Chapter 2

Numerical Solution of Solute Transport System

2.1 Numerical solution of One-Dimensional Finite Solute Transport System with First-Type Source Boundary Condition

2.1.1 Introduction

In this chapter, a sincere attempt has been taken to find the numerical solution of one-dimensional ADE for a finite system with first-type source boundary conditions, i.e., the inlet boundary has time-dependent concentration and at the outlet boundary, the concentration gradient is supposed to be zero. Initially, it is supposed that there is no solute in the aquifer. The mathematical representation of the described problem is as follows

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} - \lambda C, \tag{2.1.1}$$

under the boundary conditions

$$C = C_0, \quad x = 0, \tag{2.1.2}$$

$$\frac{\partial C}{\partial x} = 0, \quad x = L \tag{2.1.3}$$

and initial condition

$$C = 0, \quad 0 < x < L \quad \text{at} \quad t = 0, \tag{2.1.4}$$

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where $C(x,t)$ is the solute concentration, D is the coefficient of hydro-dynamic dispersion, V is the velocity of groundwater and λ is the reaction rate coefficient. During numerical computation, it is considered that the system in which velocity (V) of the groundwater is assumed to be uniform, aligned with the x-axis and constant. The coefficient of hydro-dynamic dispersion (D) is also considered to be constant. The analytical solution of the given mathematical model for the conservative system, i.e., for $\lambda = 0$ is given as (E. J. Wexler (1992))

$$C(x,t) = C_0 \left\{ 1 - 2\exp\left[\frac{Vx}{2D} - \frac{V^2 t}{4D}\right] . \sum_{i=1}^{\infty} \frac{\beta_i \sin\left(\frac{\beta_i x}{L}\right) \exp\left(\frac{\beta_i^2 Dt}{L^2}\right)}{\beta_i^2 + \left(\frac{VL}{2D}\right)^2 + \left(\frac{VL}{2D}\right)} \right\}, \quad (2.1.5)$$

where β_i are the roots of the equation $\beta \cot\beta + \frac{VL}{2D} = 0$.

We know that analytical solution is always useful for validating the numerical results. But on many occasions, it is hard to get the analytical solutions, and for those cases, the numerical solutions using various tools are very much useful. Here, the aim is to validate the proposed numerical method with the existing analytical solution for a conservative system which confirms the accuracy and efficiency of our proposed method and then applies the method to find the numerical solution of the considered problem for a non-conservative system for different particular cases.

The mathematical model considered in this chapter is a simple reaction-advection-dispersion equation. In literature, a number of analytical and numerical methods are present to solve such types of problems subject to initial and boundary conditions. In 1982, Van Genucheten and Alves (1982) considered the one-dimensional solute transport models and the computer programs had been used to solve these models. They have collectively presented most common numerous analytical solutions of the general transport models where the term accounting for convection, dispersion, linear equilibrium absorption and in some cases the effects of zero-order production and first-order decay have been taken into account. Cleary and Adrian (1973) used integral transform method to analytically solve the cation adsorption soil problem. Runkel (1996) derived the exact solution for constant parameter advection-dispersion equation (ADE) with a continuous load of finite duration. Baeumer et al. (2001) have discussed the solution of subordinated ADE for contaminant transport in their research article. Mojtabi and Deville (2014) discussed the solution of one-dimensional linear ADE with Dirichlet homogeneous boundary conditions using separation of variables for an analytical solution and finite element method for numerical solution. Luce et al. (2013) have presented an explicit analytical solution of the diurnally forced ADE to estimate bulk fluid velocity and diffusivity in streambeds. Singh et al. (2010) solved the solute transport along and against time-dependent source concentration in homogeneous finite aquifers. In 2010, Kumar et al. (2010) have given the analytical solutions of ADE converted into a diffusion equation by emitting the advective terms. In 2012, the numerical solution of one-dimensional ADE in semi-infinite media was given by Savovic and Djordjevich (2012) using explicit finite difference method for three types of dispersion problems viz., solute dispersion along steady flow through inhomogeneous medium, temporally dependent solute dispersion along uniform flow through homogeneous medium and solute dispersion along temporally dependent unsteady flow through inhomogeneous medium. In 2013, Savovic and Djordjevich (2013) numerically solved the one-dimensional ADE with variable coefficients in a semi-infinite medium using explicit finite difference method for two types of dispersion problems, temporally dependent dispersion along a uniform flow and spatially dependent dispersion along a non-uniform flow.

Here, the spectral collocation method viz., Chebyshev collocation method along with finite difference method is used to solve the considered problem. Using this method, the solution of the considered problem is approximated as a sum of shifted Chebyshev polynomial of second-kind and the roots of the second-kind shifted Chebyshev polynomial are taken as collocation points. This problem is first converted into a system of ordinary differential equations which are ultimately solved using finite difference method. The numerical results are depicted graphically for different particular cases for both conservative and non-conservative systems.

2.1.2 Preliminaries

2.1.2.1 Shifted Chebyshev Polynomials of the Second-Kind

In order to use Chebyshev polynomials in the interval $x \in [0,12]$, let us define the so-called shifted Chebyshev polynomials of the second kind $U_n^*(x)$ by introducing the change of variable with $z = \frac{x}{6} - 1$, which gives rise to

$$U_n^*(x) = U_n(\frac{x}{6} - 1), \tag{2.1.6}$$

where the logic of choosing the above length of the interval is to validate the proposed method with the existing analytical result (2.1.5) while solving the considered problem.

These polynomials are orthogonal in the interval [0, 12] as

$$\left\langle U_n^*(x), U_m^*(x) \right\rangle = \int_0^{12} \sqrt{\frac{x}{3} - \frac{x^2}{36}} U_n^*(x) U_m^*(x) dx = \begin{cases} 0, & n \neq m, \\ 3\pi, & n = m, \end{cases} \tag{2.1.7}$$

where $\sqrt{\frac{x}{3}-\frac{x^2}{36}}$ is weight function. $U_n^*(x)$ satisfies the following recurrence relations

$$U_n^*(x) = 2(\frac{x}{6}-1)U_{n-1}^*(x) - U_{n-2}^*(x), \quad n = 2,3.........; \tag{2.1.8}$$

with initial values

$$U_0^*(x) = 1, \quad U_1^*(x) = 2(\frac{x}{6}-1).$$

2.1.2.2 Function Approximation

If g(x) is squared integrable in [0, 1], it can be expressed in terms of the shifted Chebyshev polynomials of the second kind as

$$g(x) = \sum_{i=0}^{\infty} a_i U_i^*(x), \tag{2.1.9}$$

where the coefficients a_i, *i = 0,1,……,* are given by

$$a_i = \frac{1}{3\pi}\int_0^{12}\sqrt{\frac{x}{3}-\frac{x^2}{36}}\, g(x)U_i^*(x)\,dx\,. \tag{2.1.10}$$

Generally, the first *(m+1)*-terms of shifted Chebyshev polynomials of the second kind are considered in the approximate case. Thus we have

$$g_m(x) = \sum_{i=0}^{m} a_i U_i^*(x). \tag{2.1.11}$$

2.1.3 Solution of the Problem

To solve the considered problem (2.1.1) subject to the boundary conditions (2.1.2)-(2.1.3) and initial condition (2.1.4), let us approximate the solute concentration factor $C(x,t)$ by

$$C_m(x,t) = \sum_{i=0}^{m} u_i(t)U_i^*(x), \tag{2.1.12}$$

which reduces the equation (2.1.1) to

$$\sum_{i=0}^{m}\frac{du_i(t)}{dt}U_i^*(x)=D\sum_{i=0}^{m}u_i(t)\frac{d^2U_i^*(x)}{dx^2}-V\sum_{i=0}^{m}u_i(t)\frac{dU_i^*(x)}{dx}-\lambda\sum_{i=0}^{m}u_i(t)U_i^*(x). \qquad (2.1.13)$$

Collocating equation (2.1.13) with $(m+1-n)$ points as x_p, equation (2.1.13) becomes

$$\sum_{i=0}^{m}\frac{du_i(t)}{dt}U_i^*(x_p)=D\sum_{i=0}^{m}u_i(t)\frac{d^2U_i^*(x_p)}{dx^2}-V\sum_{i=0}^{m}u_i(t)\frac{dU_i^*(x_p)}{dx}-\lambda\sum_{i=0}^{m}u_i(t)U_i^*(x_p), \qquad (2.1.14)$$

where n represents the order of the problem.

The roots of the shifted Chebyshev polynomials of the second kinds $U^*_{(m+1-n)}(x)$ are suitable for the collocation points. Using equations (2.1.10) and (2.1.12), we get initial values of $u_i(t)$ in the initial case at $t=0$. Also substituting (2.1.12) in the boundary conditions (2.1.2)-(2.1.3), we get the following equations for the case $0<x<12$.

$$\sum_{i=0}^{m}(-1)^{(i+2)}(i+1)u_i(t)=C_0, \qquad \sum_{i=0}^{m}u_i(t)\left.\frac{dU_i^*(x)}{dx}\right|_{x=12}=0, \qquad (2.1.15)$$

Equations (2.1.14) with the help of equation (2.1.15) give rise to *(m+1)* ordinary differential equations, which can be solved using finite difference method to get the unknowns $u_i(t),\ i=0,1,........,m.$

Let us make an approximation with $m=3$. Equations (2.1.14) and (2.1.15) are reduced to

$$\sum_{i=0}^{3}\frac{du_i(t)}{dt}U_i^*(x_p)=D\sum_{i=0}^{3}u_i(t)\frac{d^2U_i^*(x_p)}{dx^2}-V\sum_{i=0}^{3}u_i(t)\frac{dU_i^*(x_p)}{dx}-\lambda\sum_{i=0}^{3}u_i(t)U_i^*(x_p),\ p=0,1, \qquad (2.1.16)$$

$$\sum_{i=0}^{3}(-1)^{(i+2)}(i+1)u_i(t)=C_0, \qquad \sum_{i=0}^{3}u_i(t)\left.\frac{dU_i^*(x)}{dx}\right|_{x=12}=0, \qquad (2.1.17)$$

with

$$C_3(x,t)=\sum_{i=0}^{3}u_i(t)U_i^*(x), \qquad (2.1.18)$$

where x_p's are the roots of the shifted Chebyshev polynomial of the second-kind $U_2^*(x)$.

Using equations (2.1.16) and (2.1.17), we obtain the following system of ordinary differential equations

$$\sum_{i=0}^{3} u_i^{'}(t) U_i^{*}(x_0) = \sum_{i=0}^{3} u_i(t) H_i(x_0) \tag{2.1.19}$$

$$\sum_{i=0}^{3} u_i^{'}(t) U_i^{*}(x_1) = \sum_{i=0}^{3} u_i(t) H_i(x_1) \tag{2.1.20}$$

$$u_0(t) - 2u_1(t) + 3u_2(t) - 4u_3(t) = C_0 \tag{2.1.21}$$

$$0.u_0(t) + \frac{1}{3}u_1(t) + \frac{4}{3}u_2(t) + \frac{10}{3}u_3(t) = 0, \tag{2.1.22}$$

where $H_i(x_p) = D\{U_i^{*}(x_p)\}^{''} - V\{U_i^{*}(x_p)\}^{'} - \lambda U_i^{*}(x_p)$.

Equations (2.1.19)-(2.1.22) are solved using finite difference method with the notations $T = T_{final}, 0 < t_j \le T$ and $\Delta t = T / N$, for $j = 0,1,,........., N$. Defining $u_i(t_n) = u_i^n$, the system of equations (2.1.19)-(2.1.22) is discretized in time, which gives rise to

$$\sum_{i=0}^{3} \frac{u_i^n - u_i^{n-1}}{\Delta t} U_i^{*}(x_0) = \sum_{i=0}^{3} u_i^n H_i(x_0) \tag{2.1.23}$$

$$\sum_{i=0}^{3} \frac{u_i^n - u_i^{n-1}}{\Delta t} U_i^{*}(x_1) = \sum_{i=0}^{3} u_i^n H_i(x_1) \tag{2.1.24}$$

$$u_0^n - 2u_1^n + 3u_2^n - 4u_3^n = C_0 \tag{2.1.25}$$

$$0.u_0^n + 1/3u_1^n + 4/3u_2^n + 10/3u_3^n = 0. \tag{2.1.26}$$

The above system of equations (2.1.23)-(2.1.26) can be re-written in the following matrix form as

$$AU^n = BU^{n-1} + E, \qquad \text{or} \qquad U^n = A^{-1}(BU^{n-1} + E), \tag{2.1.27}$$

where

$$A = \begin{bmatrix} U_{00} - \Delta t H_{00} & U_{10} - \Delta t H_{10} & U_{20} - \Delta t H_{20} & U_{30} - \Delta t H_{30} \\ U_{01} - \Delta t H_{01} & U_{11} - \Delta t H_{11} & U_{21} - \Delta t H_{21} & U_{31} - \Delta t H_{31} \\ 1 & -2 & 3 & -4 \\ 0 & 1/3 & 4/3 & 10/3 \end{bmatrix},$$

$$B=\begin{bmatrix}U_{00} & U_{10} & U_{20} & U_{30}\\ U_{01} & U_{11} & U_{21} & U_{31}\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}, U^n=\begin{bmatrix}u_0^n\\ u_1^n\\ u_2^n\\ u_3^n\end{bmatrix}, E=\begin{bmatrix}0\\0\\1\\0\end{bmatrix}, U_{\mathrm{ip}}=U_i(x_p),\ and\ H_{ip}=H_i(x_p)$$

for $p=0,1\ and\ i=0,1,2,3.$

In order to obtain the initial solution U^0 of equation (2.1.27), we use the initial condition $C(x,0)$ combined with equation (2.1.10). Moreover, the approximate solution of the equation (2.1.18) is obtained by substituting the analytical form of the series of the shifted Chebyshev polynomials of the second kind $U_i^*(x),\ i=0,1,2,3$ and the coefficients $u_i(t),\ i=0,1,2,3$ which are computed through equation (2.1.27).

2.1.4 Physical Problem

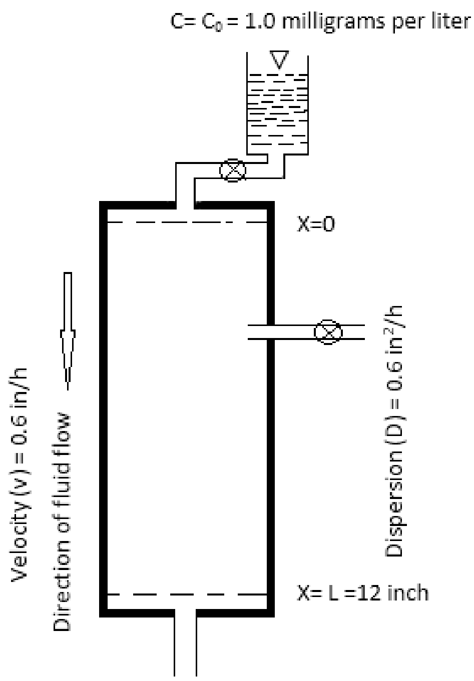

Fig. 2.1.1 Physical problem

Longitudinal dispersion (*D*) = 0.6 in^2/h, Velocity (*V*) = 0.6 in/h, System length (*L*) = 12 in, Rate coefficient (λ) = $0.693/t_{1/2}$(for Non-conservative system), Solute concentration at inflow boundary (C_0) = 1.0 mg/L.

2.1.5 Numerical Benchmarking

A comparison of the numerical results of the concentration factors versus column lengths with the existing analytical result for $t = 2.5\ hrs$ and $t = 5\ hrs$ is depicted through Fig. 2.1.2 and Fig. 2.1.3 respectively for the conservative case $(\lambda = 0)$.

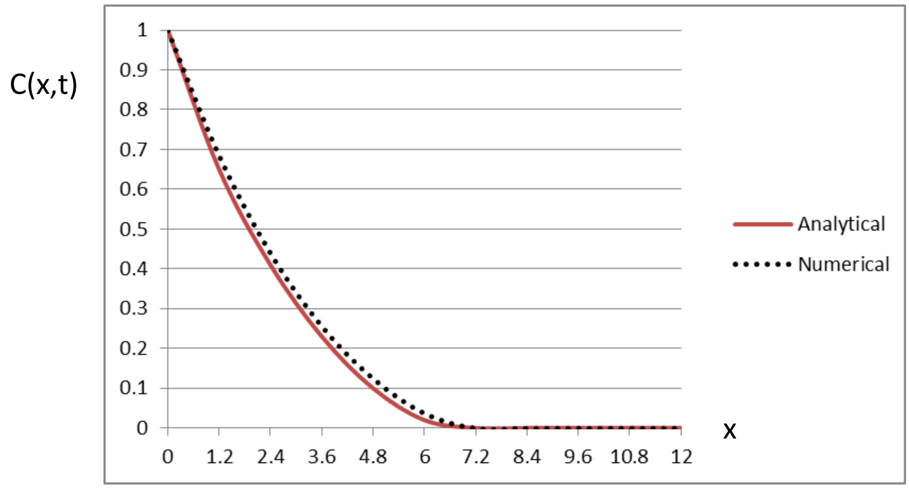

Fig. 2.1.2 Plots of analytical and numerical results of concentration factor vs. column length for the conservative system at $t = 2.5\ hrs$

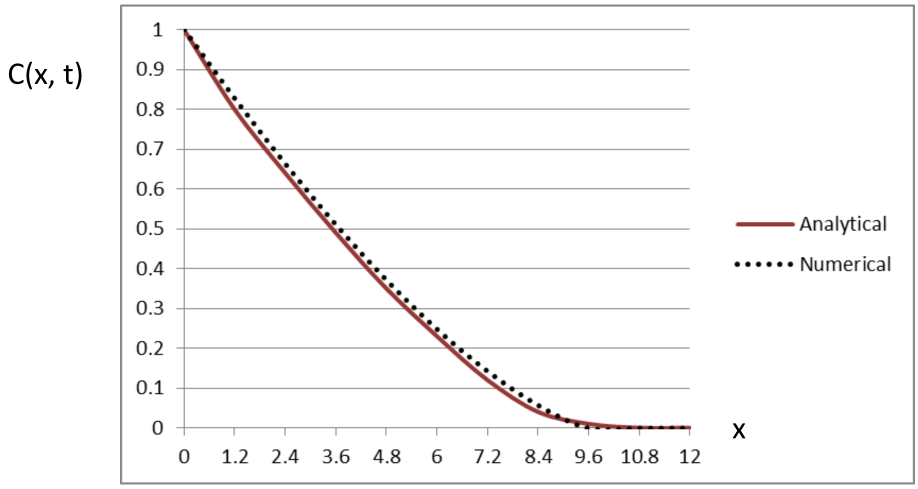

Fig. 2.1.3 Plots of analytical and numerical results of concentration factor vs. column length for the conservative system at $t = 5\ hrs$

2.1.6 Results and Discussion

In this section, the numerical values of the solute concentration factor $C(x,t)$ in finite-length system vs. column length x for different time are calculated for both conservative and non-conservative systems, which are depicted through Fig. 2.1.4 and Fig. 2.1.5 respectively. Here Fig. 2.1.4 depicts the concentration with respect to column length for different time level $t = 2.5, 5, 10, 15$ *and* 20 hrs for the conservative system. Through the figures, it is seen that as the time increases normalized concentration covers more length of the column which is physically justified. Again it is clear from the figure that as the time increases the slopes of the graphs are seen to be more flat due to the prior existence of concentration of solute in the column. The plots in the figure depict that the results obtained by our proposed numerical method are quite similar to the existing analytical results given in equation (2.1.5).

For the non-conservative system, the results depicted through Fig. 2.1.5 are similar to previous one. Here the magnitude of normalized concentration factor is less due to the presence of the sink term $(\lambda > 0)$.

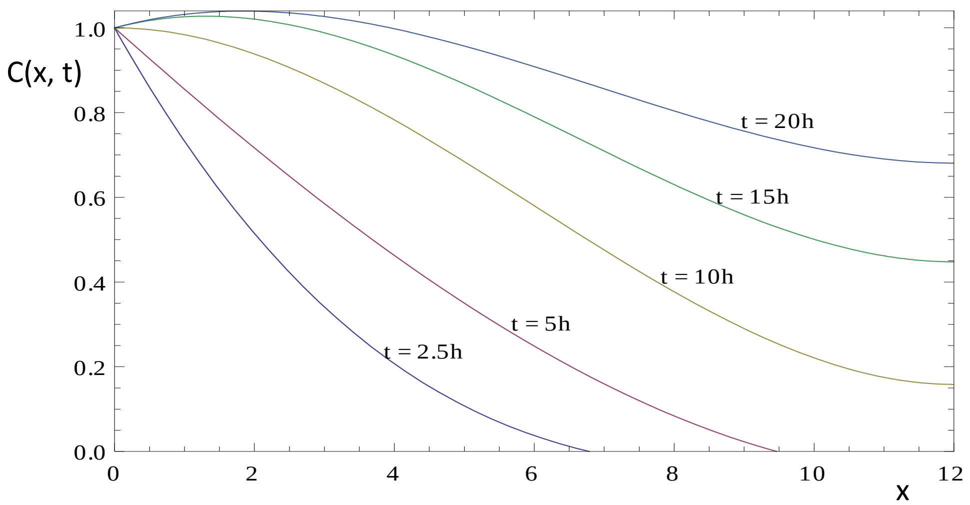

Fig. 2.1.4 Plots of concentration profiles vs. column length for a conservative finite-length system with first-type source boundary conditions at 2.5,5,10,15 and 20 hours

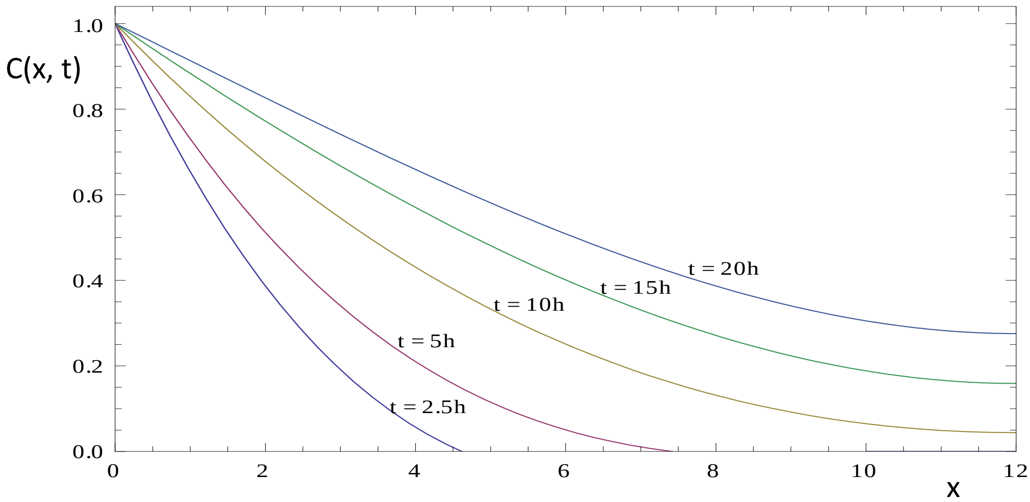

Fig. 2.1.5 Plots of concentration profiles vs. column length for a non-conservative finite-length system with first-type source boundary conditions at 2.5,5,10,15 and 20 hours

2.1.7 Conclusions

The aim of this chapter is to find the numerical solution of one-dimensional ADE having sink term with given first-type source boundary conditions and initial condition in a finite medium using spectral collocation method. The shifted Chebyshev polynomials of second-kind are properly used to reduce the considered problem into a system of ordinary differential equations which are finally converted into a system of linear equations using finite difference method. The salient feature of the present contribution is the comparison of the numerical result with the existing analytical result to validate the efficiency of the proposed method for the conservative case and then to apply the proposed method to find the approximate solution of the considered non-conservative system. Thus it can be concluded that the spectral collocation method is effective, accurate and easy to implement for solving the considered one-dimensional ADE in the finite domain and even can be useful to solve the partial differential equations with arbitrary initial and boundary conditions.

2.2 Numerical Solution of Space Fractional Order Solute Transport System

2.2.1 Introduction

In this chapter, space fractional order form of the model already considered in Section 2.1 is discussed. The fractional order form of the ADE has not yet been studied much. The growing interest in fractional advection-dispersion equation (FADE) because of their useful applications in the areas like electromagnetics, robotics and controls, acoustics, viscoelastic damping and electrochemistry and in material science has motivated the researchers to take up this exercise. The FADE is promising for an accurate description of the transportation of solute in complex media such as a porous aquifer. In the real world, fractional order ADE has comprehensive applications in engineering, physics, economics, etc. due to the non-local property of fractional order derivative. Because of this property, fractional order ADE has much more memory effect compared to standard order ADE. FADEs in time, space, time-space have been extensively applied in describing physical and engineering problems such as anomalous diffusion, medicine, biology, solute transport, random and disordered media, control, signal processing and so on. To describe and understand the dispersion phenomena, time, space, time-space FADEs have fundamental importance and have received considerable attention in recent years. The researchers and engineers are actively engaged to find the solution of ADE in fractional order system due to its greater flexibility in models, non-local behavior and ultimate convergence to the integer order system.

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Through literature survey few methods are found for solving FADE like variable transformation by Liu et al. (2003), the Green function by Huang and Liu (2005), the implicit and explicit difference method by Meerschaert and Tadjeran (2004) and the Adomian decomposition method (Momani and Odibat (2008), El-Sayed et al. (2010), Hikal and Ibrahim (2015)) etc. A new technique to solve the FADE in the reproducing kernel space is found in the research article of Jiang and Lin (2010). In 2010, El-Sayed et al. (2010) have given a numerical algorithm for the solution of an intermediate FADE. A new numerical algorithm for FADE with variable coefficients using Jacobi polynomials was given by Bhrawy (2013). A high-order numerical method for Riesz space FADE has been given by Feng et al. (2016). Analytical modeling of FADE defined in a bounded space domain has been discussed by Golbabai et al. (2011). Also some numerical methods for solving space, time and space-time FADEs can be found in Refs. (Roop (2008), Zheng and Wei (2010), Zhang et al. (2014), Parvizi (2015)). In the year 2015, Sweilam et al. (2015) solved the fractional diffusion equation using Chebyshev polynomial of the second kind, and in the next year, they solved the similar problem using Chebyshev polynomial of the third kind (Sweilam et al. (2016)). The space-dependent coefficients and the order of fractionality of time fractional order advection-diffusion solute model which shows the abnormalities of tracer in normal porous media is recently given by Maryshev et al. (2016).

Due to physical relevance and important applications, there is still plenty of scope for researchers to explore fractional order ADE, which has motivated me to propose a model of physical interest and then predict the physical nature. The proposed one-dimensional space fractional order solute transport equation having a source/sink term with given initial and boundary conditions as follows:

$$\frac{\partial C}{\partial t} = D\frac{\partial^{2\beta} C}{\partial x^{2\beta}} - V\frac{\partial^{\beta} C}{\partial x^{\beta}} - \lambda C, \qquad 0 < \beta \le 1 \tag{2.2.1}$$

under the boundary conditions

$$C = C_0, \quad x = 0 \tag{2.2.2}$$

$$\frac{\partial^{\beta} C}{\partial x^{\beta}} = 0, \quad x = L \tag{2.2.3}$$

and initial condition

$$C = 0, \quad 0 < x < L \quad at \;\; t = 0 \tag{2.2.4}$$

In this chapter, to solve the considered problems (2.2.1)-(2.2.4), the same method used in Section 2.1 is applied. In the spectral method, Chebyshev polynomial forms an orthogonal basis, and thus the coefficients can easily be determined through the application of the inner product. Since Chebyshev series or expansion is related to the Fourier cosine transform through a change of variables, the Chebyshev polynomials have eventually become important tools in numerical computation and help to achieve faster convergence of the solution. Thus due to their high accuracy and closeness to the minimax polynomials and especially for better goodness to fit, the Chebyshev polynomials are becoming more useful to the scientists and engineering compared to other orthogonal polynomials like Legendre, Hermite, and Laguerre. The convergence properties and stability analysis for Chebyshev polynomials can be found in the monographs of Canuto et al. (1988), Boyd (2000), Trefethen (2000), Peyret (2002) and Guo et al. (2012).

The considered problem is solved under the assumptions that fluid is of constant density and viscosity, the flow of the fluid is in the x-direction with constant velocity and also the longitudinal dispersion coefficient D is constant. The numerical results which are depicted through figures for different specific cases clearly exhibit that the method is effective and reliable for the solution of ADE in fractional order system. The author is optimist that the outcomes of their present model will be useful to the scientists and engineers working in the area of ADE and also to the mathematicians working in the field of applications of FDE.

2.2.2 Preliminaries

2.2.2.1 Relation between Chebyshev Polynomials and Shifted Chebyshev Polynomials of the Second-Kind

An important relation of second-kind shifted Chebyshev polynomials $U_n^*(x)$ defined in the interval $[0,12]$ with Chebyshev polynomials of the second-kind $U_n(x)$ defined in the interval $[-1,1]$ is

$$2xU_{n-1}^*(12x^2) = U_{2n-1}(x). \tag{2.2.5}$$

2.2.2.2 The Explicit Form of the Second-Kind Shifted Chebyshev Polynomials

The explicit form of the second-kind shifted Chebyshev polynomials $U_n^*(x)$ over the interval $[0,12]$ is given by

$$U_n^*(x) = \sum_{p=0}^{n} \frac{(-1)^p}{3^{n-p}} \frac{\Gamma(2n-p+2)}{\Gamma(p+1)\Gamma(2n-2p+2)} x^{n-p}, \quad n > 0. \tag{2.2.6}$$

2.2.2.3 Evaluation of the Fractional Derivative Using Second-Kind Shifted Chebyshev Polynomials

If *h(x)* be a squared integrable over [0,12], then we can derive a formula for the fractional derivative of $h_m(x)$, which is approximated through the equation (2.1.11). Now using the linearity property of the Caputo fractional derivative as discussed in Chapter 1 on $h_m(x)$, we have

$$D^\beta(h_m(x)) = \sum_{i=0}^{m} a_i D^\beta(U_i^*(x)). \tag{2.2.7}$$

Now using the linearity property of the Caputo fractional derivative with other property of Caputo derivative defined in Section 1.17.4 of Chapter 1, we get

$$D^{\beta}(U_i^*(x)) = 0, \qquad i = 0,1,........,\lceil \beta \rceil - 1, \quad \beta > 0. \tag{2.2.8}$$

and

$$D^{\beta}(U_i^*(x)) = \sum_{p=0}^{i} \frac{(-1)^p}{3^{i-p}} \frac{\Gamma(2i-p+2)}{\Gamma(p+1)\Gamma(2i-2p+2)} D^{\beta} x^{i-p}. \tag{2.2.9}$$

Again, using the properties of Caputo fractional derive in equation (2.2.9), we get

$$D^{\beta}(U_i^*(x)) = \sum_{p=0}^{i-\lceil \beta \rceil} \frac{(-1)^p}{3^{i-p}} \frac{\Gamma(2i-p+2)\Gamma(i-p+1)}{\Gamma(p+1)\Gamma(2i-2p+2)\Gamma(i+1-p-\beta)} x^{i-p-\beta}. \tag{2.2.10}$$

Now combining the equations (2.2.7) to (2.2.10), we get

$$D^{\beta}(h_m(x)) = \sum_{i=\lceil \beta \rceil}^{m} \sum_{p=0}^{i-\lceil \beta \rceil} a_i \frac{(-1)^p}{3^{i-p}} \frac{\Gamma(2i-p+2)\Gamma(i-p+1)}{\Gamma(p+1)\Gamma(2i-2p+2)\Gamma(i+1-p-\beta)} x^{i-p-\beta}, \tag{2.2.11}$$

which can be re-written as

$$D^{\beta}(h_m(x)) = \sum_{i=\lceil \beta \rceil}^{m} \sum_{p=0}^{i-\lceil \beta \rceil} a_i F_{i,p}^{(\beta)} x^{i-p-\beta}, \tag{2.2.12}$$

where

$$F_{i,p}^{(\beta)} = \frac{(-1)^p}{3^{i-p}} \frac{\Gamma(2i-p+2)\Gamma(i-p+1)}{\Gamma(p+1)\Gamma(2i-2p+2)\Gamma(i+1-p-\beta)}. \tag{2.2.13}$$

2.2.3 Solution of the Problem

During the solution of one-dimensional space fractional solute transport equation (2.2.1) using Chebyshev collocation method, with first type source boundary conditions (2.2.2) and (2.2.3), and initial condition (2.2.4), let us approximate the solute concentration *C(x,t)* as given in the equation (2.1.12) of Section 2.1. Equation (2.2.1) with the aid of equations (2.2.12) and (2.1.12) reduces to

$$\sum_{i=0}^{m}\frac{du_i(t)}{dt}U_i^*(x)=D\sum_{i=\lceil 2\beta\rceil}^{m}\sum_{p=0}^{i-\lceil 2\beta\rceil}u_i(t)F_{i,p}^{(2\beta)}x^{i-p-2\beta}-V\sum_{i=\lceil \beta\rceil}^{m}\sum_{p=0}^{i-\lceil \beta\rceil}u_i(t)F_{i,p}^{(\beta)}x^{i-p-\beta}-\lambda\sum_{i=0}^{m}u_i(t)U_i^*(x), \tag{2.2.14}$$

Now, collocating equation (2.2.14) with $(m+1-\lceil\beta\rceil)$ points as x_k, we get

$$\sum_{i=0}^{m}\frac{du_i(t)}{dt}U_i^*(x_k)=D\sum_{i=\lceil 2\beta\rceil}^{m}\sum_{p=0}^{i-\lceil 2\beta\rceil}u_i(t)F_{i,p}^{(2\beta)}x_k^{i-p-2\beta}-V\sum_{i=\lceil \beta\rceil}^{m}\sum_{p=0}^{i-\lceil \beta\rceil}u_i(t)F_{i,p}^{(\beta)}x_k^{i-p-\beta}-\lambda\sum_{i=0}^{m}u_i(t)U_i^*(x_k), \tag{2.2.15}$$

Using the roots of second-kind shifted Chebyshev polynomials $U^*_{(m+1-\lceil\beta\rceil)}(x)$ which are suitable for the collocation points and also using equations (2.1.10) and (2.1.12), we get initial values of $u_i(t)$ at $t=0$ and on substituting (2.1.12) in the boundary conditions (2.2.2)-(2.2.3) with the aid of equations (2.2.12) and (2.2.13), we get the following equations for the case $0<x<12$.

$$\sum_{i=0}^{m}(-1)^{(i+2)}(i+1)u_i(t)=C_0, \qquad \sum_{i=\lceil \beta\rceil}^{m}\sum_{p=0}^{i-\lceil \beta\rceil}u_i(t)F_{i,p}^{(\beta)}x^{i-p-\beta}\Big|_{x=12}=0. \tag{2.2.16}$$

Equation (2.2.15) with the boundary conditions given by equation (2.2.16) gives rises to $(m+1)$ ordinary differential equations, which can be solved using finite difference method to get the unknowns $u_i(t),\ i=0,1,........,m.$

Let us make an approximation with $m=3$. Then the equations (2.2.15)-(2.2.16) are reduced to

$$\sum_{i=0}^{3}\frac{du_i(t)}{dt}U_i^*(x_k)=D\sum_{i=\lceil 2\beta\rceil}^{3}\sum_{p=0}^{i-\lceil 2\beta\rceil}u_i(t)F_{i,p}^{(2\beta)}x_k^{i-p-2\beta}-V\sum_{i=\lceil \beta\rceil}^{3}\sum_{p=0}^{i-\lceil \beta\rceil}u_i(t)F_{i,p}^{(\beta)}x_k^{i-p-\beta}-\lambda\sum_{i=0}^{3}u_i(t)U_i^*(x_k), \tag{2.2.17}$$

$$\sum_{i=0}^{m}(-1)^{(i+2)}(i+1)u_i(t)=C_0, \qquad \sum_{i=\lceil \beta\rceil}^{m}\sum_{p=0}^{i-\lceil \beta\rceil}u_i(t)F_{i,p}^{(\beta)}x^{i-p-\beta}\Big|_{x=12}=0. \tag{2.2.18}$$

with $C_3(x,t)$ already given in equation (2.1.18) of Section 2.1.

Here *k=0,1* and x_k's are the roots of the second-kind shifted Chebyshev polynomial $U_2^*(x)$. Taking $0<\beta<1$, we obtain the following system of ordinary differential equations as

$$\sum_{i=0}^{3} A_i u_i^{'}(t) = B_0 u_0(t) + B_1 u_1(t) + B_2 u_2(t) + B_3 u_3(t) \tag{2.2.19}$$

$$\sum_{i=0}^{3} A_{1i} u_i^{'}(t) = B_{10} u_0(t) + B_{11} u_1(t) + B_{12} u_2(t) + B_{13} u_3(t) \tag{2.2.20}$$

$$u_0(t) - 2u_1(t) + 3u_2(t) - 4u_3(t) = C_0 \tag{2.2.21}$$

$$E_0 u_0(t) + E_1 u_1(t) + E_2 u_2(t) + E_3 u_3(t) = 0, \tag{2.2.22}$$

where $A_i = U_i^*(x_0),\ A_{1i} = U_i^*(x_1),\ B_0 = -\lambda U_0^*(x_0),\ B_1 = \{-\lambda U_1^*(x_0) - VF_{1,0}^{(\beta)} x_0^{1-\beta}\},$

$B_2 = \{-\lambda U_2^*(x_0) - V(F_{2,0}^{(\beta)} x_0^{2-\beta} + F_{2,1}^{(\beta)} x_0^{1-\beta}) + D(F_{2,0}^{(2\beta)} x_0^{2(1-\beta)})\},$

$B_3 = \{-\lambda U_3^*(x_0) - V(F_{3,0}^{(\beta)} x_0^{3-\beta} + F_{3,1}^{(\beta)} x_0^{2-\beta} + F_{3,2}^{(\beta)} x_0^{1-\beta}) + D(F_{3,0}^{(2\beta)} x_0^{3-2\beta} + F_{3,1}^{(2\beta)} x_0^{2(1-\beta)})\},$

$B_{10} = -\lambda U_0^*(x_1),\ B_{11} = \{-\lambda U_1^*(x_1) - VF_{1,0}^{(\beta)} x_1^{1-\beta}\},$

$B_{12} = \{-\lambda U_2^*(x_1) - V(F_{2,0}^{(\beta)} x_1^{2-\beta} + F_{2,1}^{(\beta)} x_1^{1-\beta}) + D(F_{2,0}^{(2\beta)} x_1^{2(1-\beta)})\},$

$B_{13} = \{-\lambda U_3^*(x_1) - V(F_{3,0}^{(\beta)} x_1^{3-\beta} + F_{3,1}^{(\beta)} x_1^{2-\beta} + F_{3,2}^{(\beta)} x_1^{1-\beta}) + D(F_{3,0}^{(2\beta)} x_1^{3-2\beta} + F_{3,1}^{(2\beta)} x_1^{2(1-\beta)})\},$

$E_0 = 0,\ E_1 = 12^{1-\beta} F_{1,0}^{(\beta)},\ E_2 = (12^{2-\beta} F_{2,0}^{(\beta)} + 12^{1-\beta} F_{2,1}^{(\beta)}),$

$E_3 = (12^{3-\beta} F_{3,0}^{(\beta)} + 12^{2-\beta} F_{3,1}^{(\beta)} + 12^{1-\beta} F_{3,2}^{(\beta)}).$

Now, the equations (2.2.19)-(2.2.22) are solved using finite difference method with the notations $T = T_{final},\ 0 < t_j \le T$ and $\Delta t = T/N$, for $j = 0,1,,.........,N$. Defining $u_i(t_n) = u_i^n$, the system of equations (2.2.19)-(2.2.22) are discretized in time and gives rise to

$$\sum_{i=0}^{3} \frac{u_i^n - u_i^{n-1}}{\Delta t} A_i = B_0 u_0(t) + B_1 u_1(t) + B_2 u_2(t) + B_3 u_3(t) \tag{2.2.23}$$

$$\sum_{i=0}^{3}\frac{u_i^n - u_i^{n-1}}{\Delta t}A_{1i} = B_{10}u_0(t) + B_{11}u_1(t) + B_{12}u_2(t) + B_{13}u_3(t) \tag{2.2.24}$$

$$u_0^n - 2u_1^n + 3u_2^n - 4u_3^n = C_0 \tag{2.2.25}$$

$$E_0u_0^n + E_1u_1^n + E_2u_2^n + E_3u_3^n = 0 \tag{2.2.26}$$

The above system of equations (2.2.23)-(2.2.26) can be re-written in the matrix form as $U^n = A^{-1}(BU^{n-1} + E)$, where

$$A = \begin{bmatrix} A_0 - \Delta tB_0 & A_1 - \Delta tB_1 & A_2 - \Delta tB_2 & A_3 - \Delta tB_3 \\ A_{10} - \Delta tB_{10} & A_{11} - \Delta tB_{11} & A_{12} - \Delta tB_{12} & A_{13} - \Delta tB_{13} \\ 1 & -2 & 3 & -4 \\ E_0 & E_1 & E_2 & E_3 \end{bmatrix},\ B = \begin{bmatrix} A_0 & A_1 & A_2 & A_3 \\ A_{10} & A_{11} & A_{12} & A_{13} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

$$U^n = \begin{bmatrix} u_0^n \\ u_1^n \\ u_2^n \\ u_3^n \end{bmatrix}, \text{and } E = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}.$$

In order to obtain the initial solution U^0 of the above matrix equation, the initial condition *C(x,0)* is used. Ultimately the approximate solution $C_3(x,t)$ is obtained after substituting analytical form of the series of the shifted Chebyshev polynomials of the second-kind $U_i^*(x),\ i = 0,1,2,3$ and the coefficients $u_i(t),\ i = 0,1,2,3$ which are computed through the above matrix equation.

2.2.4 Numerical Results and Discussion

The numerical values of the solute concentration $C(x,t)$ in the finite-length system for various time and for different values of fractional order space derivative $\beta = 0.7, 0.8, 0.9,$ and 1.0 are calculated for both conservative and non-conservative systems. During numerical computation, the model values as given in Section 2.1.4 for a standard order physical problem are used. A comparison of the results of $C(x,t)$ vs.

x between the existing analytical results given by Wexler (1992) and the results obtained by our proposed method for the standard order conservative system ($\beta = 1,\ \lambda = 0$) are same as depicted through Fig. 2.1.2 and Fig. 2.1.3 for $t = 2.5\ hrs$ and $t = 2.5\ hrs$, respectively of Chapter 1 which clearly exhibit that our proposed method is reliable and effective. Thus we may conclude that the result obtained using the proposed method is authentic for the conservative system.

The graphical plots of $C(x,t)$ vs. x for different *t's* for specific values of β are depicted through Figs. 2.2.1(a) – (d) for the conservative system ($\lambda = 0$) and Figs. 2.2.2(a) – (d) for non-conservative system ($\lambda \neq 0$). It is observed that the nature of curves for fractional order ($0 < \beta < 1$) are similar to that for the standard order case ($\beta = 1$). The variations of $C(x,t)$ vs. x for various fractional order β at specific time $t = 2.5, 5, 10, 15, and\ 20$ hrs are shown through Figs. 2.2.31(a) – (d) and Figs. 2.2.4(a) – (d) for the conservative system and non-conservative system respectively. It is seen from the figures that for both conservative and non-conservative systems, the transportation rate of solute concentration becomes faster as the system goes from standard order to fractional order, mainly due to fractional order creates closer to the actual description of porosity and permeability matrix in micro-scale. Again due to the effect of the sink term, the transportation rate is less for the non-conservative system as compared to the conservative system.

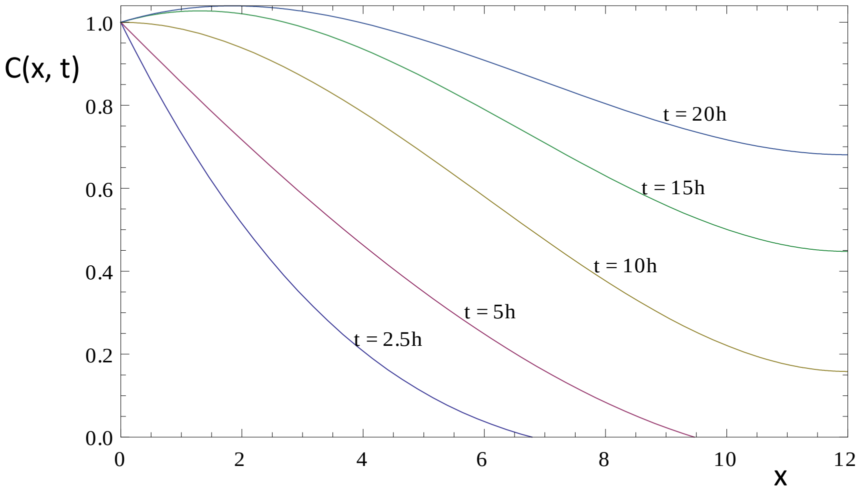

Fig. 2.2.1(a)

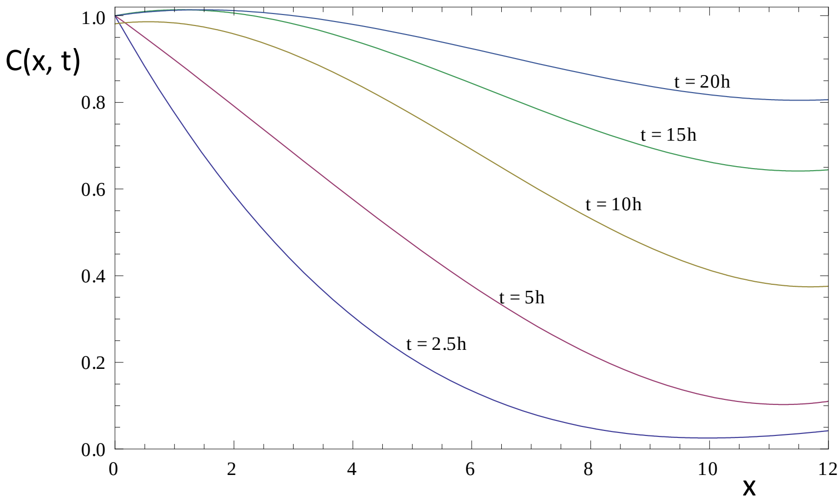

Fig. 2.2.1(b)

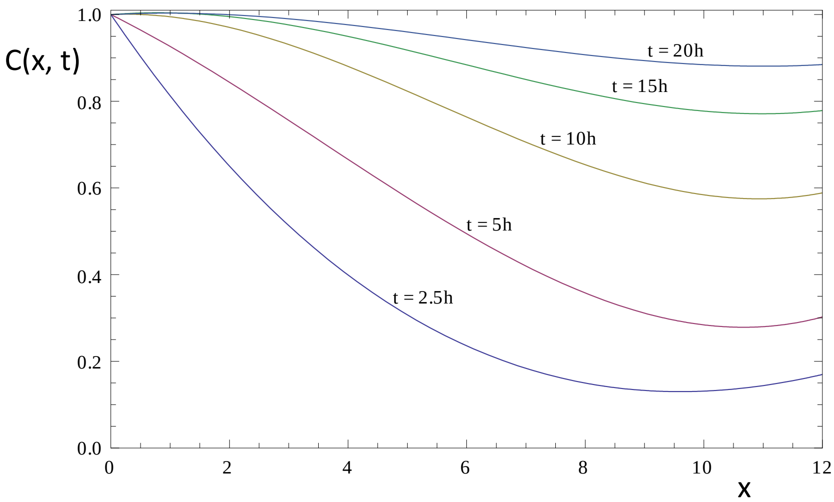

Fig. 2.2.1(c)

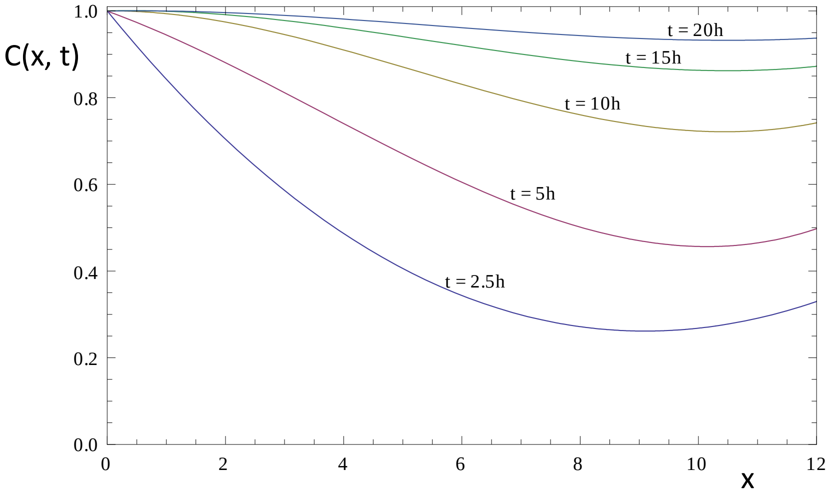

Fig. 2.2.1(d)

Fig. 2.2.1 Concentration profiles $C(x,t)$ vs. x at $t = 2.5, 5, 10, 15, and\ 20$ hrs for (a) $\beta = 1$, (b) $\beta = 0.9$, (c) $\beta = 0.8$, (d) $\beta = 0.7$, for a conservative solute

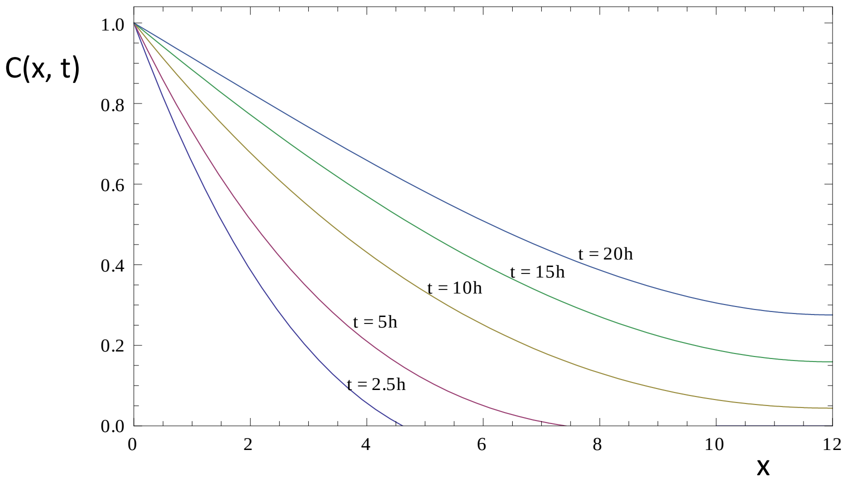

Fig. 2.2.2(a)

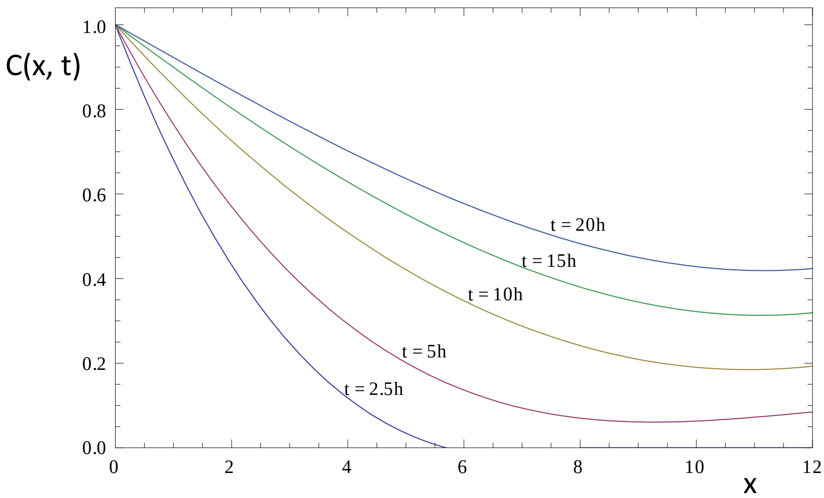

Fig. 2.2.2(b)

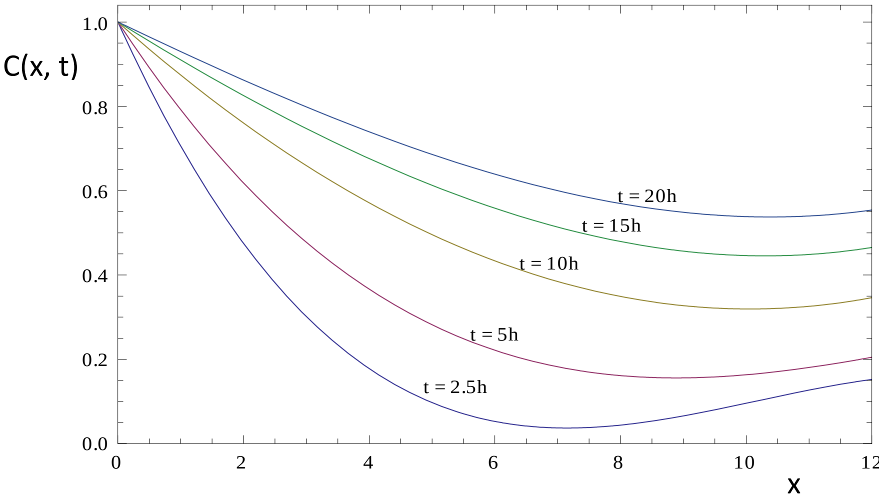

Fig. 2.2.2(c)

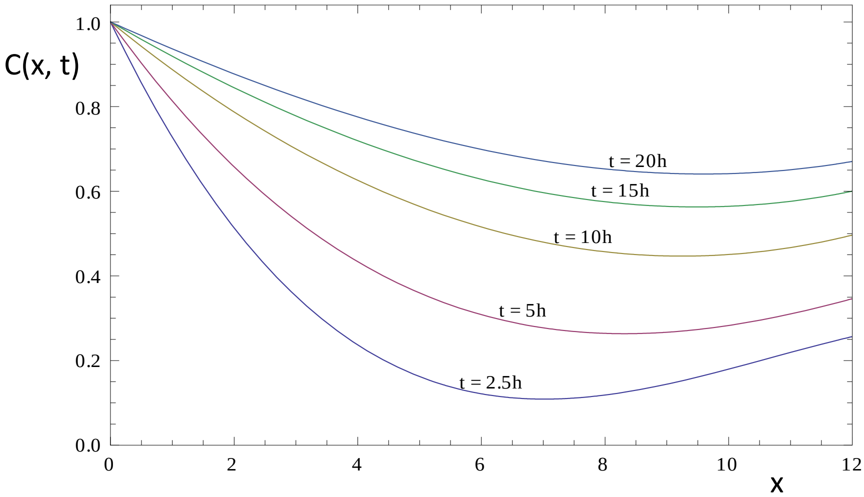

Fig. 2.2.2(d)

Fig. 2.2.2 Concentration profiles $C(x,t)$ vs. x at $t = 2.5, 5, 10, 15, and\, 20$ hrs for (a) $\beta = 1$, (b) $\beta = 0.9$, (c) $\beta = 0.8$, (d) $\beta = 0.7$, for a non-conservative solute

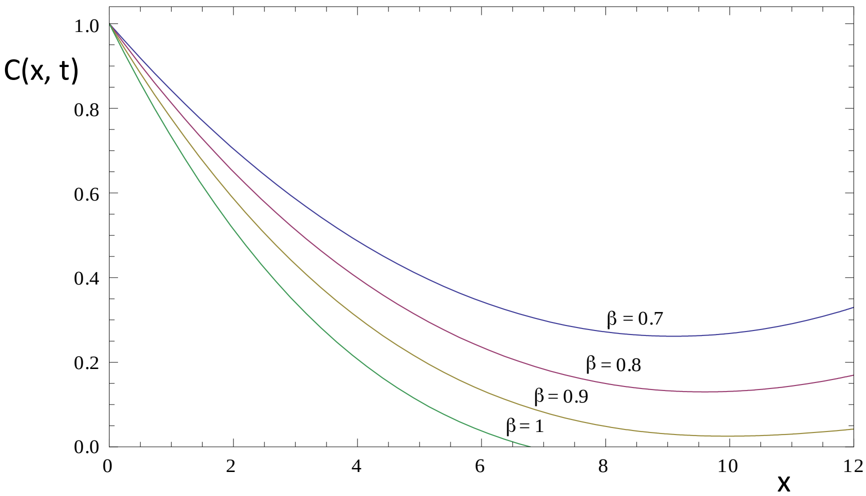

Fig. 2.2.3(a)

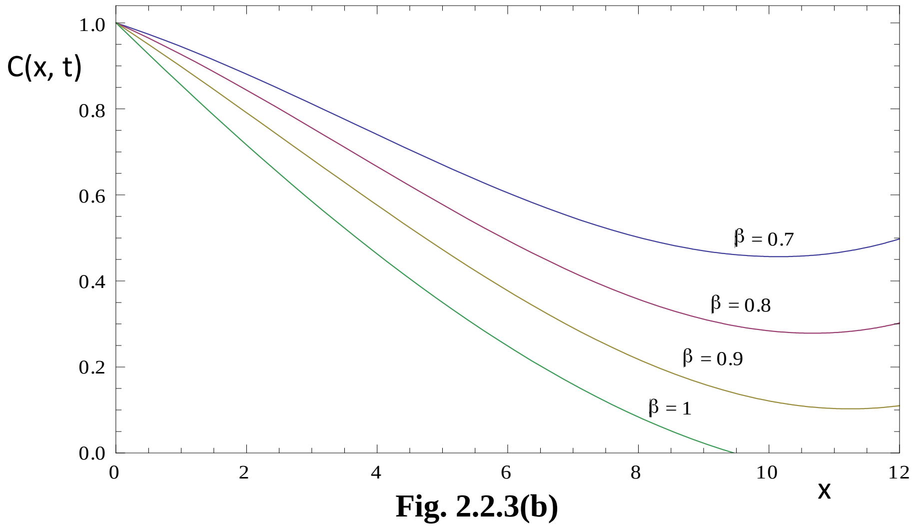

Fig. 2.2.3(b)

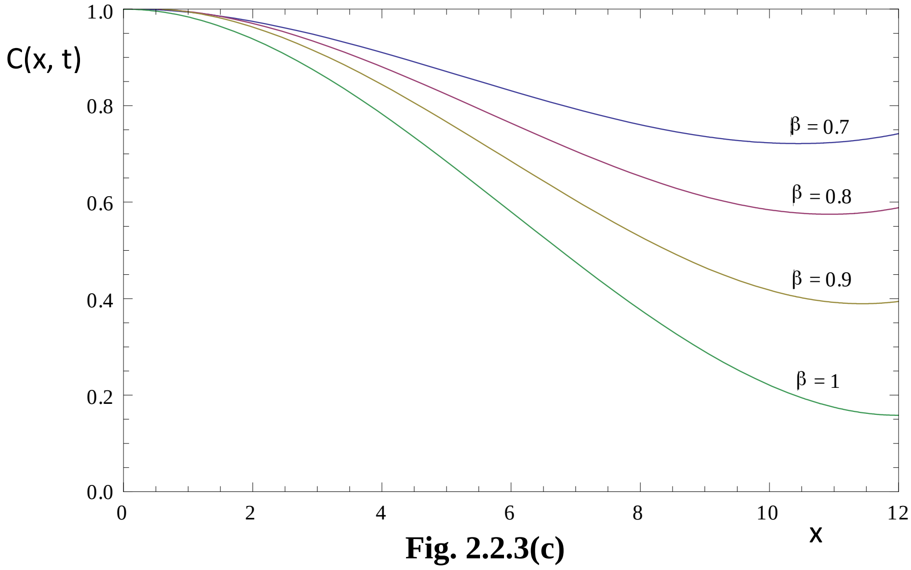

Fig. 2.2.3(c)

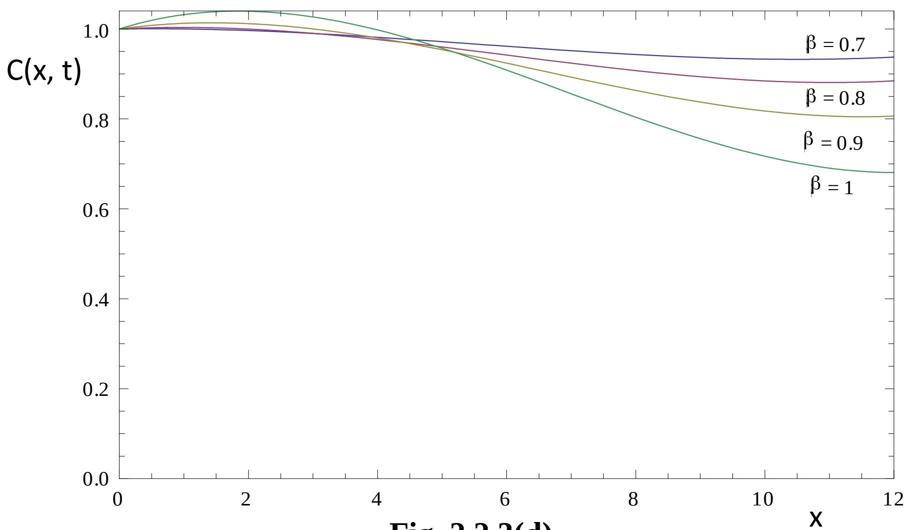

Fig. 2.2.3(d)

Fig. 2.2.3 Concentration profiles $C(x,t)$ vs. x for various β at $(a)\,t = 2.5,$ $(b)\,t = 5,$ $(c)\,t = 10,$ and $(d)\,t = 20hrs$ for a conservative solute

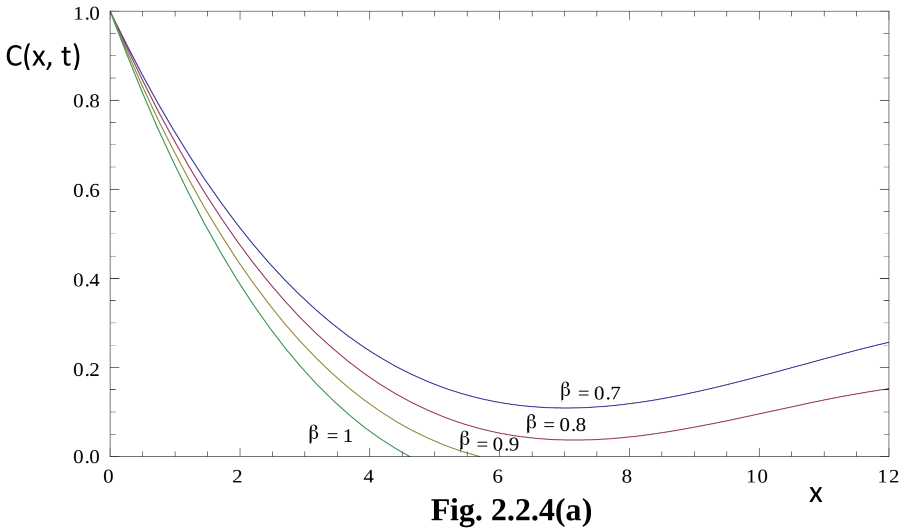

Fig. 2.2.4(a)

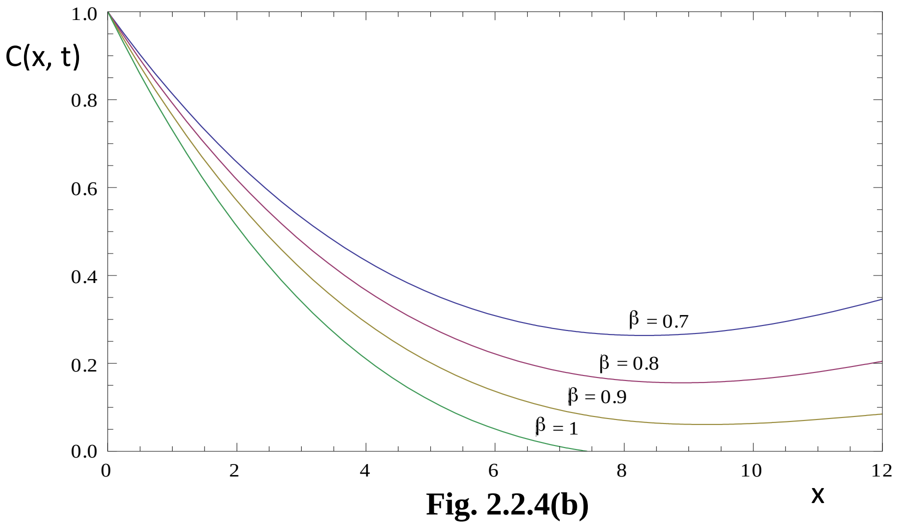

Fig. 2.2.4(b)

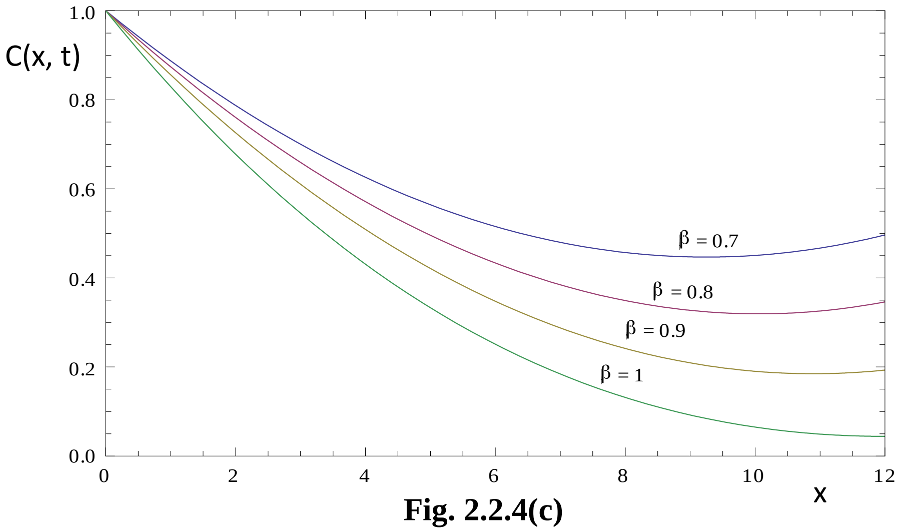

Fig. 2.2.4(c)

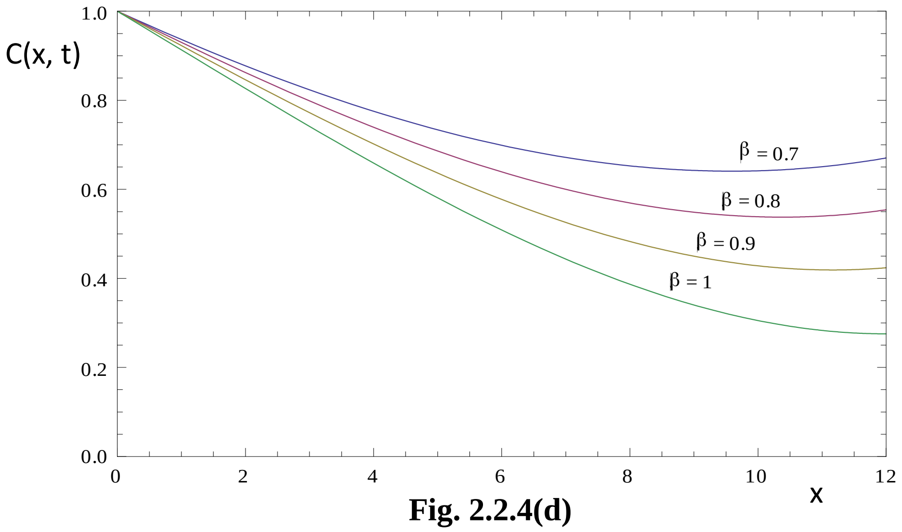

Fig. 2.2.4(d)

Fig. 2.2.4 Concentration profiles $C(x,t)$ vs. x for various β at $(a)\, t = 2.5,$ $(b)\, t = 5,$ $(c)\, t = 10,$ *and* $(d)\, t = 20hrs$ for non-conservative solute

2.2.5 Conclusions

In the present scientific contribution, three goals are achieved. First one is the effective use of shifted Chebyshev polynomials of second-degree for the solution of spatial fractional order advection-dispersion equation with source/sink term. Secondly, the graphical display of fast solute concentration as the system approaches from standard order to the fractional order for both conservative and non-conservative systems. The third one is the presentation of decay in transportation rate in the non-conservative system compared to the conservative system due to the effect of the sink term for fractional order as well as standard order case.