Chapter 3

Numerical Solution of Two-Dimensional Solute Transport System Using Operational Matrices

3.1 Introduction

Lots of researchers from different parts of the world have involved to tackle the physically relevant two-dimensional solute transport models both analytically and numerically. A large number of analytical solutions are available for solving these problems (Carslaw and Jaeger (1971); Cleary and Ungs (1978); Kumar (1983); Carnahan and Remer (1984); Barry and Sposito (1989); Lindstrom and Boersma (1989); Leij and Dane (1990); Basha and El-Habel (1993); Fry et al. (1993); Serrano (1995); Chrysikopoulos and Sim (1996); Flury et al. (1998); Sim and Chrysikopoulos (1999); Sanderson et al. (2004, 2006, 2009); Singh et al. (2008, 2009a, 2009b); Srinivasan and Clement (2008); Chrysikopoulos (2011); Shen and Reible (2015)). The analytical and experimental investigations of longitudinal and lateral dispersion in an isotropic porous medium were presented by Harleman and Rumer (1963). In semi-infinite absorbing porous media, Bruce and Street (1967) studied longitudinal and lateral dispersion with constant input concentration. The analytical solution for one-dimensional multi-species contaminant transport subject to sequential first-order decay reaction in finite porous media for constant boundary conditions is discussed by Guerrero et al. (2009), and same authors (2010) discussed it for time-varying boundary conditions in the year 2010. Konikow (2010) used the method of characteristics to solve the groundwater

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transport models by applying dispersive changes in Lagrangian particles. Lugo-Mendez et al. (2015) solved the transport model in homogeneous porous media by revisiting the up-scaling process of diffusive mass transfer of solute. The solutions of the spatially variable ADE could be found in many research articles (Ebach and White (1958); Yates (1992); Logan (1996); Lin and Ball (1998); Chen et al. (2003); Neelz (2006); Guerrero et al. (2013)). But all time it is not easy to get the analytical solutions, so one should look forward for numerical solutions (Zhao and Valliappan (1994a, 1994b); Lee (1999); Dehghan (2004); Karahan (2006); Walter et al. (2007); Huang et al. (2008); Savović and Djordjevich (2012); Djordjevich and Savović (2013); Dhawan et al. (2012); Geback and Heintz (2014); Jaiswal et al. (2017)). The solutions for two-dimensional and three-dimensional solute transport models are also available in literature (Goltz and Roberts (1986); Wexler (1992); Batu (1989, 1993); Leij et al. (1991); Chrysikopoulos (1995); Aral and Liao (1996); Anderman et al. (1996); Tartakovsky and Federico (1997); Hunt (1998); Hantush and Marino (1998); Sim and Chrysikopoulos (1998); Zoppou and Knight (1999); Tartakovasky (2000); Park and Zhan (2001); Sander and Braddock (2005); Kumar et al. (2006); Massabo et al. (2006); Singh et al. (2010); Chen et al. (2011); Assumaning and Chang (2012); Yadav et al. (2012)). In 1970, Bruce (1970) conducted an experiment for two-dimensional problems in the porous domain. A semi-analytical solution for linearized multi-component cation exchange transport in steady one, two or three-dimensional groundwater flow had been given by Samper-Calvete and Yang (2007). Fedi et al. (2010) analytically solved the two-dimensional advection-dispersion equations in porous media by considering parallel plate geometry. It is solved by the application of Laplace transform in regard to the temporal dimension and the introduction of a theta function. Discretized numerical methods are commonly used for the problems related to transport of solutes in saturated porous media, which are commonly described by the advection-dispersion equation in real domains. Xu et al. (2012) simulated the three-dimensional transport model contaminated by perchloroethylene subject to multi permeable reactive barrier remediation. Though few research works in the conservative system, have already been done, but the literature on non-conservative systems related to two-dimensional problem is not available.

In this chapter, to solve the considered two-dimensional solute transport system, the one-dimensional numerical approach is extended that has already been used in Chapter 2. Here, two-dimensional shifted Chebyshev polynomial of the first-kind is considered for approximation along with an unconditionally stable finite difference scheme discussed in the monograph of Guo et al. (2012). The numerical results are depicted graphically for different particular cases for both conservative and non-conservative systems.

3.2 Problem Formulation

For more general case, the solute transport system is given in Section. 1.14 of Chapter 1 takes place in three space dimensions, but for mathematical simplicity here two space dimensions are considered where $R = -\lambda c$ denotes the sink term with λ being reaction rate coefficient. Thus the resulting transport equation is a time-dependent reaction-advection-dispersion equation in space-time domain $\Omega \times I,$ where $\Omega \subseteq \mathbf{R}^2$, Γ is the boundary of Ω, and $I = (0, T)$ is described as

$$\frac{\partial c}{\partial t} = \nabla.(d\,\nabla c) - \nabla.(v\,c) - \lambda\,c \text{ in } \Omega \times I, \tag{3.1}$$

with initial condition

$$c(x, y, 0) = c_0(x, y) \text{ in } \Omega, \tag{3.2}$$

and boundary conditions

$$c(x,y,t) = f_- \text{ on } (\Gamma \times I)_-, \tag{3.3}$$

$$c(x,y,t) = f_+ \quad or \quad \partial_n c(x,y,t) = f_+ \text{ on } (\Gamma \times I)_+, \tag{3.4}$$

where *c* is the species concentration. *d, v* and λ are the positive quantities, and in more general case these are the functions of space and time. c_0, f_- and f_+ are the given data. $(\Gamma \times I)_-$ is the inflow boundary and $(\Gamma \times I)_+$ is the outflow boundary of the space-time boundary $(\Gamma \times I)$.

The equation (3.1) in two-dimensional form can be written as

$$\frac{\partial c}{\partial t} = d_x \frac{\partial^2 c}{\partial x^2} + d_y \frac{\partial^2 c}{\partial y^2} - v_x \frac{\partial c}{\partial x} - v_y \frac{\partial c}{\partial y} - \lambda c, \tag{3.5}$$

with boundary conditions

$$c(x,y,t) = c_0 \qquad x = 0, -l_y < y < l_y, \tag{3.6}$$

$$\frac{\partial c}{\partial x} = 0, \qquad x = l_x, -l_y < y < l_y, \tag{3.7}$$

$$\frac{\partial c}{\partial y} = 0, \qquad y = -l_y, 0 < x < l_x, \tag{3.8}$$

$$\frac{\partial c}{\partial y} = 0, \qquad y = l_y, 0 < x < l_x, \tag{3.9}$$

and initial condition

$$c(x,y,0) = 0, \qquad 0 < x < l_x, \ -l_y < y < l_y, \tag{3.11}$$

where $d_x, d_y, v_x, v_y, \lambda$ and c_0 are constants.

3.3 Preliminaries

3.3.1 One-Dimensional Chebyshev Spectral Collocation Method

In approximation theory, Chebyshev polynomials are important for approximating the function $\phi(x)$ over the finite interval $[-1,1]$ as

$$\phi(x) = \sum_{p=0}^{\infty} \hat{a}_p T_p(x), \tag{3.12}$$

where $\hat{a}_p$ is known as pseudo-spectrum of the function $\phi(x)$.

Generally the first $(N+1)$-terms of the Chebyshev polynomials are considered during the approximation. Thus, we have

$$\phi(x) = \sum_{p=0}^{N} \hat{a}_p T_p(x). \tag{3.13}$$

In spectral collocation method, the governing equation is spatially discretized at discrete Chebyshev Gauss-Lobatto points in most of the cases with the fact that the numerical solution is forced to satisfy the considered equation exactly at collocation points which are extreme points of the Chebyshev polynomials. It is defined as

$$x_p = -\cos\left(p\frac{\pi}{N}\right), \qquad p = 0,\ldots,N. \tag{3.14}$$

Since it is a technique of interpolation, it can also be expressed in terms of Lagrange polynomials of degree *N* as

$$\phi(x) = \sum_{p=0}^{N} a_p l_p^N(x) = \sum_{p=0}^{N} \hat{a}_p T_p(x), \tag{3.15}$$

where $l_p^N(x)$ is Lagrange polynomial of degree *N* defined by

$$l_p^N(x) = \prod_{i=0, i\neq p}^{N} \frac{x - x_i}{x_p - x_i}, \qquad p = 0,\ldots,N, \tag{3.16}$$

and a_p and $\hat{a}_p$ are unknown coefficients. $\hat{a}_p$ is known as pseudo-spectrum of the function $\phi(x)$ defined by

$$\hat{a}_p = \frac{2}{Nc_p} \sum_{i=0}^{N} \frac{1}{c_i} T_p(x_i) a_p, \qquad p = 0,\ldots,N. \tag{3.17}$$

with

$$c_p = \begin{cases} 2, & p = 0, N \\ 1, & otherwise \end{cases}. \tag{3.18}$$

The spatial derivative of the function $\phi(x)$ at the Chebyshev collocation points x_p is calculated using the derivatives of the Lagrange polynomials as

$$\phi^{'}(x_i) = \sum_{p=0}^{N} D_{ip} a_p = \sum_{p=0}^{N} \hat{D}_{ip} \hat{a}_p . \; i = 0,..., N, \tag{3.19}$$

where D is the Chebyshev collocation derivative matrix discussed in Section. 3.3.6, $\hat{D}$ is differentiation matrix in the pseudo-spectral space.

The relationship between D and $\hat{D}$ can be found using equation (3.17) and is given as

$$\hat{D} = T^{-1} \, D \, T, \tag{3.20}$$

where the matrix T and its inverse are given by

$$T_{pn} = T_n(x_p) = (-1)^n \cos\left(pn\frac{\pi}{N} \right), \; \left(T^{-1}\right)_{np} = \frac{2(-1)^n}{Nc_n c_p} \cos\left(pn\frac{\pi}{N} \right). \; p = 0,..., N. \tag{3.21}$$

The matrix form of equation (3.19) can be written as

$$U^{'} = D_N A = \hat{D}_N \hat{A}, \tag{3.22}$$

where $U = (\phi(x_0),... \; ,\phi(x_N))^t$, $A = (a_0,... \; ,a_N)^t$ and $\hat{A} = (\hat{a}_0,... \; ,\hat{a}_N)^t$.

The higher order derivatives are given as

$$U^k = D_N^k . A = \hat{D}_N^k . \hat{A}, \tag{3.23}$$

where D_N^k is the kth-order Chebyshev collocation derivative matrix and $\hat{D}_N^k$ can be obtained easily from the relation (3.20).

3.3.2 Two-Dimensional Chebyshev Polynomials of the First-Kind

Let us define a $(N+1)^2$ set of two-dimensional Chebyshev polynomials of the first-kind as

$$T_{pq}(x, y) = T_p(x) T_q(y), \qquad p = 0,..., N. \tag{3.24}$$

These polynomials are also orthogonal with respect to weight function $w(x,y)=\dfrac{1}{\sqrt{1-x^2}\sqrt{1-y^2}}$ on the interval $[-1,1]\times[-1,1]$ as

$$\left\langle T_{pq}(x,y),T_{rs}(x,y)\right\rangle=\int_{-1}^{1}\int_{-1}^{1}T_{pq}(x,y)\,T_{rs}(x,y)\,w(x,y)dxdy=\begin{cases}\pi^2/4, p=r\neq 0, q=s\neq 0\\ \pi^2/2, p=r=0, q=s\neq 0\\ \pi^2/2, p=r\neq 0, q=s=0\\ \pi^2, \quad p=r=0, q=s=0\\ 0, \qquad otherwise\end{cases},\tag{3.25}$$

3.3.3 Two-Dimensional Chebyshev Spectral Collocation Method

Similar to a one-dimensional problem, the Chebyshev polynomials approximation can be extended for more variables. Let us consider a two-dimensional function $\phi(x,y)$ on the physical space $[-1,1]\times[-1,1]$, which can be approximated as

$$\phi(x,y)=\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}a_{pq}\,l_{pq}(x,y)=\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\hat{a}_{pq}\,T_{pq}(x,y).\tag{3.26}$$

As one-dimensional case here also first $(N_x+1)\times(N_y+1)$ terms are considered to approximate a two-dimensional function as

$$\phi(x,y)=\sum_{p=0}^{N_x}\sum_{q=0}^{N_y}a_{pq}\,l_{pq}^{N_xN_y}(x,y)=\sum_{p=0}^{N_x}\sum_{q=0}^{N_y}\hat{a}_{pq}\,T_{pq}(x,y),\quad p=0,...,N_x,\text{ and } q=0,...,N_y.\tag{3.27}$$

or

$$\phi(x,y)=\sum_{p=0}^{N_x}\sum_{q=0}^{N_y}a_{pq}\,l_p^{N_x}(x)l_q^{N_y}(y)=\sum_{p=0}^{N_x}\sum_{q=0}^{N_y}\hat{a}_{pq}\,T_p(x)T_q(y),\ p=0,...,N_x,\text{ and } q=0,...,N_y,\tag{3.28}$$

which can be collocated with discrete Chebyshev Gauss-Lobatto points defined as

$$x_p=-\cos\left(p\frac{\pi}{N_x}\right),\ p=0,...,N_x,\qquad y_q=-\cos\left(q\frac{\pi}{N_y}\right),\ q=0,...,N_y,\tag{3.29}$$

where a_{pq} and $\hat{a}_{pq}$ are unknown coefficients. $\hat{a}_{pq}$ is the two-dimensional pseudo-spectrum of the function $\phi(x, y)$ given by

$$\hat{a}_{pq} = \frac{4}{N_x N_y c_p c_q} \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \frac{1}{c_i c_j} T_p(x_i) T_q(y_j) a_{pq}, \; p = 0,..., N_x, \text{ and } q = 0,..., N_y. \tag{3.30}$$

The spatial derivative of the two-dimensional function is discussed later in Section. 3.3.6.

3.3.4 Shifted Chebyshev Polynomials of the First-Kind

The first kind Chebyshev polynomials can be defined in any given finite range $[a,b]$ of x by making this range corresponding to the range $[-1,1]$ taking the transformation as

$$z = \frac{2x-(a+b)}{b-a} \tag{3.31}$$

Thus the shifted Chebyshev polynomials of the first kind are denoted by $T_n^*(x)$,

$$T_n^*(x) = T_n\left(\frac{2x-(a+b)}{b-a}\right). \tag{3.32}$$

This shifted Chebyshev polynomials of the first kind satisfy all the properties satisfied by the Chebyshev polynomials of the first kind and also satisfy the orthogonal condition as similar to Chebyshev polynomial with respect to weight function $w^*(x)$ corresponding to the interval $[a,b]$. It may be generated through the recurrence relation given by

$$T_n^*(x) = 2\left(\frac{2x-(a+b)}{b-a}\right)T_{n-1}^*(x) - T_{n-2}^*(x), \qquad n = 2,3,...; \tag{3.33}$$

with $T_0^*(x) = 1, T_1^*(x) = \dfrac{2x-(a+b)}{b-a}$.

3.3.5 Chebyshev Collocation Spectral Method Correspond to the Shifted Chebyshev Polynomials

A two-dimensional function $\phi(x, y)$ can be approximated by shifted Chebyshev polynomials of the first kind on any arbitrary physical space $[a_1, b_1]\times[a_2, b_2]$ as similar to Chebyshev polynomials of the first kind as

$$\phi(x,y)=\sum_{p=0}^{N_x}\sum_{q=0}^{N_y} a_{pq}\, l_{pq}^{N_x N_y}(x,y)=\sum_{p=0}^{N_x}\sum_{q=0}^{N_y}\hat{a}_{pq}\, T_{pq}^{*}(x,y),\ p=0,...,N_x,\ \text{and}\ q=0,...,N_y. \quad (3.34)$$

or

$$\phi(x,y)=\sum_{p=0}^{N_x}\sum_{q=0}^{N_y} a_{pq}\, l_p^{N_x}(x) l_q^{N_y}(y)=\sum_{p=0}^{N_x}\sum_{q=0}^{N_y}\hat{a}_{pq}\, T_p^{*}(x)T_q^{*}(y),\ p=0,...,N_x,\ \text{and}\ q=0,...,N_y. \quad (3.35)$$

which may collocate at discrete Chebyshev Gauss-Lobatto points on the space $[a_1, b_1]\times[a_2, b_2]$ defined as

$$x_p=-\frac{(b_1-a_1)}{2}\cos\left(p\frac{\pi}{N_x}\right)+\frac{a_1+b_1}{2},\ p=0,...,N_x,\ \text{and}$$

$$y_q=-\frac{(b_2-a_2)}{2}\cos\left(q\frac{\pi}{N_y}\right)+\frac{a_2+b_2}{2},\ q=0,...,N_y, \quad (3.36)$$

where $\hat{a}_{pq}$ is the two-dimensional pseudo-spectrum of the function $\phi(x, y)$ defined by

$$\hat{a}_{pq}=\frac{4}{N_x N_y c_p c_q}\sum_{i=0}^{N_x}\sum_{j=0}^{N_y}\frac{1}{c_i c_j}T_p^{*}(x_i)T_q^{*}(y_j)\, a_{pq},\qquad p=0,...,N_x,\ \text{and}\ q=0,...,N_y. \quad (3.37)$$

3.3.6 Derivative Matrix

The first-order Chebyshev collocation derivative matrix (Guo et al. (2012)) at $(N+1)\times(N+1)$ grid points is defined as

$$D_N=[d_{ij}]_{0\le i,j\le N}$$

with

$$[d_{ij}]_{0\le i,j\le N} = \begin{cases} d_{ij} = \dfrac{c_i(-1)^{i+j}}{c_j(x_i - x_j)}, \; for\, i \ne j \\ d_{ii} = -\dfrac{x_i}{2(1-x_i^2)}, \; for 1 \le i \le N-1 \\ d_{00} = \dfrac{2N^2+1}{6} = -d_{NN}, \end{cases} \tag{3.38}$$

To minimize the round-off errors during the calculation of first derivatives, one can use correction technique given by Bayliss et al. (1995) in which the diagonal entries are given as

$$D_{ii} = \sum_{\substack{j=0 \\ j\ne i}}^{N} D_{ij}. \tag{3.39}$$

The use of this technique will improve the accuracy in getting the higher-order derivatives. The second-order derivative (Peyret (2002)) can be defined as

$$D_N^2 = D_N . D_N = \begin{cases} \dfrac{(-1)^{i+j}}{c_j} \dfrac{x_i^2 + x_i x_j - 2}{(1-x_i^2)(1-x_j^2)}, & 1 \le i \le N-1, 0 \le j \le N, i \ne j \\ -\dfrac{(N^2-1)(1-x_i^2)+3}{3(1-x_i^2)^2}, & 1 \le i = j \le N-1 \\ \dfrac{2(-1)^j}{3c_j} \dfrac{(2N^2+1)(1-x_j)-6}{(1-x_j)^2}, & i = 0, 1 \le j \le N \\ \dfrac{2(-1)^{j+N}}{3c_j} \dfrac{(2N^2+1)(1-x_j)-6}{(1+x_j)^2}, & i = N, 1 \le j \le N-1 \\ \dfrac{N^4-1}{15}, & i = j = 0, i = j = N \end{cases} \tag{3.40}$$

The *n*th-order derivative matrix D_N^n is equal to the product of D_N in *n*-times, i.e., $D_N^n = D_N \times D_N \times ... n - times$. The main difficulty arises when we go from one-dimensional case to two-dimensional case to find the derivative matrix, and it is not as simpler as the one-dimensional case. To find the derivative matrix for two-dimensional case, Kronecker product comes into the picture. The first-order partial derivative relative to first space variable is obtained by using Kronecker product between I_{N_y} and

D_{N_x} denoted by $I_{N_y} \otimes D_{N_x}$ where I_{N_y} is the identity matrix of order N_y. The partial derivative related to second space variable is obtained by using the Kronecker product between D_{N_y} and I_{N_x} and denoted by $D_{N_y} \otimes I_{N_x}$. The same procedure is followed to obtain the higher order derivative matrix for the two-dimensional case in which D_N is replaced by its higher-order derivative as the one-dimensional case. For example, $I_{N_y} \otimes D_{N_x}^n$ denotes the *n*th-order partial derivative with respect to first space variable and $D_{N_y}^n \otimes I_{N_x}$ denotes the *n*th-order partial derivative with respect to second space variable. The mixed-order derivative, i.e., *m*th-order in first variable and *n*th-order in the second variable, is followed by Kronecker product $D_{N_x}^m \otimes D_{N_y}^n$.

3.3.7 Derivative Matrix Corresponding to the Shifted Chebyshev Polynomials of First-Kind defined over the Interval $[-l_x, l_x]$ and the Physical Space $[-l_x, l_x] \times [-l_y, l_y]$

The above discussed derivative matrix is only valid over the interval $[-1,1]$ and the physical space $[-1,1] \times [-1,1]$ for the one-dimensional case and two-dimensional case, respectively. For one-dimensional case, if the given interval of interest is of the form $[-l_x, l_x]$, then the first order derivative matrix is given as $\frac{1}{l_x} D_N$, i.e., the first-order derivative matrix D_N is simply multiplied by the inverse of the half of the length of interval $(1/l_x)$. The *n*th-order derivative matrix is given by $\frac{1}{l_x^n} D_N^n$. For two-dimensional case, if the given physical space of interest is $[-l_x, l_x] \times [-l_y, l_y]$ then the first-order partial derivative matrix corresponding to first space variable is given by $\frac{1}{l_x} I_{N_y} \otimes D_{N_x}$, and the first-order partial derivative matrix corresponding to the second space variable is given by $\frac{1}{l_y} D_{N_y} \otimes I_{N_x}$. The same procedure is followed to compute the *n*th-order partial derivative matrix for two-dimensional problem by replacing the l_x, l_y, D_{N_x}, and D_{N_y} by $l_x^n, l_y^n, D_{N_x}^n$, and $D_{N_y}^n$, respectively. The mixed order partial derivative matrix, i.e., *m*th-order in first space variable and *n*th-order in second space variable, is given by $\frac{1}{l_x^m l_y^n} D_{N_x}^m \otimes D_{N_y}^n$.

3.3.8 Derivative Matrix Corresponding to the Shifted Chebyshev Polynomials of First-Kind defined over the Interval $[a,b]$ and the Physical Space $[a_1,b_1]\times[a_2,b_2]$

From the above discussion, it is clear that for any arbitrary interval like $[a,b]$ the first-order derivative matrix for the one-dimensional case is given as $\frac{2}{(b-a)} D_N$, i.e., first-order derivative matrix D_N given for the interval $[-1,1]$ is simply multiplied by the inverse of the half of the length of the interval. The *n*th-order derivative matrix is given by $\frac{2^n}{(b-a)^n} D_N^n$. For two-dimensional case, if the given physical space of interest is $[a_1,b_1]\times[a_2,b_2]$, then the partial first-order derivative matrix corresponding to first space variable is given by $\frac{2}{(b_1-a_1)} I_{N_y} \otimes D_{N_x}$ and the partial first-order derivative matrix corresponding to the second space variable is given by $\frac{2}{(b_2-a_2)} D_{N_y} \otimes I_{N_x}$. The same procedure is followed to compute the *n*th-order partial derivative matrix for two-dimensional problem by replacing the $\frac{2}{(b_1-a_1)}$, $\frac{2}{(b_2-a_2)}$, D_{N_x} and D_{N_y} by $\frac{2^n}{(b_1-a_1)^n}$, $\frac{2^n}{(b_2-a_2)^n}$, $D_{N_x}^n$ and $D_{N_y}^n$ respectively. The mixed-order partial derivative matrix, i.e., *m*th-order in first space variable and *n*th-order in second space variable, is given by $\frac{2^{m+n}}{(b_1-a_1)^m(b_2-a_2)^n} D_{N_x}^m \otimes D_{N_y}^n$.

3.4 Numerical Method

The considered solute transport system (3.5) can be re-written as

$$c_t = d_x c_{xx} + d_y c_{yy} - v_x c_x - v_y c_y - \lambda c \tag{3.41}$$

Let us approximate $c(x, y, t)$ toward finding the solution of the considered problem in the physical domain $(x, y) \in [a_1, b_1] \times [a_2, b_2]$ as

$$c(x, y, t) = \sum_{p=0}^{N_x}\sum_{q=0}^{N_y} c_{pq}\, l_p^{N_x}(x) l_q^{N_y}(y) = \sum_{p=0}^{N_x}\sum_{q=0}^{N_y} \hat{c}_{pq}\, T_p^*(x) T_q^*(y),\ p = 0,..., N_x,\ and\ q = 0,...N_y, \tag{3.42}$$

where $T_p^*(x)$ and $T_q^*(y)$ are shifted Chebyshev polynomials over the interval $[a_1, b_1]$ and $[a_2, b_2]$, respectively.

To overcome with the time derivative present on the left-hand side of the governing equation, let us use finite difference scheme as discussed in the monograph of Guo et al. (2012) as

$$c_t = \frac{\frac{3}{2}c^{k+1} - \left(2c^k - \frac{1}{2}c^{k-1}\right)}{\delta t}, \text{with } t = k\delta t \text{ and } k = 0,1,...,\infty. \tag{3.43}$$

Therefore, the time-discrete version of equation (3.41) is

$$\frac{\frac{3}{2}c^{k+1}-\left(2c^{k}-\frac{1}{2}c^{k-1}\right)}{\delta t}=d_x c_{xx}^{k+1}+d_y c_{yy}^{k+1}-v_x c_x^{k+1}-v_y c_y^{k+1}-\lambda c^{k+1},\ k=0,1,...,\infty. \quad (3.44)$$

or,

$$d_x c_{xx}^{k+1}+d_y c_{yy}^{k+1}-v_x c_x^{k+1}-v_y c_y^{k+1}-\lambda c^{k+1}-\frac{3}{2\delta t}c^{k+1}=-\frac{1}{\delta t}\left(2c^{k}-\frac{1}{2}c^{k-1}\right),\ k=0,1,...,\infty. \quad (3.45)$$

with the initial condition

$$c(x,y,0)=c^{(0)}(x,y)=c_0(x,y)\ . \quad (3.46)$$

The polynomial $c_0(x,y)$ can be determined by equation (3.42) together with the pseudo-spectrum relation given in equation (3.37). During numerical computation $c^{(-1)}(x,y)$ arising for $k=0$ is given as

$$c^{(-1)}(x,y)=c^{(0)}(x,y). \quad (3.47)$$

Equation (3.45) indicates that we evaluate equation (3.41) at the time $t=(k+1)\delta t$. This temporal scheme is unconditionally stable and accurate up to second order in time (Isaacson and Keller (1966); Canuto et al. (1988)).

Before discretizing the above equation at Chebyshev collocation points, we need to approximate $c_{xx}, c_{yy}, c_x,\ and\ c_y$ using Chebyshev differentiation matrix as discussed above. We get

$$c_{xx}\approx\left(\frac{2^2}{(b_1-a_1)^2}I_{N_y}\otimes D_{N_x}^2\right).C, \qquad c_{yy}\approx\left(\frac{2^2}{(b_2-a_2)^2}D_{N_y}^2\otimes I_{N_x}\right).C,$$

$$c_x\approx\left(\frac{2}{(b_1-a_1)}I_{N_y}\otimes D_{N_x}\right).C, \text{ and } c_y\approx\left(\frac{2}{(b_2-a_2)}D_{N_y}\otimes I_{N_x}\right).C, \quad (3.48)$$

where $C=[c_{pq}]^t\in M_{(N_x+1)(N_Y+1)\times 1}$ will denote the matrix representation of c_{pq} at Chebyshev collocation points defined as

$$C=(\underbrace{c_{00},\dots,c_{N_x0}},\underbrace{c_{01},\dots,c_{N_x1}},\dots,\dots,\underbrace{c_{0N_y},\dots,c_{N_xN_y}})^t, \tag{3.49}$$

in which each block corresponds to a given y position in C.

Equation (3.44) gives the matrix representation as

$$\left(E+F+G+H-(\lambda+\frac{3}{2\delta t})I\right).C^{k+1}=-\frac{1}{\delta t}\left(2C^k-\frac{1}{2}C^{k-1}\right), \tag{3.50}$$

where $E=d_x\left(\frac{2^2}{(b_1-a_1)^2}I_{N_y}\otimes D_{N_x}^2\right)$, $F=d_y\left(\frac{2^2}{(b_2-a_2)^2}D_{N_y}^2\otimes I_{N_x}\right)$,

$$G=-v_x\left(\frac{2}{(b_1-a_1)}I_{N_y}\otimes D_{N_x}\right),\ H=-v_y\left(\frac{2}{(b_2-a_2)}D_{N_y}\otimes I_{N_x}\right) \text{ and } I=I_{N_x}\otimes I_{N_y}. \tag{3.51}$$

The matrix representation (3.50) is taken only for inner elements of the matrix $C=[c_{pq}]$, which is corresponding to inner Chebyshev collocation points of space grid, i.e., those with $1\le i\le N_x-1$ and $1\le j\le N_y-1$ (Fig. 3.1). The boundary conditions are used to calculate c_{0q}, c_{N_xq}, c_{p0}, and c_{pN_y}, which are the outer elements corresponding to boundary Chebyshev collocation points of space grid.

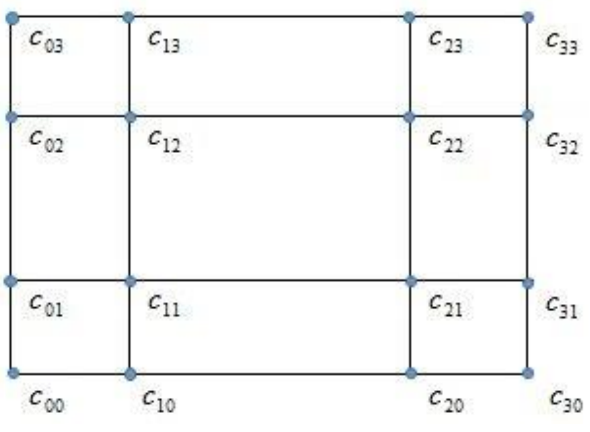

Fig. 3.1 Chebyshev Gauss-Lobatto grid for $N_x=3=N_y$ together with c_{pq}'s

3.4.1 Implementation of Boundary Conditions

General forms of boundary conditions are

$$\begin{cases} \alpha_1 c(a_1, y) + \beta_1 c_x(a_1, y) = f_1(y), \\ \alpha_2 c(b_1, y) + \beta_2 c_x(b_1, y) = f_2(y), \\ \alpha_3 c(x, a_2) + \beta_3 c_y(x, a_2) = f_3(x), \\ \alpha_4 c(x, b_2) + \beta_4 c_y(x, b_2) = f_4(x). \end{cases} \tag{3.52}$$

If $\alpha_i \neq 0, \beta_i = 0,$ then it simply denotes the Dirichlet boundary condition, if $\alpha_i = 0, \beta_i \neq 0,$ then it denotes the Neumann boundary condition and if $\alpha_i \neq 0, \beta_i \neq 0$ then it denotes the Robin boundary conditions.

For the implementation of given boundary conditions, let us first approximate it with considered approximation function given in equation (3.42) then collocate at Chebyshev collocation points given in equation (3.36). For c_x and c_y Chebyshev derivative matrix is used as discussed in Section 3.3.8. From here a matrix representation of considered boundary values is obtained which corresponds to boundary Chebyshev collocation points of space grid. The first two equations of (3.52) give c_{0q}, and $c_{N_x q}$, $0 \le q \le N_y$ and the last two equation of (3.52) give c_{p0}, and c_{pN_y}, $0 \le p \le N_x$. From here we get matrix form for given boundary conditions as

$$A.C = F, \tag{3.53}$$

where A is the matrix of the order $(N_x+1)(N_y+1) \times (N_x+1)(N_y+1)$ corresponding to the boundary points of space grid. C is the column matrix discussed in equation (3.49) and $F = [f_i]^t \in M_{(N_x+1)(N_Y+1)\times 1}$ is the column matrix corresponding to the R.H.S of equation (3.52).

The considered boundary conditions are

$$\begin{cases} \mathrm{c(x,y,t)} = \mathrm{c}_0,\ x = 0, -l_y < y < l_y, \\ \dfrac{\partial c}{\partial x} = 0, x = l_x, -l_y < y < l_y, \\ \dfrac{\partial c}{\partial y} = 0, y = -l_y, 0 < x < l_x, \\ \dfrac{\partial c}{\partial y} = 0, y = l_y, 0 < x < l_x. \end{cases}$$

If we take $N_x = 3 = N_y$, then the matrix form of the corresponding boundary conditions is

$$\begin{bmatrix}
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{bmatrix} . C = \begin{bmatrix} 0\\0\\0\\0\\c_i\\0\\0\\0\\0\\c_i\\0\\0\\0\\0\\0\\0 \end{bmatrix},$$

$$\frac{2}{l_x}\begin{bmatrix}
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&D_{30}&D_{31}&D_{32}&D_{33}&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
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0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{bmatrix} . C = \begin{bmatrix} 0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0 \end{bmatrix},$$

$$\frac{1}{l_y}\begin{bmatrix} D_{00} & 0 & 0 & 0 & D_{01} & 0 & 0 & 0 & D_{02} & 0 & 0 & 0 & D_{03} & 0 & 0 & 0 \\ 0 & D_{00} & 0 & 0 & 0 & D_{01} & 0 & 0 & 0 & D_{02} & 0 & 0 & 0 & D_{03} & 0 & 0 \\ 0 & 0 & D_{00} & 0 & 0 & 0 & D_{01} & 0 & 0 & 0 & D_{02} & 0 & 0 & 0 & D_{03} & 0 \\ 0 & 0 & 0 & D_{00} & 0 & 0 & 0 & D_{01} & 0 & 0 & 0 & D_{02} & 0 & 0 & 0 & D_{03} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} .C = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

$$\frac{1}{l_y}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ D_{30} & 0 & 0 & 0 & D_{31} & 0 & 0 & 0 & D_{32} & 0 & 0 & 0 & D_{33} & 0 & 0 & 0 \\ 0 & D_{30} & 0 & 0 & 0 & D_{31} & 0 & 0 & 0 & D_{32} & 0 & 0 & 0 & D_{33} & 0 & 0 \\ 0 & 0 & D_{30} & 0 & 0 & 0 & D_{31} & 0 & 0 & 0 & D_{32} & 0 & 0 & 0 & D_{33} & 0 \\ 0 & 0 & 0 & D_{30} & 0 & 0 & 0 & D_{31} & 0 & 0 & 0 & D_{32} & 0 & 0 & 0 & D_{33} \end{bmatrix} .C = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

These boundary conditions along with equation (3.50) give a system of linear equations which completely describe the considered problem. From here the unknown coefficients c_{pq} are obtained and use those in equation (3.42) to get the approximate solution of the considered problem.

3.5 Numerical Results and Discussion

The numerical values of normalized solute concentration $c(x, y, t)/c_0$ in the two-dimensional finite-length homogeneous porous medium system for different time are calculated for both conservative $(\lambda = 0)$ and non-conservative $(\lambda \neq 0)$ systems with c_0 being equal to unity. During numerical computation, a porous medium is assumed with the following arbitrary transport parameters: $d_x = 25 cm^2/day,\ \ d_y = 5 cm^2/day,$ $v_x = 50 cm/day,\ \ v_y = 0,$ for the conservative system and for the non-conservative system in the physical space $\Omega \in [0,40] \times [-10,10]$. The inlet concentration is $c_i = 1 mg/cm$. The graphical plots of normalized concentration $c(x, y, t)/c_0$ vs. physical domain (x, y) are depicted through Fig. 3.2(a) – (d) for the conservative system and through Fig. 3.3(a) – (d) for the non-conservative system at various time $t = 0.25, 0.5, 0.75$ and 1 day. Figures 3.4 and 3.5 show the comparisons at different time levels for conservative and non-conservative systems, respectively. Figure 3.6 shows the comparison between conservative and non-conservative system at $t = 0.5$ day which shows that the rate of transportation for the non-conservative system $(\lambda \neq 0)$ is less compared to the conservative system $(\lambda = 0)$ due to the effect of reaction term.

It is seen from the figures that the solute covers the more space in both the directions as time increases which is physically justified. Also, it is clear from the graphs that the slope of planes is going to be more flat as time increases due to the prior existence of solute concentration in the physical space, i.e., it moves towards the saturation. Fig. 3.7(a) – (d) and Fig. 3.8(a) – (d) show the nature of the normalized concentration $c(x, y, t)/c_0$ based on similar choices of parameters for fixed $y = 10$ cm at a various time $t = 0.25, 0.5, 0.75$ and 1 day for conservative and non-conservative systems, respectively. Figures 3.9 and 3.10 show the comparisons for $y = 10$ cm at different time levels for conservative and non-conservative systems, respectively.

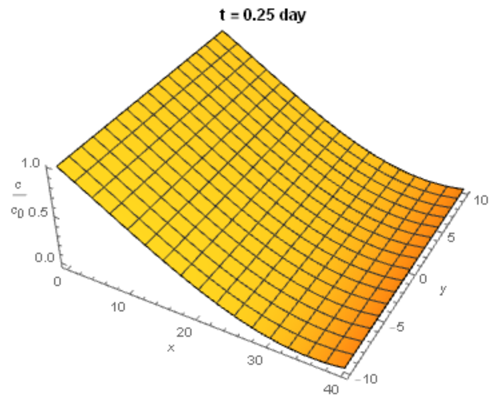

Fig. 3.2(a)

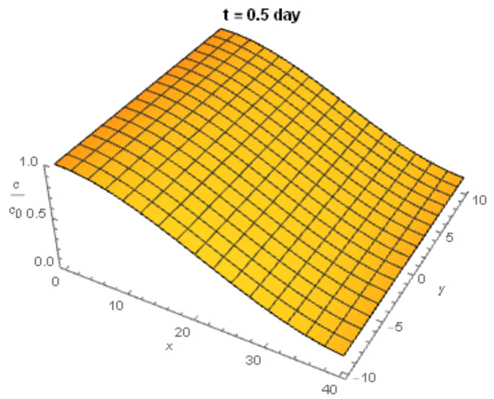

Fig. 3.2(b)

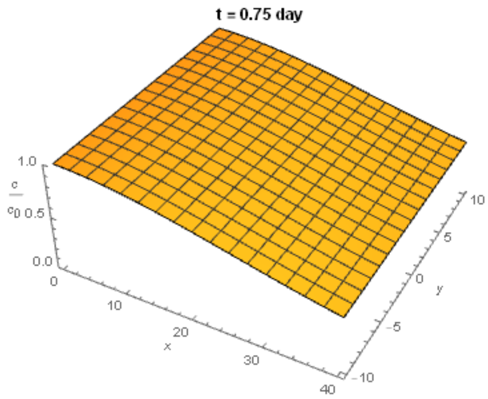

Fig. 3.2(c)

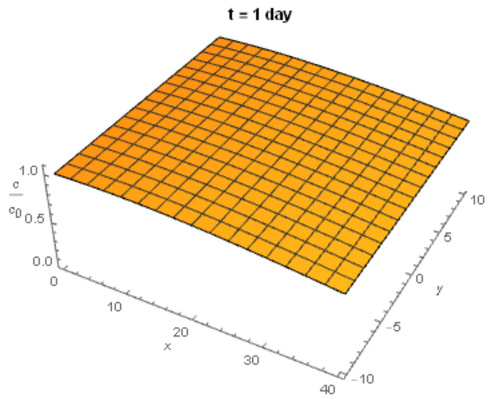

Fig. 3.2(d)

Fig. 3.2 Normalized concentration distributions for conservative system at different time levels (a) $t = 0.25$day, (b) $t = 0.5$day, (a) $t = 0.75$day, (a) $t = 1$day

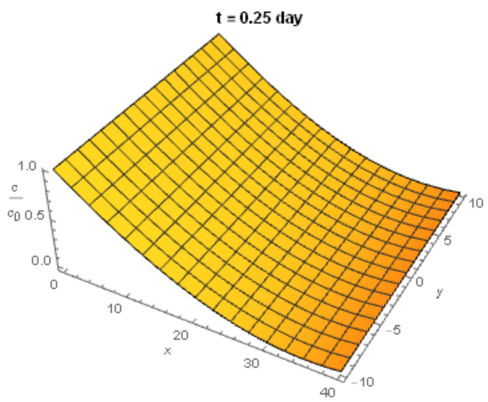

Fig. 3.3(a)

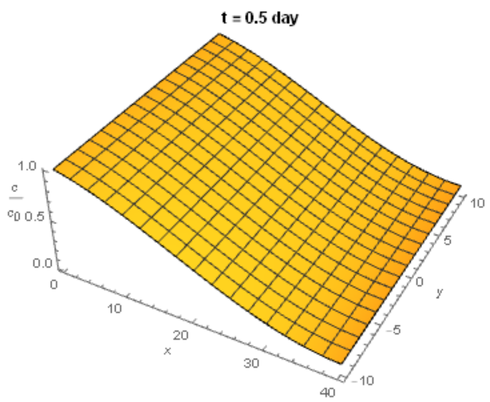

Fig. 3.3(b)

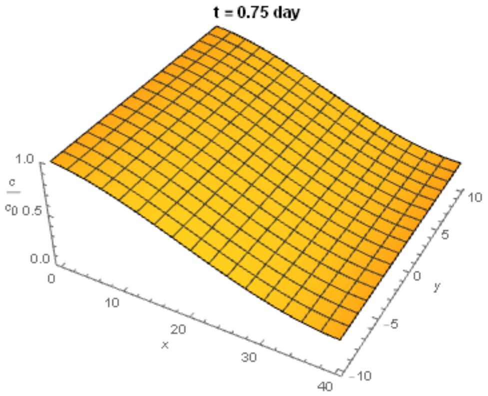

Fig. 3.3(c)

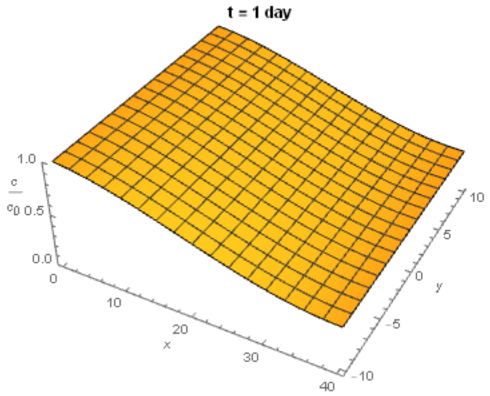

Fig. 3.3(d)

Fig. 3.3 Normalized concentration distributions for non-conservative system at different time levels (a) $t = 0.25$day, (b) $t = 0.5$day, (a) $t = 0.75$day, (a) $t = 1$day

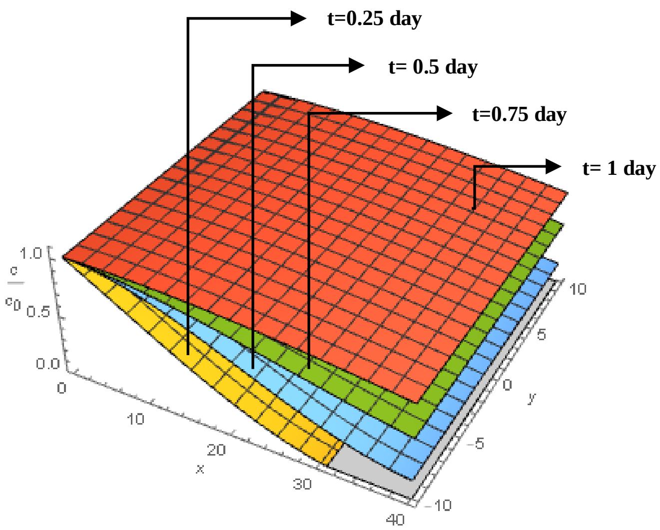

Fig. 3.4 Comparison of normalized concentration distributions for the conservative system at different time levels

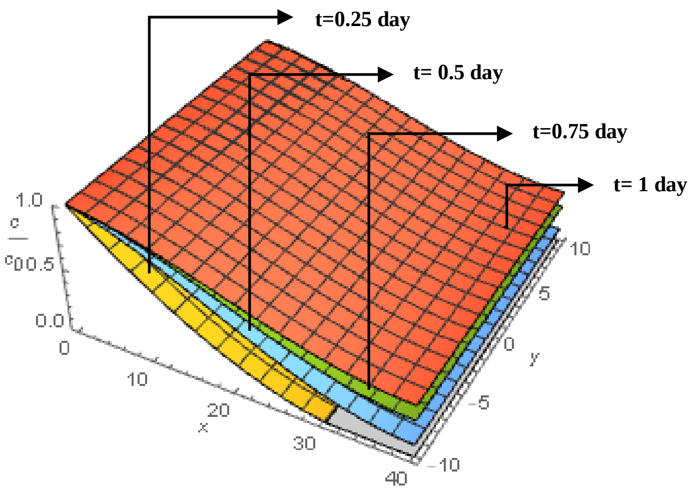

Fig. 3.5 Comparison of normalized concentration distributions for the non-conservative system at different time levels

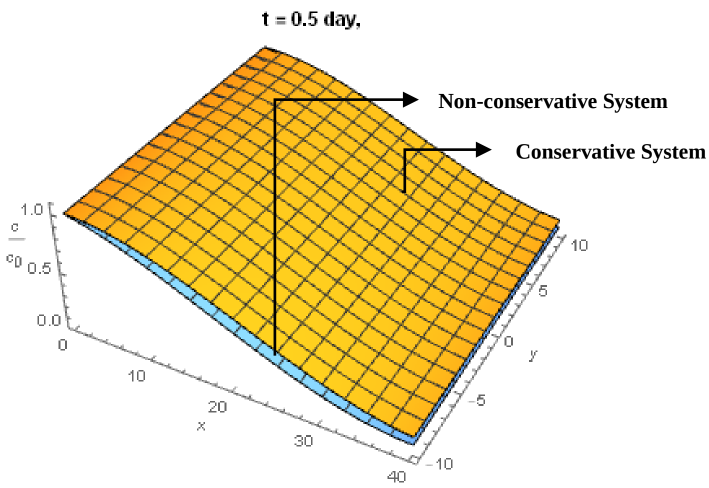

Fig. 3.6 Comparison between conservative and non-conservative system at $t = 5$ day

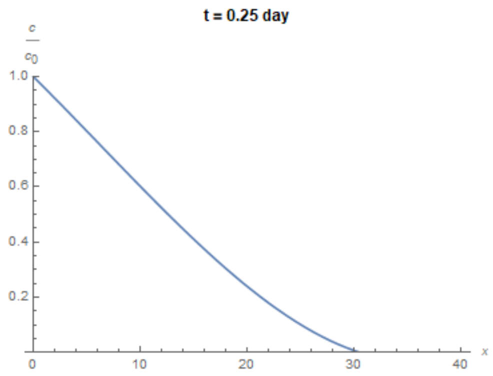

Fig. 3.7(a)

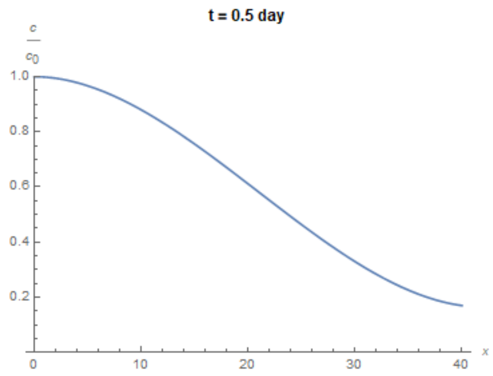

Fig. 3.7(b)

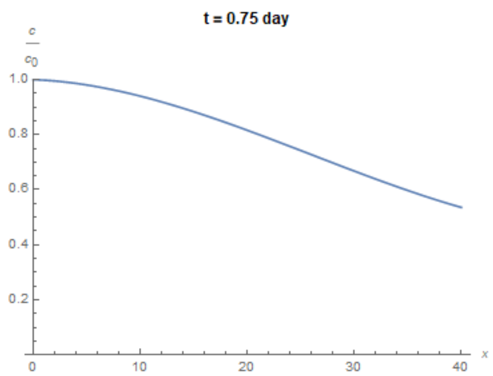

Fig. 3.7(c)

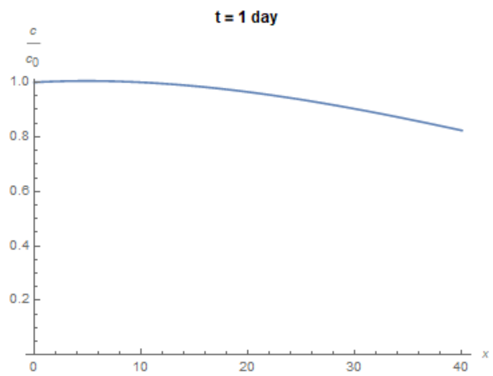

Fig. 3.7(d)

Fig. 3.7 Normalized concentration distributions for conservative system for $y = 10$ cm at different time levels (a) $t = 0.25$ day, (b) $t = 0.5$ day, (a) $t = 0.75$ day, (a) $t = 1$ day

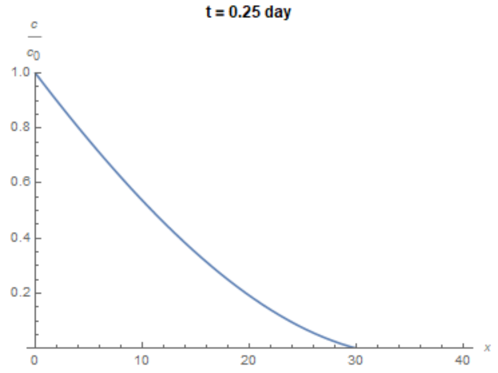

Fig. 3.8(a)

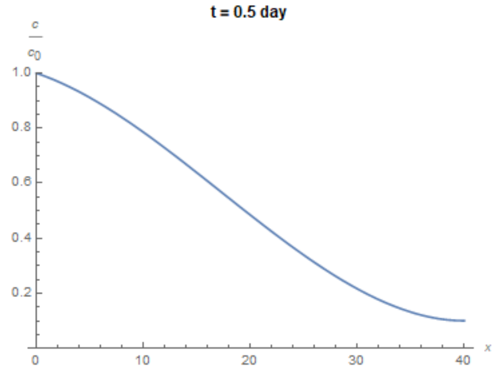

Fig. 3.8(b)

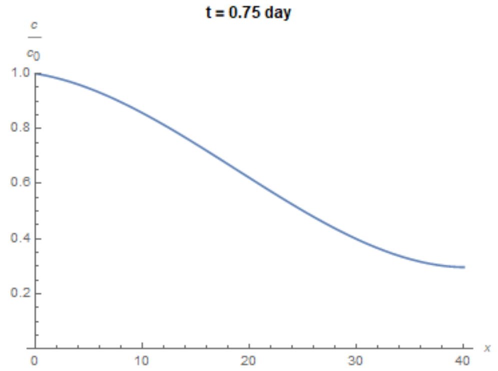

Fig. 3.8(c)

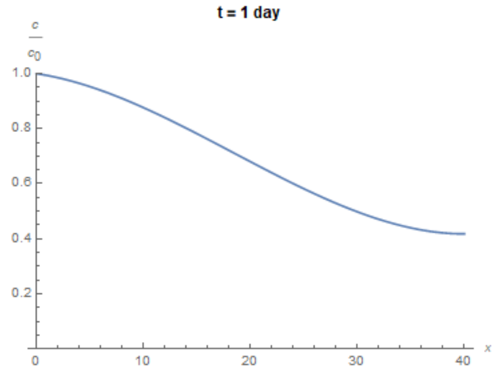

Fig. 3.8(d)

Fig. 3.8 Normalized concentration distributions for non-conservative system for $y = 10$ cm at different time levels (a) $t = 0.25$ day, (b) $t = 0.5$ day, (a) $t = 0.75$ day, (a) $t = 1$ day

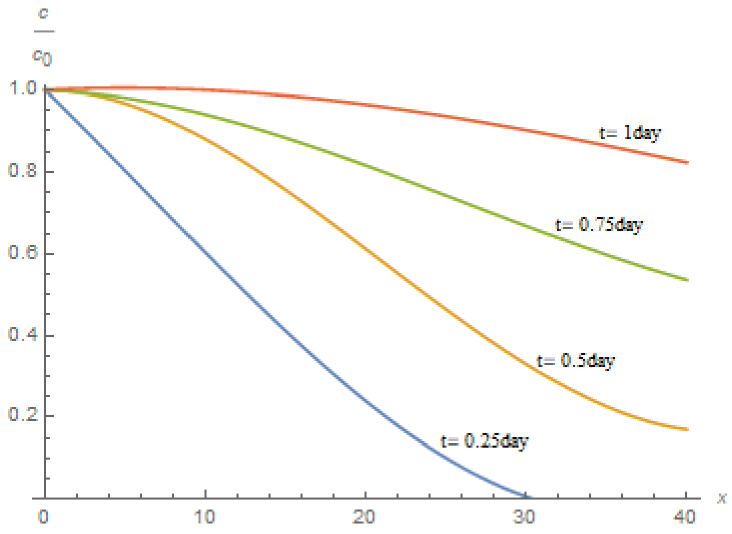

Fig. 3.9 Normalized concentration distributions for a conservative system for $y = 10$ cm at different time levels

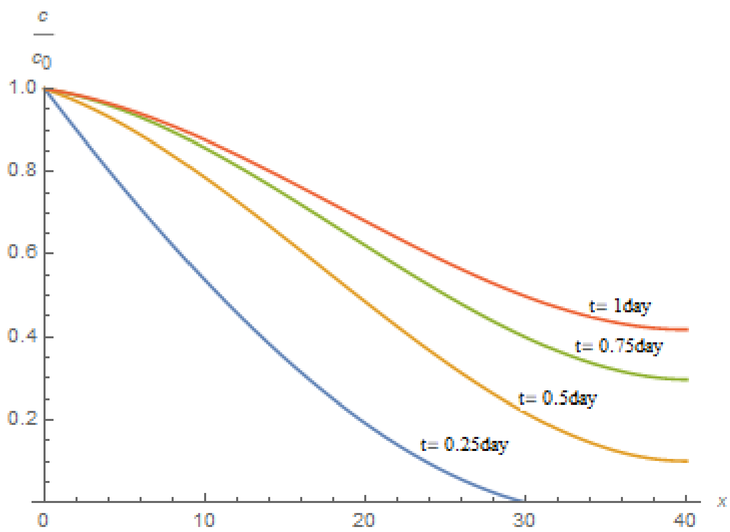

Fig. 3.10 Normalized concentration distributions for a non-conservative system for $y = 10$ cm at different time levels

3.6 Conclusions

Through the present scientific contribution, five goals have been achieved. First one is the effective use of shifted Chebyshev polynomials of the first kind. Second one is the derivation of the Chebyshev differentiation matrix in an arbitrary physical space. Third one is the effective use of Chebyshev differentiation matrix to overcome the spatial derivative. Fourth one is the use of unconditionally stable difference scheme to overcome the temporal derivative. The last one is the graphical exhibition of the lesser rate of transportation for non-conservative system compared to the conservative system due to the effect of sink term.