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

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Abstract In this study, the numerical solution of the two-dimensional solute transport system in a homogeneous porous medium of finite length is obtained. The considered transport system has the terms accounting for advection, dispersion and first-order decay with first-type source boundary conditions. Initially, the aquifer is considered solute free, and a constant input concentration is considered at inlet boundary. The solution is describing the solute concentration in rectangular inflow region of the homogeneous porous media. The numerical solution is derived using a powerful method, viz. spectral collocation method. The numerical computation and graphical presentations exhibit that the method is effective and reliable during the solution of the physical model with complicated boundary conditions even in the presence of reaction term.

Keywords Two-dimensional solute transport system · Spectral collocation method · Chebyshev polynomials · Chebyshev differentiation matrix

1 Introduction

It is known fact that the 70% area of the planet is covered by water, of which only 3% is fresh water, more than two third of its covered by the glacier and ice caps. So the groundwater is one of the most important source of freshwater toward the fulfillment of basic needs like agriculture, industries and also as an important source of drinking water in both urban and rural areas. For drinking water, half of the population of USA depends on groundwater. Ninety-seven percent of freshwater comes from groundwater. Unfortunately, it is persuadable to pollutants. The source of groundwater contaminations can be natural or human activities. The natural

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contamination depends on material through which the groundwater moves. During movement, it may pick up a wide range of compounds such as magnesium, calcium and chlorides. Naturally occurring minerals and metallic deposits in rock and soil also create groundwater contamination. Manmade products like gasoline, oil, road salts and chemicals get mingled with groundwater and create groundwater contamination. Due to the increase in population, it is overexploited and thus contaminated by various point and non-point sources like storage tank, disposal sites, industry waste disposal sites, accidental spills, leaking gasoline, landfills, fertilizers, pesticides and herbicides (Fried 1975; USEPA 1989, 1990; Anderson and Woessner 1992; Charbeneau 2000; Kebew 2001; Sharma and Reddy 2004; Rai 2004; Rausch et al. 2005; Thangarajan 2007). Near the coast, a vacuum is created by over pumping an aquifer which can quickly be filled up with salty seawater, due to which water supply may become undrinkable and useless for irrigation. Groundwater pumping has exceeded the rate of replenishment. In our country, the contamination of groundwater is caused by human activities such as sewage disposal, refuse disposal, pesticides and use of fertilizers, industrial discharges, and toxic waste disposal. Improper management of groundwater resources is also a major issue leading to increase in the problem of drinking water and as a result the water level is getting down fast in several parts of India because of excessive extraction of groundwater as reported by National Water Policy (1987). Since non-point source materials are used over large area, it can have large impact on the water in an aquifer compared to point source. Contaminated groundwater is very harmful for environment, human health and widely effect the wildlife. It may not damage humans and animal health immediately but can be harmful after long-term exposure. Groundwater contamination through septic tank waste can have serious effects on human health. Various diseases like cancer, hepatitis and dysentery may be caused by polluted water. Different actions are being taken by different countries to remediate the surface and ground water. Compared to surface water, groundwater contamination is more difficult to abate because it can move very large distance in unseen aquifers. If groundwater is contaminated overall, then the rehabilitation is deemed to be too difficult and expensive. And as a result, it may become unusable for decades. Then, finding the other source of water is the only option which is seen impossible.

The declination of groundwater has increased research interests in the field of solute transport by porous media (Bear 1972; Vafai 2005), since most of the structure through which groundwater moves is porous type structure. Through the advection and dispersion processes, pollutants create a contaminant plume within an aquifer, the movement of which in an aquifer is described by transport model. One of the very rich transport model is advection–dispersion equation which is used to describe the transport phenomena in different fields of science and engineering such as chemical science, thermal science and hydrology with varying initial and boundary conditions (Javandel et al. 1984; Bear and Verruijt 1987; Rao 1995; Rai 2004). The advection–dispersion equation can be also derived from mass balance principles, which is very much useful to describe transport in natural soils. Solute transport modeling is helpful to predict the solute concentration in aquifers, rivers, lakes and streams too. The general transport equation is

$$\frac{\partial c}{\partial t} = \nabla \cdot (d \nabla c) - \nabla \cdot (vc) + R, \tag{1}$$

where c describes the species concentration for mass transfer problem and temperature for heat transfer problem, d is the mass diffusivity for particle motion and thermal diffusivity for heat transfer, v is the average velocity and for flows in porous media v is the superficial velocity, and R is the source or sink of c.

Adequate literature is available on the topics like groundwater hydrology, fluid mechanics, hydraulics, chemical engineering and environmental engineering on the dispersion of pollutants in general (Marino 1978; Latinopoulos et al. 1988; Aral and Tang 1992; Chen et al. 1996; Kumar and Kumar 2002). Thus, lot of researchers from different parts of the world were involved to tackle this physically relevant model analytically and numerically. A large number of analytical solutions are available for solving these problems (Carslaw and Jaeger 1971; Cleary and Adrian 1973; Cleary and Ungs 1978; Van Genucheten and Alves 1982; Kumar 1983; Carnahan and Remer 1984; Barry and Sposito 1989; Lindstrom and Boersma 1989; Leij and Dane 1990; Chrysikopoulos 2011; Basha and El-Habel 1993; Fry et al. 1993; Serrano 1995; Runkel 1996; Chrysikopoulos and Sim 1996; Flury et al. 1998; Sim and Chrysikopoulos 1999; Baeumer et al. 2001; Sanderson et al. 2006, 2009; Singh et al. 2008, 2009a, b, 2010; Srinivasan and Clement 2008; Kumar et al. 2010; Luce et al. 2013; Deville and Mojtabi 2014; Shen and Reible 2015). The analytical and experimental investigation of longitudinal and lateral dispersion in an isotropic porous medium is 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 discussed it for time-varying boundary conditions in the year 2010. Konikow (2010) used the method of characteristics to solve the groundwater transport models by applying dispersive changes in Lagrangian particles. Lugo-Mendez et al. (2015) has solved the transport model in homogeneous porous media by revisiting the up-scaling process of diffusive mass transfer of solute. 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). These solutions also solve the spatially variable advection–dispersion equation (Ebach and White 1958; Yates 1992; Fry et al. 1993; 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, b; Lee 1999; Dehghan 2004; Karahan 2006; Walter et al. 2007; Huang et al. 2008; Savović and Djordjevich 2012, 2013; Djordjevich and Savovic' 2013; Dhawan et al. 2012; Gebäck 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 1989; Batu 1989, 1993; Leij et al. 1991; Chrysikopoulos 1995; Aral and Liao 1996; Anderman et al. 1996; Tartakovsky and Federico 1977; Hunt 1998; Hantush and Marino 1998; Sim and Chrysikopoulos 1998; Zoppou and Knight 1999; Tartakovasky 2000; Park and Zhan 2001; Chen et al. 2003; Sander and Braddock 2005; Kumar et al. 2006; Massabò et al. 2006; Singh et al. 2010; Chen et al. 2011; Assumaning and Chang 2012; Yadav et al. 2012). Bruce (1970) conducted a series of two-dimensional dispersion experiments in a one and two layered porous medium with the combined effect of longitudinal and lateral dispersion which verified the theoretical and the numerical solution both of which describe the two-dimensional dispersion of a miscible, second fluid through a unidirectional, seepage flow. 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 the few research works in conservative system have already been done, the literature on non-conservative systems related to two-dimensional problem is not available.

In this article, one of the powerful methods, viz., spectral collocation method (Canuto et al. 1988; Boyd 2000; Trefethen 2000), is used to find the numerical solution of a two-dimensional solute transport system in non-conservative case. The reason behind choosing this powerful method is its exponential rate of convergence due to which it provides highly accurate solutions to linear/nonlinear differential equations even using a small number of grids. Using this method, first the solution of the considered problem is approximated as a sum of certain basic functions like orthonormal functions and as a result accurate difference between the exact solution and approximate solution can be shown. The choice of collocation points in this method are most important for the convergence and efficiency of the collocation approximation. The considered 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 Problem Formulation

For more general case, Eq. (1) takes place in three space dimensions, but for numerical 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 time-dependent advection–dispersion reaction equation in space–time domain $\Omega \times I$, where $\Omega \subseteq \Re^2$, Γ is the boundary of Ω, and $I = (0, T)$ is described as

$$\frac{\partial c}{\partial t} = \nabla \cdot (d \nabla c) - \nabla \cdot (vc) - \lambda c \text{ in } \Omega \times I, \tag{2}$$

with initial condition

$$c(x, y, 0) = c_0(x, y) \text{ in } \Omega, \tag{3}$$

and boundary conditions

$$c(x, y, t) = f_- \text{ on } (\Gamma \times I)_-, \tag{4}$$

$$c(x, y, t) = f_+ \text{ or } \partial_n c(x, y, t) = f_+ \text{ on } (\Gamma \times I)_+, \tag{5}$$

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 $(\Gamma \times I)$.

Equation (2) in two-dimensional form can be written as

$$\frac{\partial c}{\partial t} = d_x \frac{\partial^2 c}{\partial x^2} + d_y \frac{\partial^2 c}{\partial y^2} - v_x \frac{\partial c}{\partial x} - v_y \frac{\partial c}{\partial y} - \lambda c, \tag{6}$$

with boundary conditions

$$c(x, y, t) = c_0, \quad x = 0, -l_y < y < l_y, \tag{7}$$

$$\frac{\partial c}{\partial x} = 0, \quad x = l_x, -l_y < y < l_y, \tag{8}$$

$$\frac{\partial c}{\partial y} = 0, \quad y = -l_y, 0 < x < l_x, \tag{9}$$

$$\frac{\partial c}{\partial y} = 0, \quad y = l_y, 0 < x < l_x, \tag{10}$$

and initial condition

$$c(x, y, 0) = 0, \qquad 0 < x < l_x, -l_y < y < l_y, \tag{11}$$

where d_x, d_y, v_x, v_y, λ and c_0 are constants.

3 Preliminaries

3.1 One-Dimensional Chebyshev Polynomials of the First Kind

The Chebyshev polynomials $T_n(x)$ of the first kind of degree n in x are defined on the interval $[-1, 1]$ as

$$T_n(x) = \cos(n \cos^{-1} x), \tag{12}$$

where $x = \cos\theta$ and $\theta \in [0, \pi]$ (Mason 1993; Mason and Handscomb 2003). The polynomials $T_n(x)$ are orthogonal on $[-1, 1]$ with respect to the inner products

$$\langle T_{\mathrm{n}}(x), T_m(x)\rangle = \int_{-1}^{1} \frac{T_n(x)T_m(x)}{\sqrt{1-x^2}}\mathrm{d}x = \begin{cases} 0, & n \neq m, \\ \pi, & n = m = 0 \\ \pi/2 & n = m, \end{cases} \tag{13}$$

where $\frac{1}{\sqrt{1-x^2}}$ is weight function.$T_n(x)$ may be generated by using the recurrence relations

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x), \quad n = 2, 3, \ldots \tag{14}$$

with $T_0(x) = 1,\ T_1(x) = x.$

3.2 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

$$\phi(x) = \sum_{p=0}^{\infty} \hat{a}_p T_p(x)., \tag{15}$$

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

$$\phi(x) = \sum_{p=0}^{N} \hat{a}_p T_p(x). \tag{16}$$

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

$$x_p = -\cos\left(p\frac{\pi}{N}\right), \qquad p = 0, \ldots, N. \tag{17}$$

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

$$\phi(x) = \sum_{p=0}^{N} a_p l_p^N(x) = \sum_{p=0}^{N} \hat{a}_p T_p(x). \tag{18}$$

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

$$l_p^N(x) = \prod_{i=0, i\neq p}^{N} \frac{x - x_i}{x_p - x_i}, \quad p = 0, \ldots, N. \tag{19}$$

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

$$\hat{a}_p = \frac{2}{Nc_p} \sum_{i=0}^{N} \frac{1}{c_i} T_p(x_i) a_p, \quad p = 0, \ldots, N. \tag{20}$$

$$\text{with} \qquad c_p = \begin{cases} 2 & p = 0, N \\ 1 & \text{otherwise} \end{cases}. \tag{21}$$

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

$$\phi'(x_i) = \sum_{p=0}^{N} D_{ip} a_p = \sum_{p=0}^{N} \hat{D}_{ip} \hat{a}_p {\cdot} i = 0, \ldots, N, \tag{22}$$

where D is the Chebyshev collocation derivative matrix discussed later in Sect. 3.7 and $\hat{D}$ is differentiation matrix in the pseudo-spectral space.

The relationship between D and $\hat{D}$ can be found using Eq. (20) and given as

$$\hat{D} = T^{-1} D T, \tag{23}$$

where the matrix T and its inverse are given by

$$T_{pn} = T_n(x_p) = (-1)^n \cos\left(pn\frac{\pi}{N}\right), \left(T^{-1}\right)_{np} = \frac{2(-1)^n}{Nc_n c_p} \cos\left(pn\frac{\pi}{N}\right) .n,\, p = 0, \ldots, N. \tag{24}$$

The matrix form of Eq. (22) can be written as

$$U' = D_N A = \hat{D}_N \hat{A}, \tag{25}$$

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

The higher-order derivatives can be given as

$$U^k = D_N^k \cdot A = \hat{D}_N^k . \hat{A}, \tag{26}$$

where D_N^k is the kth-order Chebyshev collocation derivative matrix and $\hat{D}_N^k$ can be obtained easily from the relation (23).

3.3 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

$$T_{pq}(x, y) = T_p(x)T_q(y), \quad p, q = 0, \dots, N. \tag{27}$$

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

$$\langle T_{pq}(x, y), T_{rs}(x, y) \rangle = \int_{-1}^{1}\int_{-1}^{1} T_{pq}(x, y)T_{rs}(x, y)w(x, y)\mathrm{d}x\mathrm{d}y$$
$$= \begin{cases} \pi^2/4, & p = r \neq 0, q = s \neq 0 \\ \pi^2/2, & p = r = 0, q = s \neq 0 \\ \pi^2/2, & p = r \neq 0, q = s = 0 \\ \pi^2, & p = r = 0, q = s = 0 \\ 0, & \text{otherwise} \end{cases}, \tag{28}$$

3.4 Two-Dimensional Chebyshev Spectral Collocation Method

Similar to 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

$$\phi(x, y) = \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} a_{pq}l_{pq}(x, y) = \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} \hat{a}_{pq}T_{pq}(x, y). \tag{29}$$

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

$$\phi(x, y) = \sum_{p=0}^{N_x}\sum_{q=0}^{N_y} a_{pq}l_{pq}^{N_x N_y}(x, y)$$
$$= \sum_{p=0}^{N_x}\sum_{q=0}^{N_y} \hat{a}_{pq}T_{pq}(x, y), \quad p = 0, \dots, N_x \text{ and } q = 0, \dots, N_y \tag{30}$$

or

$$\phi(x, y) = \sum_{p=0}^{N_x}\sum_{q=0}^{N_y} a_{pq}l_p^{N_x}(x)l_q^{N_y}(y)$$
$$= \sum_{p=0}^{N_x}\sum_{q=0}^{N_y} \hat{a}_{pq}T_p(x)T_q(y), p = 0, \dots, N_x \text{ and } q = 0, \dots, N_y, \tag{31}$$

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

$$x_p = -\cos\left(p\frac{\pi}{N_x}\right), p = 0, \dots, N_x; \qquad y_q = -\cos\left(q\frac{\pi}{N_y}\right), \qquad q = 0, \dots, N_y, \tag{32}$$

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

$$\hat{a}_{pq} = \frac{4}{N_x N_y c_p c_q} \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \frac{1}{c_i c_j} T_p(x_i) T_q(y_j) a_{pq}, \; p = 0, \ldots, N_x \text{ and } q = 0, \ldots, N_y. \tag{33}$$

The spatial derivative of the two-dimensional functions is discussed later in Sect. 3.7.

3.5 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

$$z = \frac{2x - (a + b)}{b - a} \tag{34}$$

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

$$T_n^*(x) = T_n \left(\frac{2x - (a + b)}{b - a} \right). \tag{35}$$

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

$$T_n^*(x) = 2 \left(\frac{2x - (a + b)}{b - a} \right) T_{n-1}^*(x) - T_{n-2}^*(x), \quad n = 2, 3, \ldots \tag{36}$$

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

3.6 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 first kind on any arbitrary physical space $[a_1, b_1] \times [a_2, b_2]$ as similar to Chebyshev polynomials of first kind as

$$\begin{aligned} \phi(x, y) &= \sum_{p=0}^{N_x} \sum_{q=0}^{N_y} a_{pq} l_{pq}^{N_x N_y}(x, y) \\ &= \sum_{p=0}^{N_x} \sum_{q=0}^{N_y} \hat{a}_{pq} T_{pq}^*(x, y), \quad p = 0, \ldots, N_x \text{ and } q = 0, \ldots, N_y. \end{aligned} \tag{37}$$

or

$$\begin{aligned} \phi(x, y) &= \sum_{p=0}^{N_x} \sum_{q=0}^{N_y} a_{pq} l_p^{N_x}(x) l_q^{N_y}(y) \\ &= \sum_{p=0}^{N_x} \sum_{q=0}^{N_y} \hat{a}_{pq} T_p^*(x) T_q^*(y), \; p = 0, \ldots, N_x \text{ and } q = 0, \ldots, N_y, \end{aligned} \tag{38}$$

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

$$x_p = -\frac{(b_1 - a_1)}{2}\cos\left(p\frac{\pi}{N_x}\right) + \frac{a_1 + b_1}{2},\ p = 0, \ldots, N_x \text{ and}$$
$$y_q = -\frac{(b_2 - a_2)}{2}\cos\left(q\frac{\pi}{N_y}\right) + \frac{a_2 + b_2}{2},\ q = 0, \ldots, N_y, \tag{39}$$

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

$$\hat{a}_{pq} = \frac{4}{N_x N_y c_p c_q}\sum_{i=0}^{N_x}\sum_{j=0}^{N_y}\frac{1}{c_i c_j}T_p^*(x_i)T_q^*(y_j)a_{pq}, \quad p = 0, \ldots, N_x \text{ and } q = 0, \ldots, N_y. \tag{40}$$

3.7 Derivative Matrix

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

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

with

$$[d_{ij}]_{0\le i,j\le N} = \begin{cases} d_{ij} = \frac{c_i(-1)^{i+j}}{c_j(x_i - x_j)}, & \text{for } i \ne j \\ d_{ii} = -\frac{x_i}{2(1-x_i^2)}, & \text{for } 1 \le i \le N-1 \\ d_{00} = \frac{2N^2+1}{6} = -d_{NN}, & \end{cases} \tag{41}$$

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

$$D_{ii} = \sum_{\substack{j=0\\ j\ne i}}^{N} D_{ij}. \tag{42}$$

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

$$D_N^2 = D_N \cdot D_N = \begin{cases} \frac{(-1)^{i+j}}{c_j}\frac{x_i^2 + x_i x_j - 2}{(1-x_i^2)(1-x_j^2)}, & 1 \le i \le N-1,\ 0 \le j \le N,\ i \ne j \\ -\frac{(N^2-1)(1-x_i^2)+3}{3(1-x_i^2)^2}, & 1 \le i = j \le N-1 \\ \frac{2(-1)^j}{3c_j}\frac{(2N^2+1)(1-x_j)-6}{(1-x_j)^2}, & i = 0,\ 1 \le j \le N \\ \frac{2(-1)^{j+N}}{3c_j}\frac{(2N^2+1)(1-x_j)-6}{(1+x_j)^2}, & i = N,\ 1 \le j \le N-1 \\ \frac{N^4-1}{15}, & i = j = 0,\ i = j = N \end{cases} \tag{43}$$

The nth-order derivative matrix D_N^n is equal to the product of D_N n-times, i.e., $D_N^n = D_N \times D_N \times \ldots n$ 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 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 two-dimensional case in which D_N is replaced by its higher-order derivative as one-dimensional case. For example, $I_{N_y} \otimes D^n_{N_x}$ denotes the nth-order partial derivative with respect to first space variable and $D^n_{N_y} \otimes I_{N_x}$ denotes the nth-order partial derivative with respect to second space variable. The mixed-order derivative, i.e., mth order in first variable and nth order in second variable, is followed by Kronecker product $D^m_{N_x} \otimes D^n_{N_y}$.

3.8 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 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., first-order derivative matrix D_N is simply multiplied by the inverse of the half of the length of interval $(1/l_x)$. The nth-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 partial first-order derivative matrix corresponding to first space variable is given by $\frac{1}{l_x} I_{N_y} \otimes D_{N_x}$ and the partial first-order 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 nth-order partial derivative matrix for two-dimensional problem by replacing the l_x, l_y, D_{N_x} and D_{N_y} by $l^n_x, l^n_y, D^n_{N_x}$ and $D^n_{N_y}$, respectively. The mixed-order partial derivative matrix, i.e., mth order in first space variable and nth order in second space variable, is given by $\frac{1}{l^m_x l^n_y} D^m_{N_x} \otimes D^n_{N_y}$.

3.9 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 can be concluded that for any arbitrary interval like $[a, b]$ the first-order derivative matrix for 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 interval. The nth-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 nth-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 $\frac{2^n}{(b_1-a_1)^n}$, $\frac{2^n}{(b_2-a_2)^n}$, $D^n_{N_x}$ and $D^n_{N_y}$, respectively. The mixed-order partial derivative matrix, i.e., mth order in first space variable and nth order in second space variable, is given by $\frac{2^{m+n}}{(b_1-a_1)^m (b_2-a_2)^n} D^m_{N_x} \otimes D^n_{N_y}$.

4 Numerical Methods

The considered solute transport system (6) can be re-written as

$$c_t = d_x c_{xx} + d_y c_{yy} - v_x c_x - v_y c_y - \lambda c \tag{44}$$

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

$$\begin{aligned} c(x, y, t) &= \sum_{p=0}^{N_x} \sum_{q=0}^{N_y} c_{pq} l_p^{N_x}(x) l_q^{N_y}(y) \\ &= \sum_{p=0}^{N_x} \sum_{q=0}^{N_y} \hat{c}_{pq} T_p^*(x) T_q^*(y), \quad p = 0, \ldots, N_x \text{ and } q = 0, \ldots, N_y. \end{aligned} \tag{45}$$

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 the time derivative present in 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

$$c_t = \frac{\frac{3}{2} c^{k+1} - \left(2c^k - \frac{1}{2} c^{k-1}\right)}{\delta t}, \text{ with } t = k\delta t \text{ and } k = 0, 1, \ldots, \infty. \tag{46}$$

Therefore, the time-discrete version of Eq. (44) is

$$\frac{\frac{3}{2} c^{k+1} - \left(2c^k - \frac{1}{2} c^{k-1}\right)}{\delta t} = d_x c_{xx}^{k+1} + d_y c_{yy}^{k+1} - v_x c_x^{k+1} - v_y c_y^{k+1} - \lambda c^{k+1}, \quad k = 0, 1, \ldots, \infty \tag{47}$$

or,

$$\begin{aligned} & d_x c_{xx}^{k+1} + d_y c_{yy}^{k+1} - v_x c_x^{k+1} - v_y c_y^{k+1} - \lambda c^{k+1} - \frac{3}{2\delta t} c^{k+1} \\ &= -\frac{1}{\delta t} \left(2c^k - \frac{1}{2} c^{k-1}\right), \quad k = 0, 1, \ldots, \infty, \end{aligned} \tag{48}$$

with the initial condition

$$c(x, y, 0) = c^{(0)}(x, y) = c_0(x, y). \tag{49}$$

The polynomial $c_0(x, y)$ can be determined by Eq. (45) together with the pseudo-spectrum relation given in Eq. (40). During numerical computation $c^{(-1)}(x, y)$ arising for $k = 0$ is given as

$$c^{(-1)}(x, y) = c^{(0)}(x, y). \tag{50}$$

Equation (48) indicates that we evaluate the equation (44) at 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 (39), we need to approximate c_{xx}, c_{yy}, c_x and c_y using Chebyshev differentiation matrix as discussed above. We get

$$
\begin{aligned}
c_{xx} &\approx \left(\frac{2^2}{(b_1-a_1)^2} I_{N_y} \otimes D_{N_x}^2\right)\cdot C, \qquad c_{yy} \approx \left(\frac{2^2}{(b_2-a_2)^2} D_{N_y}^2 \otimes I_{N_x}\right)\cdot C,\\
c_x &\approx \left(\frac{2}{(b_1-a_1)} I_{N_y} \otimes D_{N_x}\right)\cdot C, \text{ and } c_y \approx \left(\frac{2}{(b_2-a_2)} D_{N_y} \otimes I_{N_x}\right)\cdot C,
\end{aligned}
\tag{51}
$$

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

$$
C = (\underleftrightarrow{c_{00}, \ldots, c_{N_x 0}}, \underleftrightarrow{c_{01}, \ldots, c_{N_x 1}}, \ldots, \underleftrightarrow{c_{0N_y}, \ldots, \ldots, c_{N_x N_y}})^t, \tag{52}
$$

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

Equation (47) gives the matrix representation as

$$
\left(E + F + G + H - \left(\lambda + \frac{3}{2\delta t}\right) I\right)\cdot C^{k+1} = -\frac{1}{\delta t}\left(2C^k - \frac{1}{2}C^{k-1}\right), \tag{53}
$$

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

$$
\begin{aligned}
G &= -v_x\left(\frac{2}{(b_1-a_1)} I_{N_y} \otimes D_{N_x}\right),\\
H &= -v_y\left(\frac{2}{(b_2-a_2)} D_{N_y} \otimes I_{N_x}\right) \text{ and } I = I_{N_x} \otimes I_{N_y}\cdot
\end{aligned}
\tag{54}
$$

The matrix representation (53) 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. 1). The boundary conditions are used to calculate c_{0q}, $c_{N_x q}$, c_{p0} and c_{pN_y}, which are the outer elements corresponding to boundary Chebyshev collocation points of space grid.

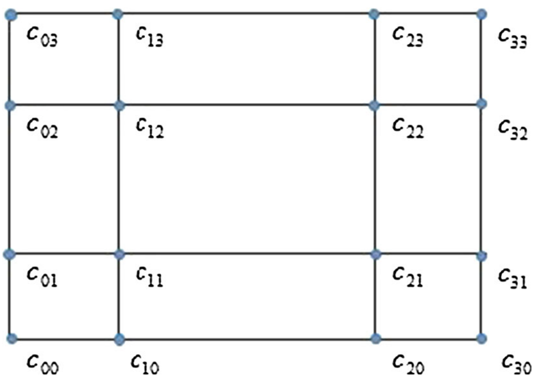

Fig. 1 Chebyshev Gauss–Lobatto grid for $N_x = 3 = N_y$ together with c_{pq}'s

4.1 Implementation of Boundary Conditions

General form of boundary conditions are

$$\begin{cases} \alpha_1 c(a_1, y) + \beta_1 c_x(a_1, y) = f_1(y), \\ \alpha_2 c(b_1, y) + \beta_2 c_x(b_1, y) = f_2(y), \\ \alpha_3 c(x, a_2) + \beta_3 c_y(x, a_2) = f_3(x), \\ \alpha_4 c(x, b_2) + \beta_4 c_y(x, b_2) = f_4(x), \end{cases} \tag{55}$$

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 implementation of given boundary conditions, let us first approximate it with considered approximation function given in Eq. (45) and then collocate at Chebyshev collocation points given in Eq. (39). For c_x and c_y, Chebyshev derivative matrix is used as discussed in Sect. 3.9. 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 (55) gives c_{0q} and $c_{N_x q}$, $0 \leq q \leq N_y$ and the last two equation of (55) give c_{p0} and c_{pN_y}, $0 \leq p \leq N_x$. From here we get matrix form for given boundary conditions as

$$A \cdot C = F, \tag{56}$$

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 (52) 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 Eq. (55).

The considered boundary conditions are

$$\begin{cases} c(x, y, t) = c_0, x = 0, & -l_y < y < l_y, \\ \frac{\partial c}{\partial x} = 0, x = l_x, & -l_y < y < l_y, \\ \frac{\partial c}{\partial y} = 0, y = -l_y, & 0 < x < l_x, \\ \frac{\partial c}{\partial y} = 0, y = l_y, & 0 < x < l_x, \end{cases}$$

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

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

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

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

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

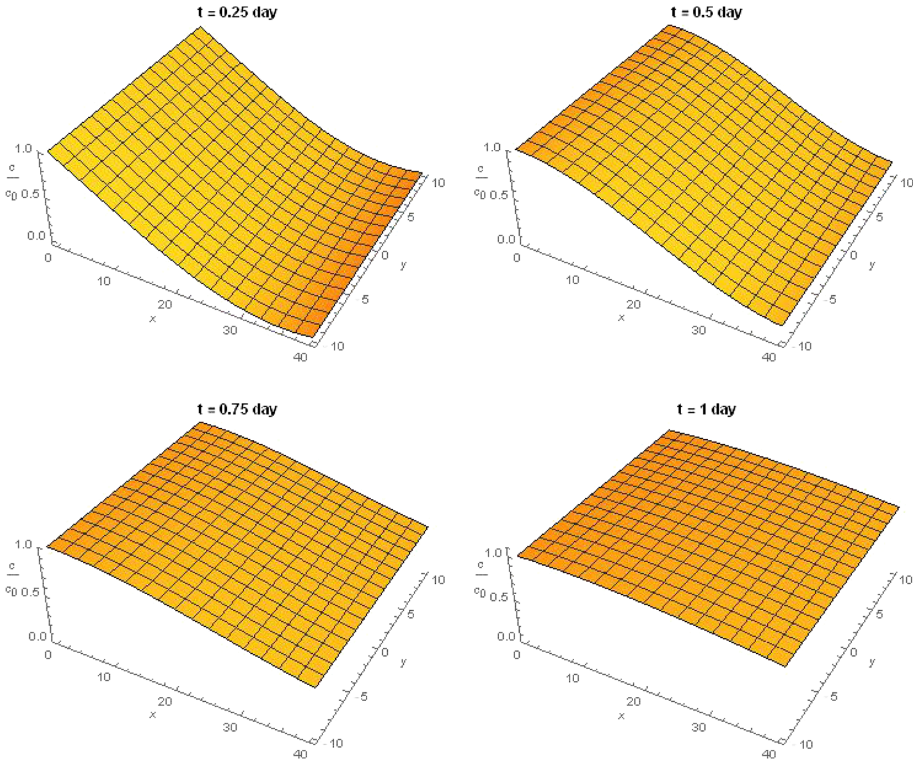


Fig. 2 Normalized concentration distributions for conservative system at different time levels

These boundary conditions along with Eq. (53) 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 Eq. (46) to get the approximate solution of the considered problem.

5 Numerical Results and Discussion

The numerical values of normalized solute concentration $c(x, y, t)/c_0$ in 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, we assumed a porous medium with the following arbitrary transport parameters: $d_x = 25\,\text{cm}^2/\text{day}$, $d_y = 5\,\text{cm}^2/\text{day}$, $v_x = 50\,\text{cm/day}$, $v_y = 0$, for conservative system and for non-conservative system in the physical space $\Omega \in [0, 40] \times [-10, 10]$. The inlet concentration is $c_i = 1\,\text{mg/cm}$. The graphical plots of normalized concentration $c(x, y, t)/c_0$ vs. physical domain (x, y) are depicted through Fig. 2 for conservative system and through Fig. 3 for non-conservative system at various time $t = 0.25, 0.5, 0.75$ and 1 day. Figures 4 and 5 show the comparisons at different time levels for conservative and non-conservative systems, respectively. Figure 6 shows the comparison between conservative and non-conservative system at $t = 0.5$ day which shows that the rate of transportation for non-conservative system ($\lambda \neq 0$) is less compared to conservative system ($\lambda = 0$) due to the effect of reaction term.

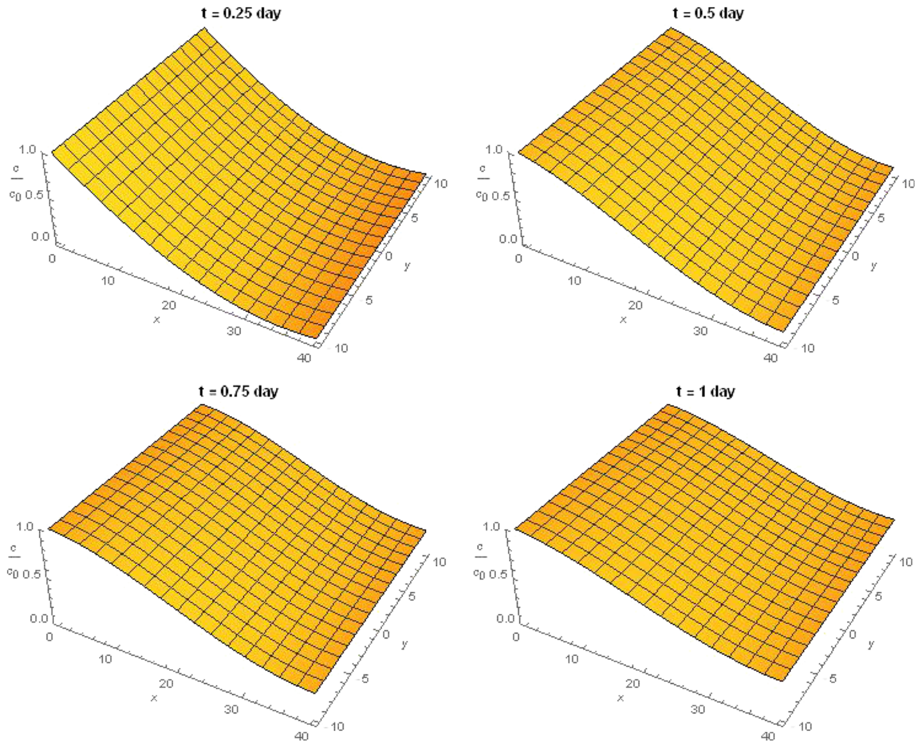
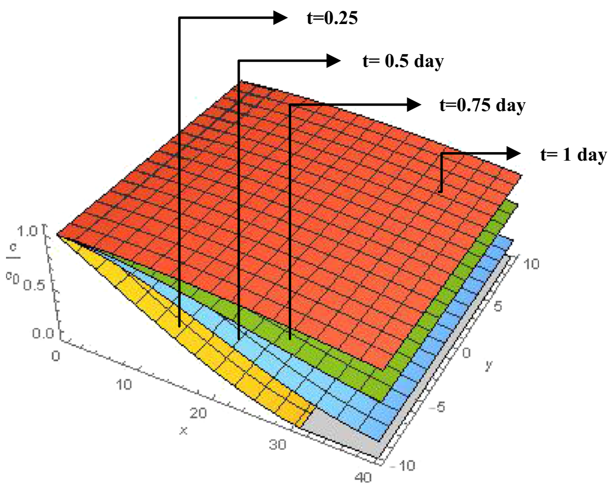


Fig. 3 Normalized concentration distributions for non-conservative system at different time levels

Fig. 4 Comparison of normalized concentration distributions for conservative system at different time levels



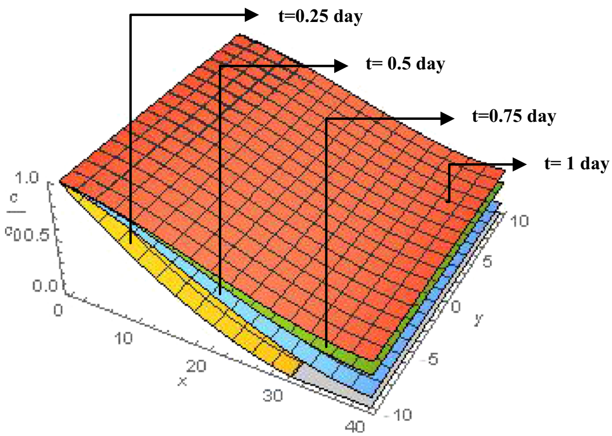


Fig. 5 Comparison of normalized concentration distributions for non-conservative system at different time levels

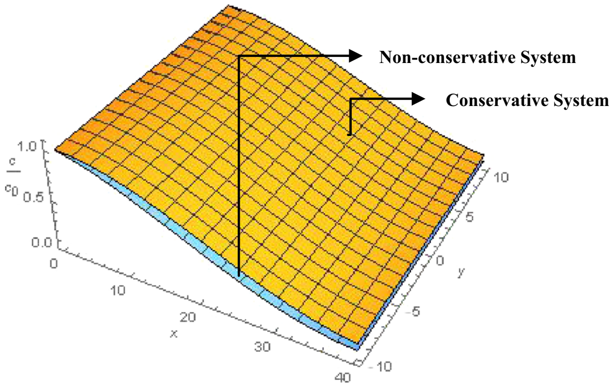


Fig. 6 Comparison between conservative and non-conservative system at $t = 0.5$ day

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 prior existence of solute concentration in the physical space, i.e., it moves toward the saturation. Figures 7 and 8 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 various time $t = 0.25, 0.5, 0.75$ and 1 day for conservative and non-conservative systems, respectively.

6 Conclusions

In the present article, spectral collocation method, which is unconditionally stable, efficient and spectrally accurate, is applied to solve the two-dimensional advection–dispersion reaction equation on a rectangular inflow region. During numerical computation, shifted Chebyshev polynomials of first kind are calculated and the Chebyshev differentiation matrix for any arbitrary physical space is derived using Kronecker tensor product with the Cheby-

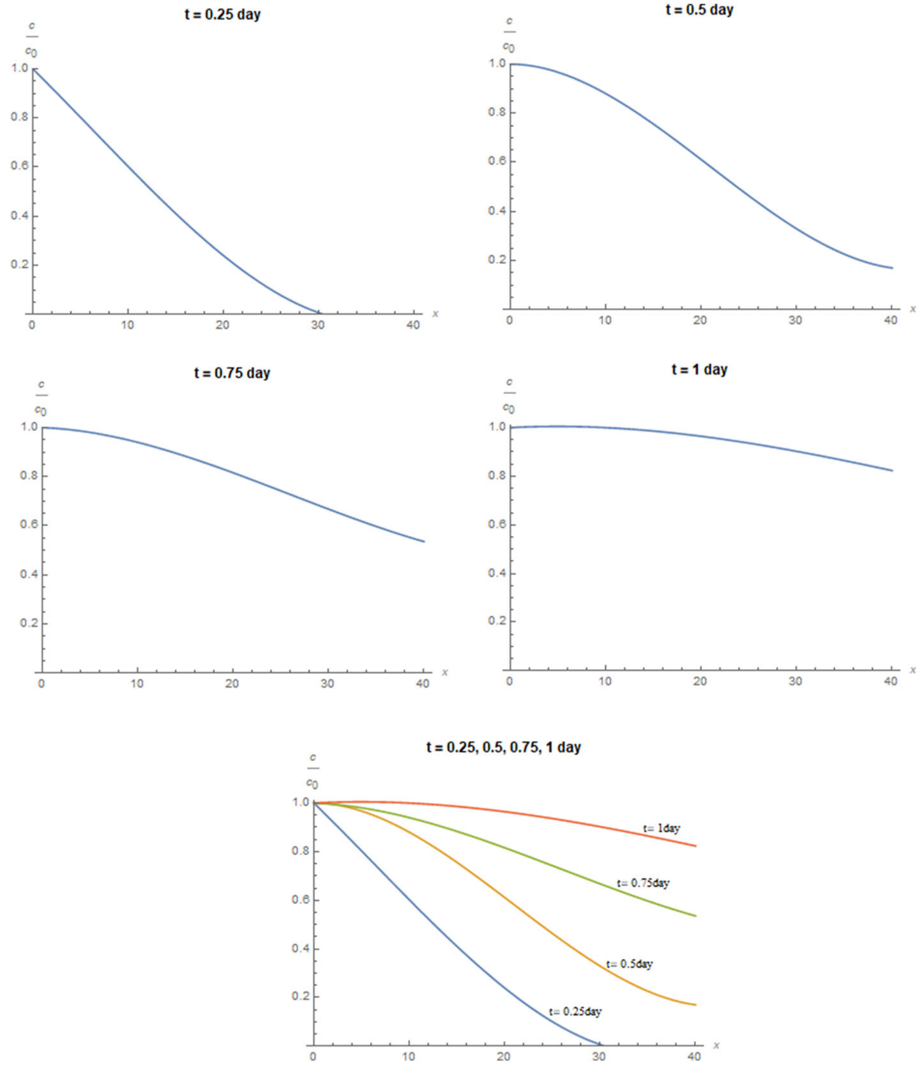


Fig. 7 Normalized concentration distributions for conservative system at different time level at $y = 10\,\text{cm}$

shev differentiation matrix given in the interval $[-1, 1]$. Here Chebyshev collocation method together with finite difference scheme is used to convert the considered mathematical model into a system of linear equations which can be solved easily. The present study shows that the behavior of the solute is not uniform and it decreases as it moves away from source along either direction or horizontal plane. During numerical computation, the considered method is applied for constant parameters' problems while it can be applied for some non-constant parameters' problems.

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

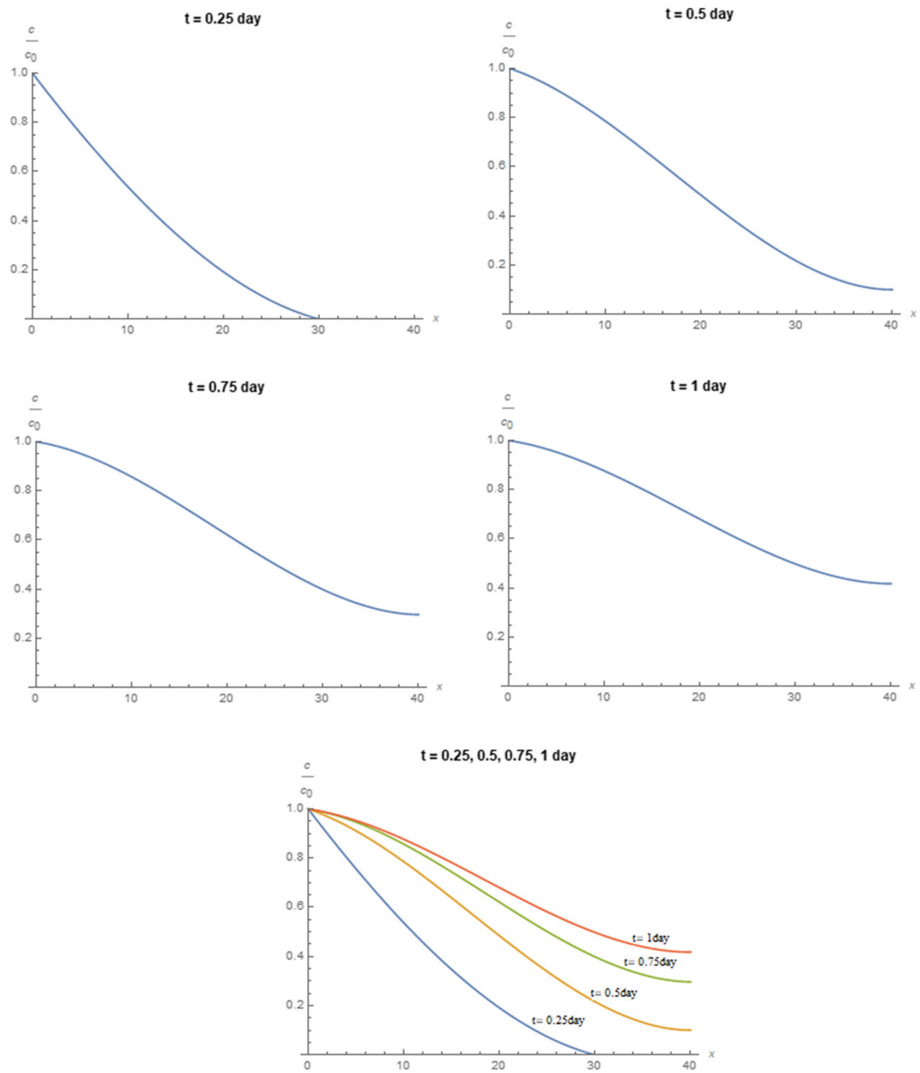


Fig. 8 Normalized concentration distributions for Non-conservative system at different time levels at $y = 10\,\text{cm}$

use of unconditionally stable difference scheme to overcome the temporal derivative. The last one is the graphical exhibition of lesser rate of transportation for non-conservative system compared to conservative system due to effect of sink term.

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