(\beta^2 - \frac{u_0^2}{4D_0}\right)T - \left(\frac{\beta}{\sqrt{D_0}} - \frac{u_0}{2D_0}\right)x\right\}\operatorname{erfc}\left(\frac{x}{2\sqrt{D_0T}} - \beta\sqrt{T}\right)\right.$$
$$+ \frac{1}{4\beta}\left(2\beta T + \frac{x}{\sqrt{D_0}}\right)\exp\left\{\left(\beta^2 - \frac{u_0^2}{4D_0}\right)T + \left(\frac{\beta}{\sqrt{D_0}} + \frac{u_0}{2D_0}\right)x\right\}\operatorname{erfc}\left(\frac{x}{2\sqrt{D_0T}} + \beta\sqrt{T}\right)$$
$$- \frac{2\sqrt{D_0}}{u_0}\{\sqrt{\frac{T}{\pi}}\exp\left(\frac{u_0x}{2D_0} - \frac{x^2}{4D_0T} - \frac{u_0^2T}{4D_0}\right)$$
$$+ \frac{1}{4\beta}\left(1 - \frac{\beta x}{\sqrt{D_0}} + 2\beta^2T\right)\exp\left\{\left(\beta^2 - \frac{u_0^2}{4D_0}\right)T - \left(\frac{\beta}{\sqrt{D_0}} - \frac{u_0}{2D_0}\right)x\right\}\operatorname{erfc}\left(\frac{x}{2\sqrt{D_0T}} - \beta\sqrt{T}\right)$$
$$\left. - \frac{1}{4\beta}\left(1 + \frac{\beta x}{\sqrt{D_0}} + 2\beta^2T\right)\exp\left\{\left(\beta^2 - \frac{u_0^2}{4D_0}\right)T + \left(\frac{\beta}{\sqrt{D_0}} + \frac{u_0}{2D_0}\right)x\right\}\operatorname{erfc}\left(\frac{x}{2\sqrt{D_0T}} + \beta\sqrt{T}\right)\}\right] \tag{23b}$$

$$G'(x,T) = \left[\sqrt{\frac{T}{\pi}}\exp\left(\frac{u_0x}{2D_0} - \frac{x^2}{4D_0T} - \frac{u_0^2T}{4D_0}\right) + \frac{\sqrt{D_0}}{2u_0}\operatorname{erfc}\left(\frac{x}{2\sqrt{D_0T}} - \frac{u_0}{2}\sqrt{\frac{T}{D_0}}\right)\right.$$
$$\left. - \frac{\sqrt{D_0}}{2u_0}\left(1 + \frac{u_0x}{D_0} + \frac{u_0^2T}{D_0}\right)\exp\left(\frac{u_0x}{D_0}\right)\operatorname{erfc}\left(\frac{x}{2\sqrt{D_0T}} + \frac{u_0}{2}\sqrt{\frac{T}{D_0}}\right)\right] \tag{23c}$$

$$H'(x,T)=\left[\frac{1}{2\left(\sqrt{D_0}\alpha+\frac{u_0}{2\sqrt{D_0}}\right)}exp\left\{\left(D_0\alpha^2-\frac{u_0^2}{4D_0}\right)T-\left(\alpha-\frac{u_0}{2D_0}\right)x\right\}erfc\left(\frac{x}{2\sqrt{D_0T}}-\alpha\sqrt{D_0T}\right)\right.$$
$$-\frac{1}{2\left(\sqrt{D_0}\alpha-\frac{u_0}{2\sqrt{D_0}}\right)}exp\left\{\left(D_0\alpha^2-\frac{u_0^2}{4D_0}\right)T+\left(\alpha+\frac{u_0}{2D_0}\right)x\right\}erfc\left(\frac{x}{2\sqrt{D_0T}}+\alpha\sqrt{D_0T}\right)$$
$$\left.+\frac{u_0}{2\sqrt{D_0}\left(D_0\alpha^2-\frac{u_0^2}{4D_0}\right)}exp\left(\frac{u_0x}{D_0}\right)erfc\left(\frac{x}{2\sqrt{D_0T}}+\frac{u_0}{2}\sqrt{\frac{T}{D_0}}\right)\right] \tag{23d}$$

$$J(x,T)=c'+c_i\,exp\left\{\left(D_0\alpha^2-\frac{u_0^2}{4D_0}\right)T-\left(\alpha-\frac{u_0}{2D_0}\right)x\right\} \tag{23e}$$

where, $\alpha=\gamma+\frac{u_0}{2D_0}$ $\quad \beta^2=\frac{u_0^2}{4D_0}+\mu_0$ $\quad and \quad u_1=\frac{c'w}{\theta\mu_0\,|sin(mt)|}$

2.3 Numerical Solution with Explicit Finite Difference Method

Owing to the form and algebraic simplicity of the equation resulting from the finite-difference approximations and development of solution algorithms are relatively easier (Huyakorn, and Pinder, 1983). The usage of finite difference in surface flow modelling began with Peaceman and Rachford (1955). It appears that the first application of the finite difference theory to the groundwater flow was studied (Remson et al., 1965). In the mid of 1970s, USGS released two publicly available finite difference computer codes for groundwater flow modelling (Trescott, 1975; Trescott and Larson, 1976). In the last quarter of the 20th century, the number of the publications and computer codes for groundwater flow and groundwater solute transport modelling increased significantly. Following the methodology and applications of finite difference method, we adopted the similar concept with an explicit finite-difference method in this work. To obtain the numerical solution, the semi-infinite domain is converted into a finite domain using the following transformation:

$$x'=1-exp(-x) \tag{24}$$

Using equation (24) in equations (10)-(13), one can get as follows:

$$\frac{\partial C}{\partial T}=D_0(1-x')^2\frac{\partial^2 C}{\partial x'^2}-(D_0+u_0)(1-x')\frac{\partial C}{\partial x'}-\mu_0 C+\frac{c'w}{\theta\,|sin(mt)|} \tag{25}$$

$$C(x',T)=c'+c_i\phi(1-x');\quad x'\geq 0,\quad T=0 \tag{26}$$

$$C(x',T)=c'+c_0(2-mT);\quad x'=0,\quad T>0 \tag{27}$$

$$\frac{\partial C}{\partial x'}=0;\quad x'=1,\quad T=0 \tag{28}$$

where, $\phi=exp(\gamma)$

Using explicit finite-difference approximation with a forward time and central-space (FTCS) scheme in equations (25)-(28), we get as follows:

$$C_{i,j+1} = C_{i,j} - \mu_0 C_{i,j}\Delta T + \frac{c'w}{\theta|\sin(mt)|}\Delta T + D_0(1-x'_i)^2(C_{i+1,j} - 2C_{i,j} + C_{i-1,j})\frac{\Delta T}{\Delta x'^2}$$
$$-(D_0 + u_0)(1-x'_i)(C_{i+1,j} - C_{i-1,j})\frac{\Delta T}{2\Delta x'} \qquad (29)$$

$$C_{i,0} = c' + c_i\phi(1-x'_i); \quad i > 0 \qquad (30)$$

$$C_{0,j} = c' + c_0(2 - mT_j); \quad j > 0 \qquad (31)$$

$$C_{M,j} = C_{M-1,j}; \quad j > 0 \qquad (32)$$

The numerical approximation for the Cauchy-type boundary condition in equation (21) can be written as,

$$C_{0,j} = \frac{D_0}{(D_0 + u_0\Delta x')}C_{1,j} + \frac{u_0\Delta x'}{(D_0 + u_0\Delta x')}\{c' + c_0(2 - mT_j)\}; \quad j > 0 \qquad (33)$$

In discretization process, the model domain is represented by a network of grid cells or elements and the simulation time is presented by time steps. An accuracy of numerical model depends on the model input data, the size of the space and time discretization, and the numerical method used to solve the model equations. In the above equations (29)-(33) the subscript $i =$ space, the subscript $j =$ time, $\Delta T =$ the time increment and $\Delta x' =$ the space increment. The contaminant concentration is at a point in the space x'_i with j^{th} subinterval of time T defined by $C_{i,j}$. The domains x' and T are discretized by a rectangular grid of step sizes given below:

$$x'_i = x'_{i-1} + \Delta x'; \qquad i = 1,2,...,M, \quad x'_0 = 0, \quad \Delta x' = 0.02 \qquad (34)$$

$$T_j = T_{j-1} + \Delta T; \qquad j = 1,2,...,N, \quad T_0 = 0, \quad \Delta T = 0.0001 \qquad (35)$$

3. Stability Analysis

Simth (1978) proposed the matrix method to determine the stability criteria of FTCS scheme for the advection dispersion equation. This technique was also used by Notodarmojo et al. (1991). To determine the stability condition, the governing parabolic type partial differential equation is written in the form of finite difference scheme as,

$$C_{i,j+1} = (\xi_1 + \xi_2)C_{i-1,j} + (1 - 2\xi_1 - \xi_3)C_{i,j} + (\xi_1 - \xi_2)C_{i+1,j}\frac{c'w}{\theta|\sin(mt)|}\Delta T \qquad (36)$$

where, $\xi_1 = D_0\frac{\Delta T}{\Delta x^2}$, $\xi_2 = u_0\frac{\Delta T}{2\Delta x}$, $\xi_3 = \mu_0\Delta T$

Equation (36) can be written in matrix form as,

$$[C]^{j+1} = A[C]^j + \frac{c'w}{\theta|\sin(mt)|}\Delta T \qquad (37)$$

According to Smith (1978), the finite difference equation is stable if the modulus of eigenvalues of matrix A is less than or equal to unity. Following the approach of Notodarmojo et al. (1991) and using Gerschgorin's circle theorem, we determine the stability criteria for the time as

$$\Delta T \le \frac{1}{\frac{2D_0}{\Delta x^2} + \frac{\mu_0}{2}} \qquad (38)$$

where, Δx is the increment of space variable.

4. Accuracy of the Solution

To set the numerical accuracy the Root Mean Square error (RMS), Relative error and Percentage error are also explored. RMS error is defined as,

$$RMS = \sqrt{\frac{1}{N}\sum_{i=1}^{N}|\Delta C_i|^2}$$

where, $\Delta C = C_{Analytical} - C_{numerical}$ and N is the number of data.

Relative error is obtained as,

$$Relative\ error = \frac{|\Delta C|}{Analytical\ value}$$

and the percentage error is obtained as,

$$Percentage\ error = \frac{|\Delta C|}{Analytical\ value} \times 100$$

In Table 1 and Table 2, the Relative, Percentage and R.M.S. error for the solution with Dirichlet-type boundary condition are obtained in gravel ($\theta = 0.32$) and clay($\theta = 0.55$) mediums respectively. Similarly, the Relative, Percentage and R.M.S. error for the solution with Cauchy-type boundary condition are obtained and it is shown in Table 3 and Table 4 respectively for the gravel and clay mediums.

Table 1: Relative, Percentage and R.M.S error for solution with Dirichlet-type boundary condition with time t=1 year in gravel medium (0:32)

Distance(km)	0	0.02	0.04	0.06	0.08	R.M.S. Error
Analytical Results	0.7246	0.6477	0.5704	0.4957	0.4263	0.0333
Numerical Results	0.6996	0.6218	0.5405	0.4591	0.3814	
Relative Error	0.0345	0.0399	0.0525	0.0738	0.1053	
Percentage Error	3.45%	3.99%	5.25%	7.38%	10.53%	

Table 2: Relative, Percentage and R.M.S error for solution with Dirichlet-type boundary condition with time t=1 year in clay medium (0:55)

Distance(km)	0	0.02	0.04	0.06	0.08	R.M.S. Error
Analytical Results	0.7142	0.6372	0.5599	0.4853	0.4158	0.0232
Numerical Results	0.6996	0.6218	0.5405	0.4591	0.3814	
Relative Error	0.0204	0.0241	0.0346	0.0539	0.0827	
Percentage Error	2.04%	2.41%	3.46%	5.39%	8.27%	

Table 3: Relative, Percentage and R.M.S error for solution with Cauchy-type boundary condition with time t=1 year in gravel medium (0.32)

Distance(km)	0	0.02	0.04	0.06	0.08	R.M.S. Error
Analytical Results	0.2174	0.1962	0.1778	0.1621	0.1492	0.00301
Numerical Results	0.2147	0.1941	0.1752	0.1586	0.1445	
Relative Error	0	0.0107	0.0146	0.0215	0.0315	
Percentage Error	0%	1.07%	1.46%	2.15%	3.15%	

Table 4: Relative, Percentage and R.M.S error for solution with Cauchy-type boundary condition with time t=1 year in clay medium (0.55)

Distance(km)	0	0.02	0.04	0.06	0.08	R.M.S. Error
Analytical Results	0.2192	0.1977	0.1790	0.1630	0.1498	

Numerical Results	0.2147	0.1941	0.1752	0.1586	0.1445	0.00436
Relative Error	0.0205	0.0182	0.0212	0.0269	0.0353	
Percentage Error	2.05%	1.82%	2.12%	2.69%	3.53%	

5. Results and Discussions

The effect of the model parameters, periodic seepage velocity, dispersion coefficients, elemental recharge rate and first-order decay term on the transport of dissolved substance are presented. The concentration values are determined from the analytical solutions given in equation (19) for Dirichlet-type boundary condition and equation (22) for Cauchy-type boundary condition in a finite domain $0 \le x(km) \le 1$. The other input values are considered as

$c' = 0.1, c_0 = 0.3, c_i = 0.01, D_0 = 0.9(km^2 / year),$

$u_0 = 1.0(km / year), m = 0.05(year^{-1}), \gamma = 0.01, \mu_0 = 0.05, w = 0.0002, \theta = 0.32$ (for gravel), $\theta = 0.37$ (for sand), $\theta = 0.55$ (for clay medium) (Singh and Das, 2015). For the numerical approximations, we take $\Delta x = 0.02$ *and* $\Delta T = 0.0001$.

The concentration pattern for the solution given in equation (19) is shown in the Fig.2 for clay medium ($\theta = 0.55$) at the four different time intervals 1, 1.5, 2 and 2.5 years. It is observed that, the contaminant concentration values increase with time and decreases with distance travelled. From Fig.3, it is observed that the nature of the graphs, drawn for contaminant concentration, are remains same in both gravel and clay mediums. The concentration values are lesser in clay medium than the gravel medium at each point.

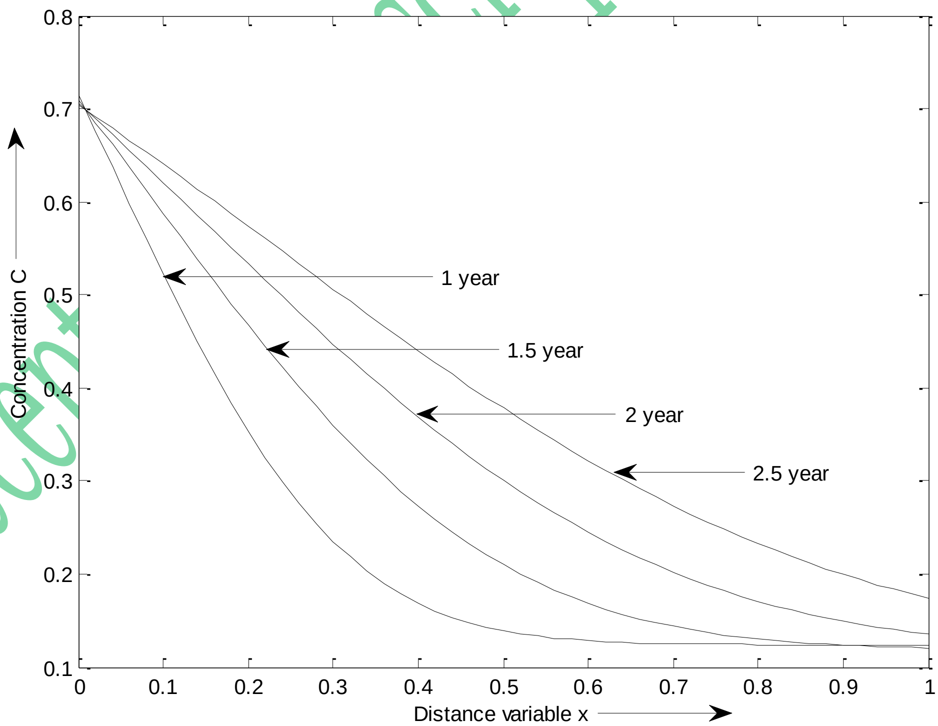

Fig-2: Concentration distribution pattern for Dirichlet or first-type boundary condition at four different time intervals with average porosity of clay medium ($\theta = 0.55$)

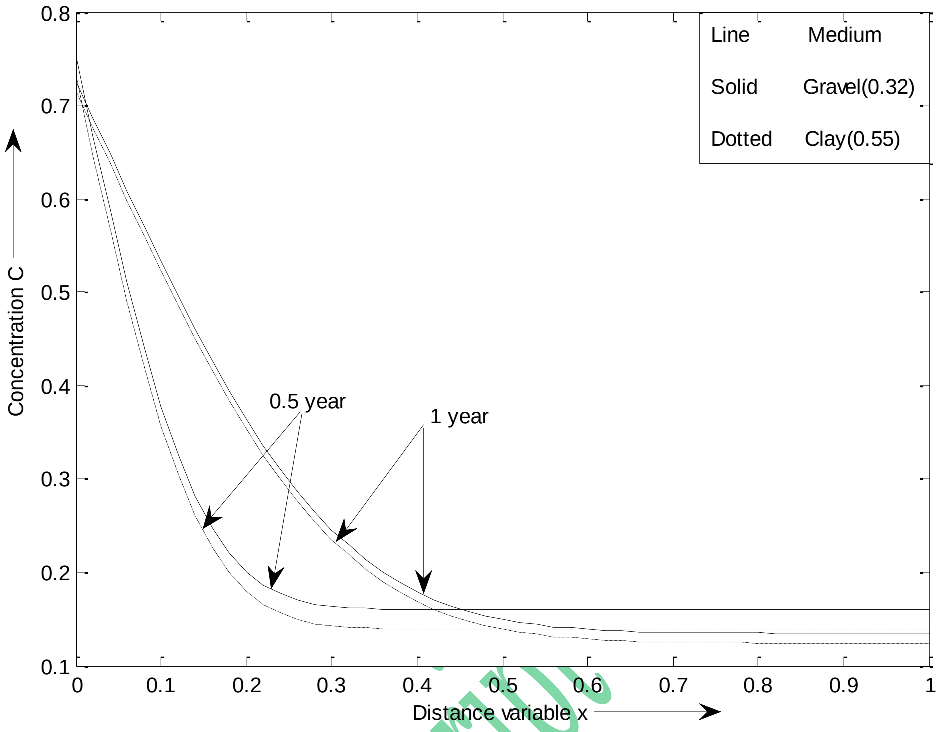

Fig-3: Concentration distribution pattern for different geological formations for Dirichlet-type BC

The concentration values for all the three mediums are also shown in tabular form i.e., in Table 5 (for Dirichlet-type BC) and Table 6 (for Cauchy-type BC). The comparison between the analytical and numerical results are shown in Fig.4, and observed a good agreement between them. The natures of the graphs for both analytical and numerical results are remains same and the slight deviations among these two results are observed only because of the truncation of higher order terms in Taylor series expansion.

Table 5: Concentration distribution (for Dirichlet-type BC) in different layer of aquifer with their average porosity Gravel (0.32), Sand (0.37), Clay (0.55) at t=1 year

x(km)	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Gravel	0.725	0.532	0.363	0.246	0.179	0.149	0.139	0.136	0.134	0.134	0.134
Sand	0.721	0.529	0.361	0.242	0.176	0.146	0.135	0.132	0.131	0.131	0.131
Clay	0.714	0.522	0.353	0.235	0.169	0.139	0.128	0.125	0.124	0.124	0.124

Table 6: Concentration distribution (for Cauchy-type BC) in different layer of aquifer with their average porosity Gravel (0.32), Sand (0.37), Clay (0.55) at t=1 year

x(km)	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Gravel	0.217	0.169	0.139	0.122	0.114	0.111	0.110	0.110	0.109	0.109	0.109
Sand	0.217	0.170	0.139	0.122	0.114	0.111	0.110	0.110	0.109	0.109	0.109
Clay	0.219	0.171	0.139	0.122	0.114	0.111	0.110	0.110	0.109	0.109	0.109

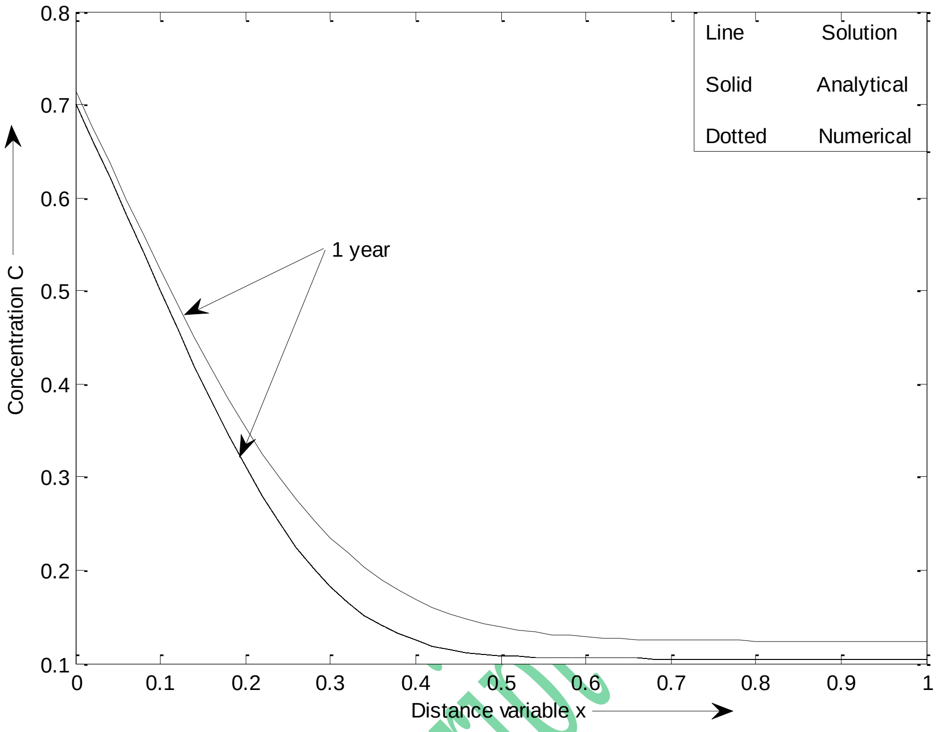

Fig-4: Comparison of the analytical and numerical results with Dirichlet-type boundary condition at $t = 1$ year with average porosity of clay medium

The source term added with the governing partial differential equation significantly contributing towards the contaminant concentration values. If we remove the source term, then it becomes the advection-dispersion equation with first-order decay. To remove the source term, we took $c' = 0$ and the concentration distribution patterns are shown in Fig.5 for three different time intervals 1, 2 and 3 years. It is seen that the concentration values without the source term at each point as well as at each time interval are lower than the concentration values with the source term. It is easily understood from Fig.5, without the source term the concentration values become zero earlier than the concentration values with the source term. So we can say that if the source concentration is properly treated before entering into the system, the concentration could be controlled and even less harmful to the end-users.

Groundwater recharge rate is a very important parameter in solute transport modeling. The concentration distribution patterns with three different recharge rates $w = 0.0002, 0.0008, 0.002$ are predicted and shown in Fig.6. The distribution pattern for $w = 0.002$ takes higher values as compared to other two values of recharge rates. The minimum concentration values attain for the elemental recharge rate $w = 0.0002$ at each of the position in the domain. So, we observed form Fig.6 that concentration values increase as the recharge rate increases. This is due to increasing recharge rate, an amount of water increases in the groundwater reservoir and by this process an amount of solute meets the aquifer, which increases the level of contaminant concentration.

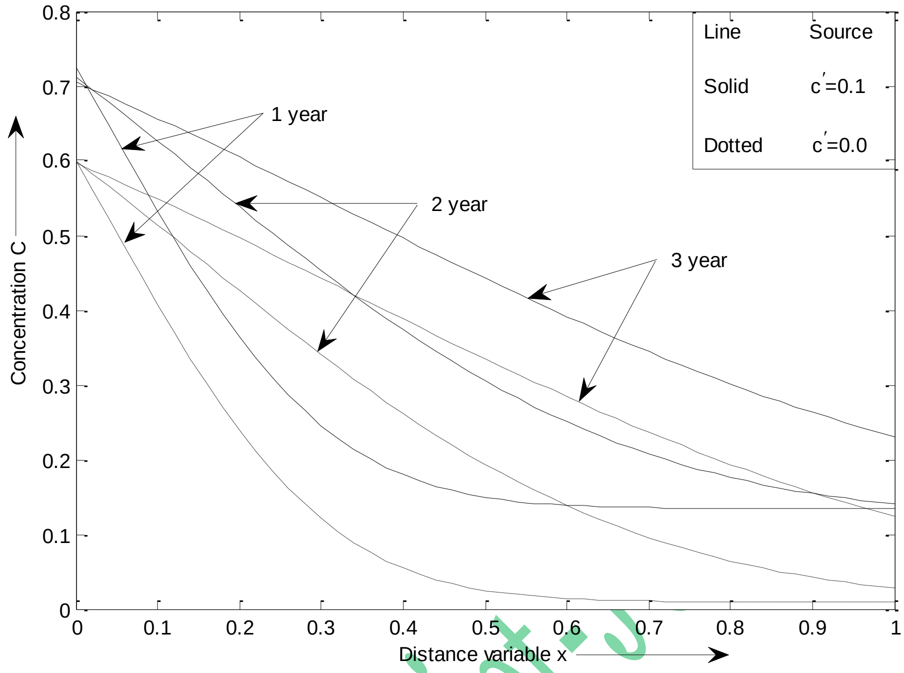

Fig-5: Contaminant concentration distribution for Dirichlet-type boundary condition in sand medium ($\theta = 0.37$) for with the source term (i.e., when $c' = 0.1$) and without the source term (i.e., whe $c' = 0.0$)

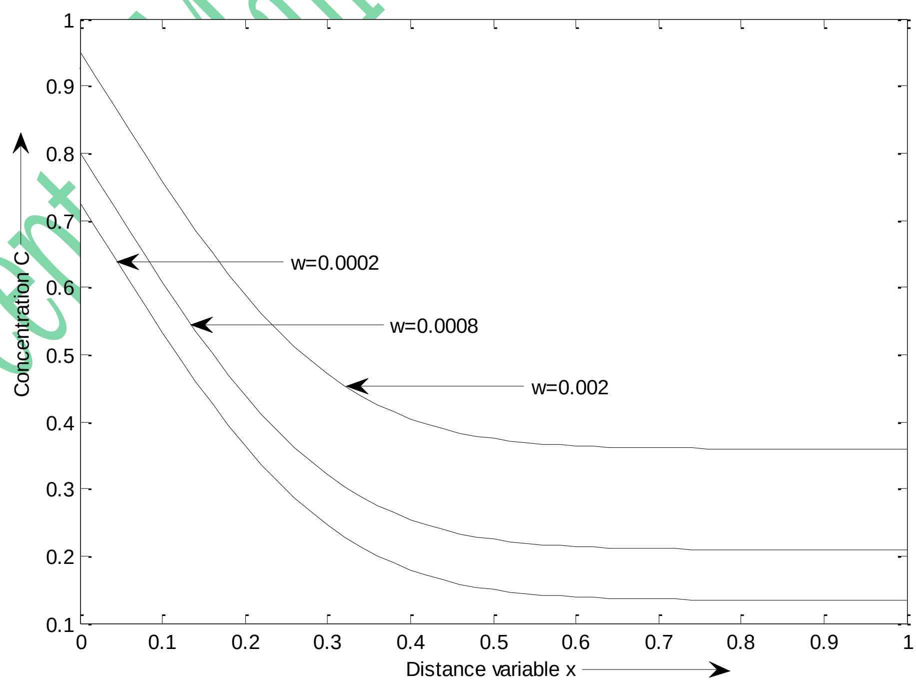

Fig-6: Contaminant concentration pattern (Dirichlet-type boundary condition) for different recharge rate (w) of aquifer in gravel medium

Contaminant concentration in sand medium for Cauchy-type boundary condition is predicted and shown in Fig.7 at $t = 1,2$ and $t = 3$ years. It is seen that the solute concentration decreases with the space variable and reaches minimum values of concentration at an exit boundary. It increases with time except at the initial stage where concentration takes the maximum value for $t = 1$ year in comparison to $t = 2$ and $t = 3$ years. In Fig.8, analytical and numerical results are compared for the Cauchy-type boundary condition in gravel medium for 1year.

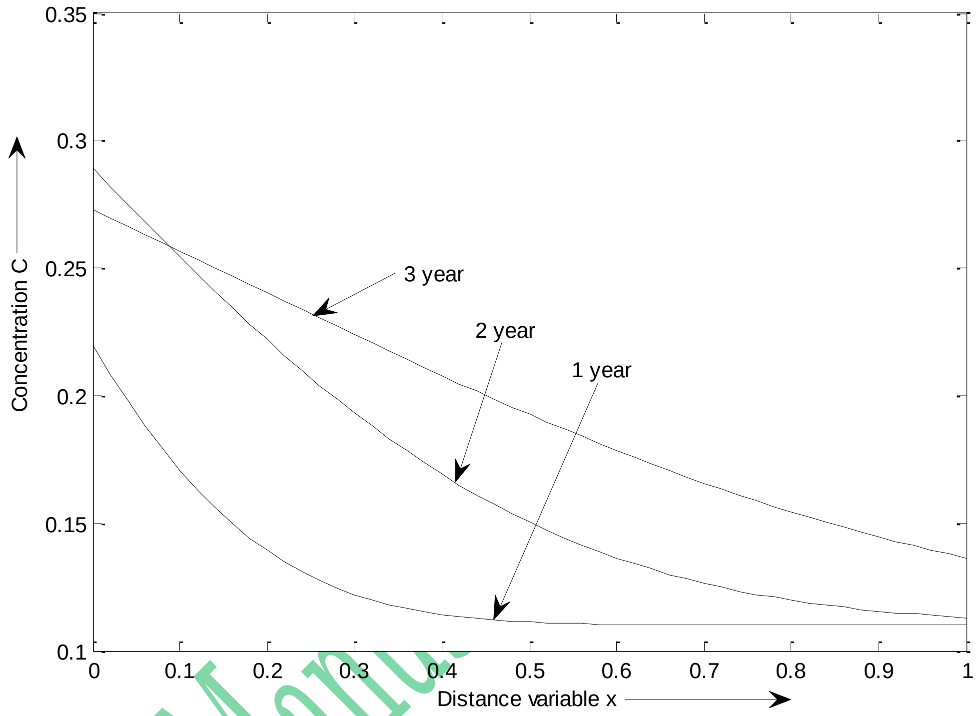

Fig-7: Concentration distribution patter for Cauchy-type boundary condition at different time intervals in clay medium ($\theta = 0.55$)

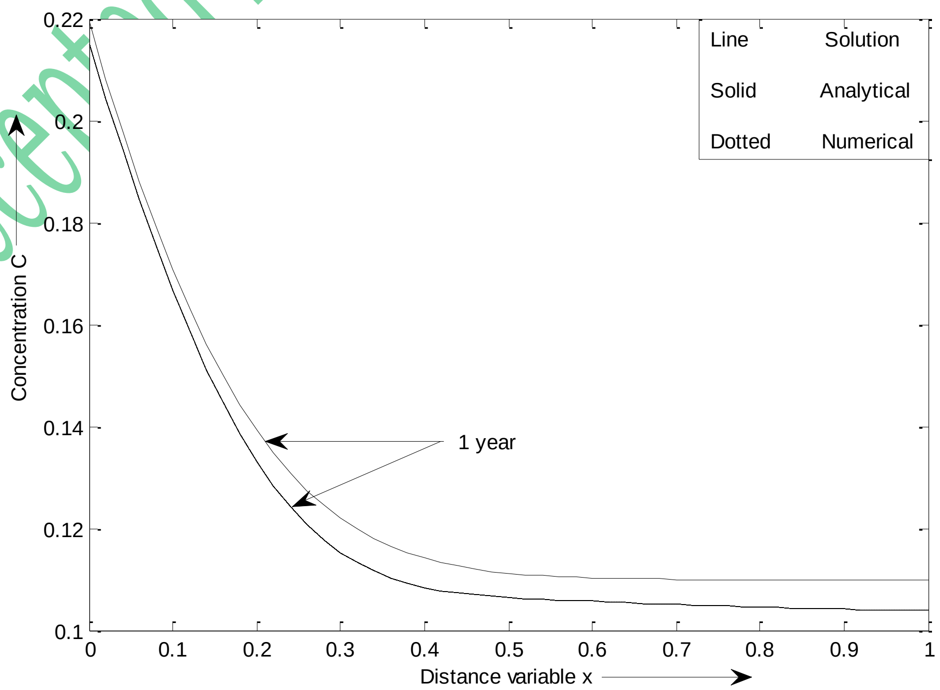

Fig-8: Comparison of the analytical and numerical results with Cauchy-type boundary condition at a fixed time 1 year in clay medium ($\theta = 0.55$)

The flow resistance coefficient m is another important parameter that changes the nature of the concentration pattern. From Fig.9, the concentration distribution pattern is explored with Dirichlet-type boundary condition for different values of m (=0.03, 0.08, 0.13, 0.3). It is observed that concentration values increase with the increases value of m. The concentration pattern with Cauchy-type boundary condition for $m = 0.03, 0.08$ and $m = 0.13$ is also explored and shown in Fig.10. It is seen that the concentration values increase with the increases value of m. An impact of first-order decay parameter μ_0 is also depicted in Fig.11 for the three different values of first-order decay parameter $\mu_0 = 0.01, 0.02, 0.05$. From Fig. 11, it is observed that the concentration values decrease with the increases value of first-order decay term.

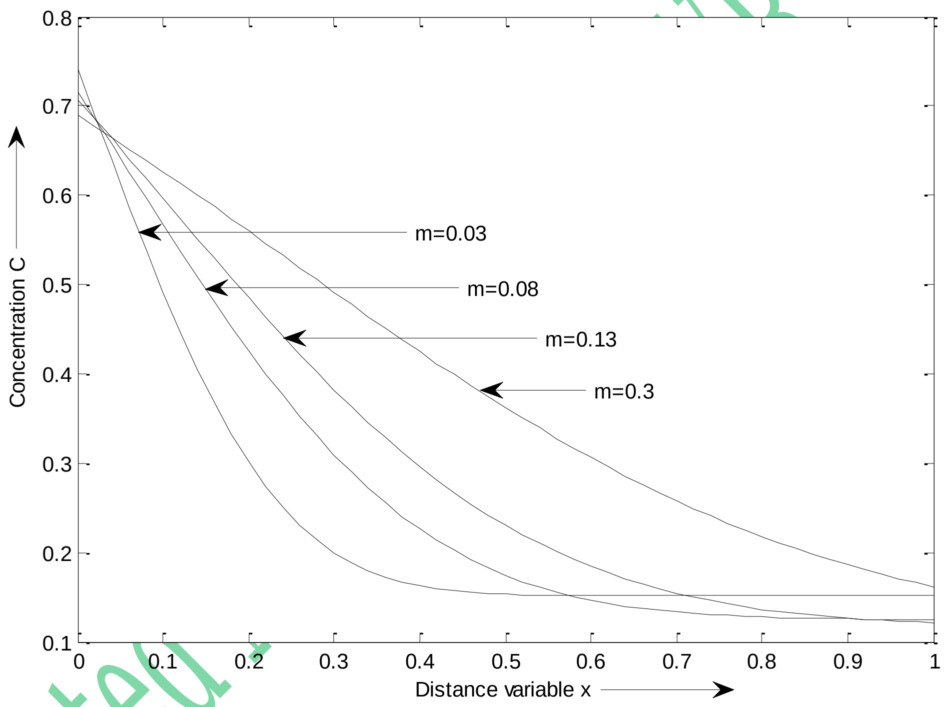

Fig-9: Concentration pattern with Dirichlet-type boundary condition for different values of flow resistance coefficient (m)

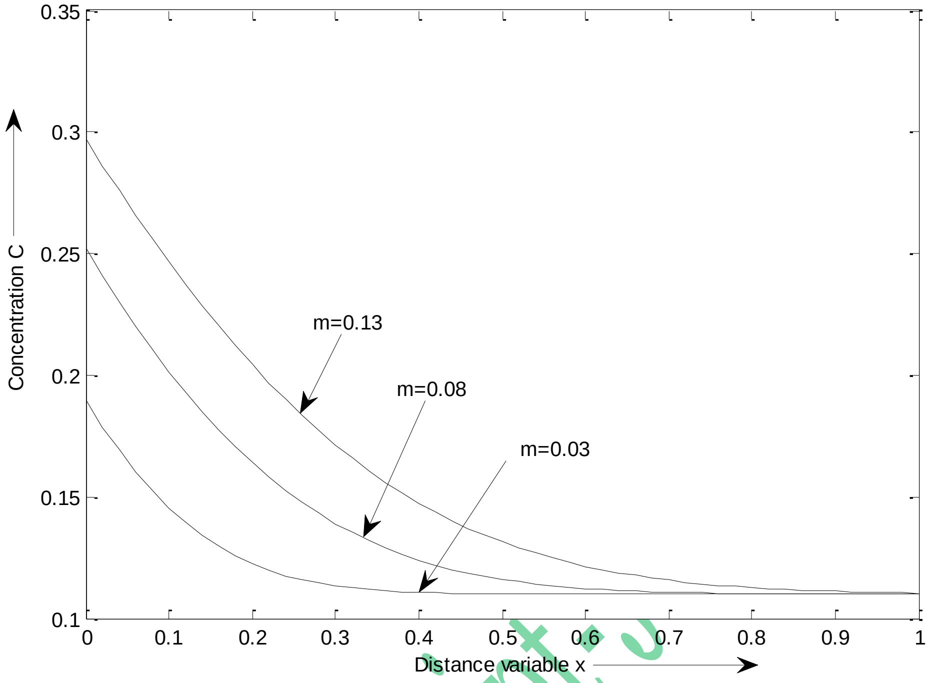

Fig-10: Concentration pattern for different values of flow resistance coefficient (m) for increasing input condition (i.e., for Cauchy-type boundary condition)

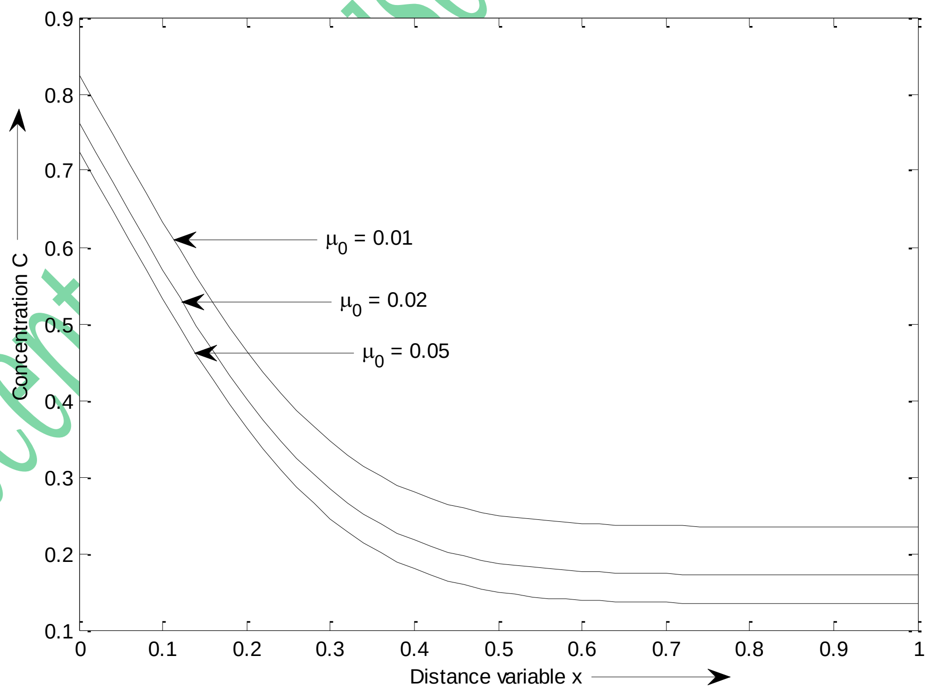

Fig-11: Concentration distribution with Dirichlet-type BC for different values of first-order decay term (μ_0)

The Courant number depends on velocity, cell size and time step and is typically calculated for each cell in the numerical solution. The Courant number will accordingly change a bit when we have a static mesh and constant time step. The Courant number for one-dimension is defined as, $C_r = \frac{u_0 \Delta T}{\Delta x}$. Here, we fixed the mesh and time step and change the velocity to get different Courant numbers that will increase with the increases value of velocity. The concentration pattern for different Courant numbers are depicted and shown in Fig.12. It is observed that the concentration values increase at each point with the increases Courant number. It is also important to explore one another non-dimensional parameter σ which is known as 'strength of contaminant decay' and defined as- $\sigma = \frac{x\mu_0}{u_0\theta}$. From Fig.13, it is seen that the concentration value decreases as the value of σ increases.

Peclet number is a dimensionless parameter indicates the relative importance of advection and dispersion to solute transport equation. When the Peclet number is high, advection term dominates and when the Peclet number is low, dispersion term dominates. Generally, the Peclet number is defined as the ratio of the advective and dispersive components of solute transport with the small spatial variation in space, i.e., $Pe = \frac{u_0 x}{\theta D_0}$. The value of Peclet number decreases with increases porosity i.e., value of θ. It can be seen from Fig.14 that the concentration of pollutant decreases as Peclet number increases. So, we can say that, the Peclet number is high in gravel medium in comparison to clay medium, the impact of Peclet number on pollutant concentration is less in clay medium.

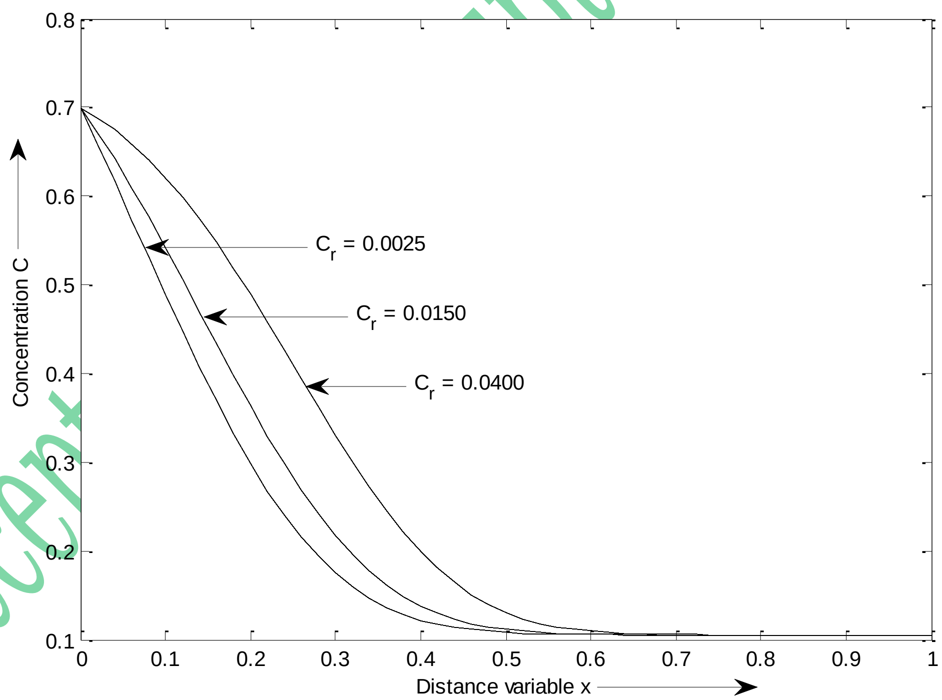

Fig-12: Contaminant concentration distribution for first-type BC for different courant number (C_r)

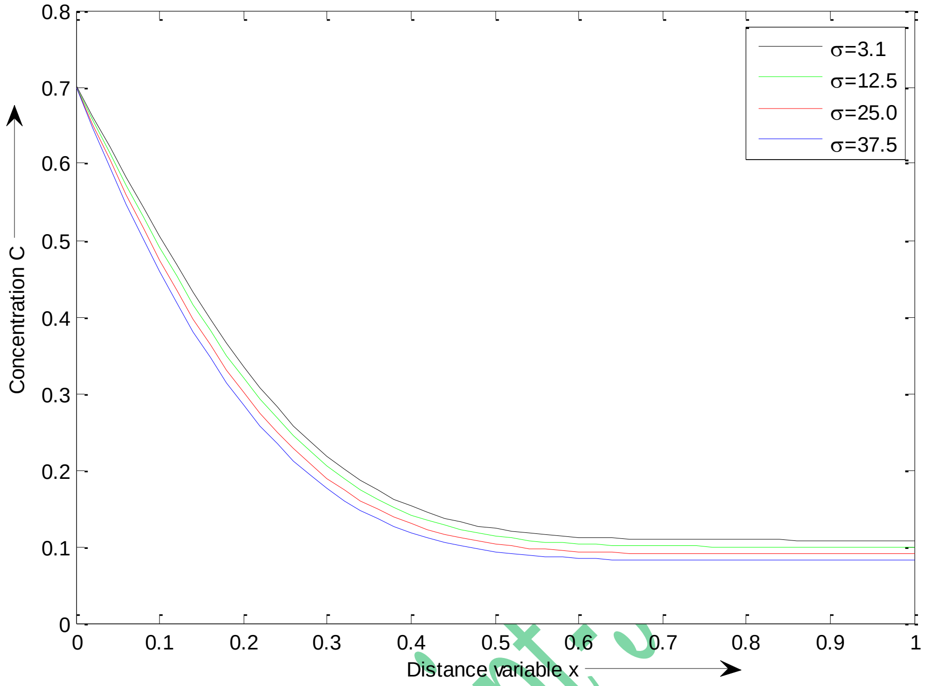

Fig-13: Contaminant concentration distribution with first-type BC for different values of strength of contaminant decay (σ)

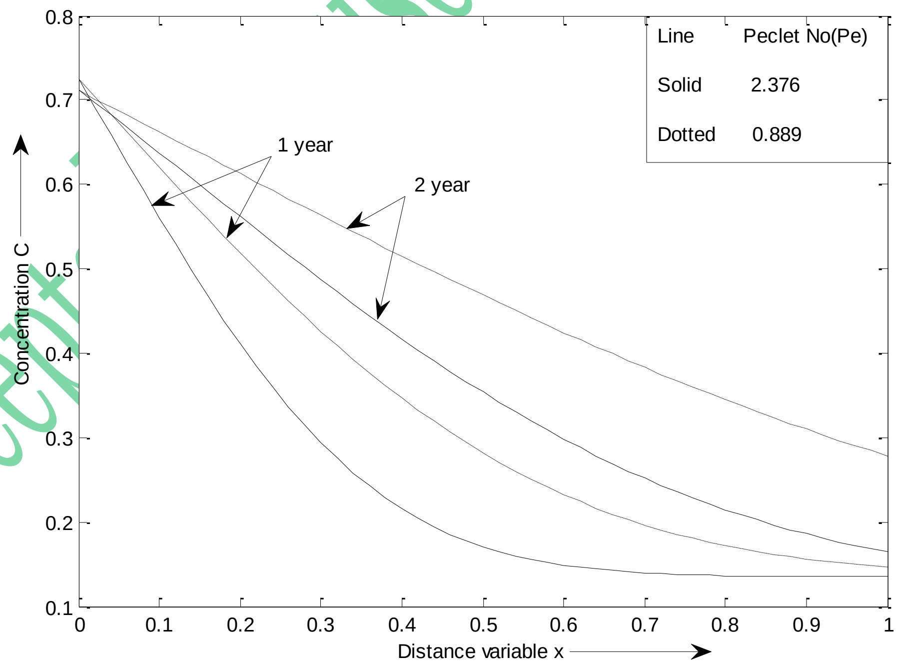

Fig-14: Contaminant concentration distribution for different values of peclet number (Pe)

6. Summary and Conclusions

The concentration distribution behaviour of contaminants is discussed through analytical solutions of the advection-dispersion-reaction (ADR) equation with an impact of elemental recharge rate and time-dependent periodic boundary condition. The ADR equation is solved analytically using Laplace Integral Transform Technique (LITT) whereas Numerical solution is obtained using Explicit Finite Difference (EFD) method. An effect of elemental recharge rate, first-order decay term and flow resistant coefficient are explored and found that the concentration values increases with time and decreases with distance. The concentration values are lower or higher depending upon the parameters increases or decreases. The Courant number, Peclet number and strength of contaminant decay parameter are also explored.

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Corresponding Author

Sultana Begam

Department of Mathematics and Computing

Indian Institute of Technology (Indian School of Mines) Dhanbad-826004

Email: sultanabegam26@gmail.com

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