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Numerical Solution of Nonlinear Reaction–Advection–Diffusion Equation

In the present article, the advection–diffusion equation (ADE) having a nonlinear type source/sink term with initial and boundary conditions is solved using finite difference method (FDM). The solution of solute concentration is calculated numerically and also presented graphically for conservative and nonconservative cases. The emphasis is given for the stability analysis, which is an important aspect of the proposed mathematical model. The accuracy and efficiency of the proposed method are validated by comparing the results obtained with existing analytical solutions for a conservative system. The novelty of the article is to show the damping nature of the solution profile due to the presence of the nonlinear reaction term for different particular cases in less computational time by using the reliable and efficient finite difference method. [DOI: 10.1115/1.4042687]

Keywords: advection–diffusion equation, solute transport system, groundwater contamination, nonlinear reaction term, finite difference

1 Introduction

Nonlinear partial differential equations (PDEs) are widely used in recent years to evaluate the various physical phenomena in science and engineering. These are used to describe complex phenomena in fluid mechanics, plasma physics, quantum mechanics, nonlinear optics, solid-state physics, physical chemistry, and numerous areas of mathematical modeling. Since it is difficult to obtain the analytical solutions of nonlinear PDEs, a number of numerical methods have been proposed by the researchers to solve these nonlinear PDEs. The reaction–advection–diffusion equation (RADE) forms a very important particular class of partial differential equations. Due to the parabolic nature of the PDE, the solution or approximation of the RADE is a formidable task and has become a subject of great interest to researchers. RAD PDEs have been widely applied in mathematical modeling of a diverse range of natural phenomena. For instance, in environmental engineering, the RADE serves as an important water quality model since water pollution is a serious problem for living things. Contamination of groundwater, for example, from septic tank waste can have serious health effects if used for drinking and may cause diseases such as hepatitis and dysentery. Contaminated groundwater can also harm wildlife. The harmful chemical deposits into groundwater go through porous media from surface water to groundwater. It is noticed that over a long period of time in groundwater reservoirs, many chemicals are seen to undergo reactive decay. It is also seen as surface water is transported to the groundwater through the open fractures and caverns without filtering. Nonlinear advection–diffusion equations (ADEs) are mathematical models for groundwater hydrology to model the transportation of passive tracers carried by fluid flow in a porous medium. Discussions on the role of mathematical modeling in groundwater resources management can be found in Ref. [1]. The analysis of the resource potential and prediction of future impact on the environment in groundwater modeling have been studied by many researchers. Sufficient research works in experiments and theoretical studies toward the prediction of movement and behavior of solute concentration are found during the literature survey. A large number of scientists and engineers are engaged to investigate the possibilities of contamination of the subsurface environment, which have contributed a tremendous impact on the research of solute transport phenomena in porous media.

Presently, water-quality problems involve the application of the ADE. The ADE with specific initial and boundary conditions explains special and temporal variations in solute concentration. In case of steady and uniform flow, the advection–diffusion equation may be considered with a constant parameter, which is the simple form of the governing equation. The considered system, which is physically a transported phenomenon, is one-dimensional (1D) in which solute concentration is well mixed horizontally and vertically such that concentration varies only in the longitudinal or downstream direction. The steady and uniform flow field is imposed and as result effects of diffusion are spatially constant. Any biogeochemical processes may be described in term of the first-order reaction.

The mathematical model, which describes the solute transport in groundwater, was presented by Fried [2], Bear and Verruijt [3], Gómez-Aguilar et al. [4], Jaiswal et al. [5], etc. The mathematical model of ADE describes phenomena where various physical quantities viz., particles, energy, or other quantities are transferred to a physical system due to diffusion and advection processes. In the present article, the mass transport of a dissolved solute or movement of a component in a gas mixture is proposed. Diffusion will take place in the soil column due to concentration gradients and if there is bulk fluid motion, then advection will also contribute to the flux of chemical species. The determination of the combined effect of both advection and diffusion with reaction term on the solution profile is not an easy task. Thus, the present article deals with computation for mathematical models described

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Contributed by the Design Engineering Division of ASME for publication in the Journal of Computational and Nonlinear Dynamics. Manuscript received April 17, 2018; final manuscript received January 16, 2019; published online February 15, 2019. Assoc. Editor: Dumitru Baleanu.

above with a reliable technique that requires less computational work compared to the existing methods used to solve nonlinear systems. The concentration distribution behavior with space and time is a PDE of parabolic type. The general one-dimensional advection–diffusion equation with nonlinear reaction term is defined as

$$\frac{\partial u(x,t)}{\partial t} + V\ \frac{\partial u(x,t)}{\partial x} = D\ \ \frac{\partial^2 u(x,t)}{\partial x^2} + \lambda f(u) \qquad (1)$$

where $u(x,t)$ is the solute concentration, x is the spatial coordinate, t is the time, D is the diffusion coefficient, V is the average fluid velocity, λ is rate coefficient, and $f(u)$ is the reaction term representing the capacity of the internal source or sink. The dispersion term in Eq. (1) causing the spreading of fluid is composed of molecular and mechanical dispersions, which generally cannot be distinguished in Darcy scale. The mechanical dispersion increases with the increase in the speed of the fluid flow. If $\lambda = 0$, Eq. (1) represents simply a linear ADE whose center of mass is Vt and a measure of dispersion is $2Dt$. If $\lambda < 0$, Eq. (1) is called the RADE. Here, the reaction term causes the damping of the solute concentration. If $f(u) = u$, then $<X^2(t)> \sim t^{3/2}$, which shows that the linear reaction–advection–diffusion equation represents an evolutionary process. This has motivated the authors to the study of ADE with the presence of a nonlinear reaction term.

The ADE physically interprets the phenomena that particles' activities vary with time due to the transportation of fluid streams, and its spreading and mass transfers through the channel in which the streams flow. The said equation derived from the conservative principle of continuum mechanics and phenomenology laws is considered in a microscopic sense without reference to any microscopic analysis. When a particle is undergoing in Brownian motion, its displacement and velocity directions will change with time unit. But in a shorter time scale, it is found to be a continuous ballistic path, which will be revealed by the random walk with uncorrelated steps. In this case, to describe the motion of a particle, a deterministic model is more suitable than a stochastic model. The equation is widely used in physics and engineering for the descriptions of earth surface processes related to sediment transport, landscape evolution, solute transport, suspended transport and also in the investigations on the evolution of braiding rivers, suspension and bedload transport, etc.

There are many analytic and numerical solutions present in the literature [6–10] for one, two, and three-dimensional (3D) linear advection–diffusion equations with different forms of initial and boundary conditions. The modeling of solute transport and its analytical solution was given by San Jose Martinez et al. [11]. In 2012, Savovic and Djordjevich [12] solved the one-dimensional advection–diffusion equation in semi-infinite media using an explicit finite difference method (FDM). In the following year, the authors [13] have used the same method to solve the two-dimensional (2D) solute transport-diffusion equation. Recently, one-dimensional advection–diffusion equation with linear type reaction term in groundwater problem was solved by Jaiswal et al. [14]. But to the best of the authors' knowledge, the problem with nonlinear reaction term with prescribed initial and boundary conditions has not yet been done by any researcher.

In 1928, the fundamental theoretical article on the solution of the problem of mathematical physics using FDM had been published by R. Courant, K. O. Friedrichs, and H. Lewy. A discrete analog of Dirichlet's principle was used in the article to define five-point approximation solution of Laplace equation. Considerable progress in FDM was made later for time-dependent problems. There are many researchers viz., J. Crank, P. Nicolson, J. Douglas, D. Lees, O. Widlund, and others who played major contributions during the 1950s and 1960s. The Poisson equation is the equation of Poiseuille flows in arbitrary cross section, which was calculated numerically by T. Fukuchi using the forward time centered space. During computation, a rectangular as well as rotating square cross section domain had been considered. The computed results were confirmed with the analytical solution for any grid dispositions. T. Fukuchi calculated the stability analysis of forward time centered space using bisection method, which was very important and difficult to calculate.

Finite difference method is the oldest method for solving the partial differential equations, which use a topologically square network of lines toward discretization of the PDEs. In the case of Cartesian coordinate systems, the method can be applied to numerical analysis over any complex domain. Due to the complexity of complex domain when taken for geometry of immersed body in a fluid, an analytical domain of arbitrary configuration is considered. For structured grids, the method is simple and effective, and for regular grids, it is accessible to obtain higher order schemes. Since during discretization by FDM, the lengths of the intervals for both time and space decrease, it will provide more accurate result. Again, the method is simple and easy to implement in a structured domain. The numerical scheme is easy to debug codes. For these reasons, this numerical method has become an important and efficient tool for solving nonlinear problems. The advantage of the concerned method over the other existing methods is that it provides the flexibility to reduce the linear/nonlinear problem into the system of linear/nonlinear algebraic equations, which can be computed easily for different discretized points. The strong historical background and the simplicity and efficiency of the method showed that this method may continue to flourish and be an active field of research on nonlinear fluid flow problems. Due to its potential in solving many unsolved problems, FDM was treated as a novel method in the field of computations. The limitations of the method in the requirement of long memory due to unavailability of resources in research laboratories had been well taken care of by the researchers after the invention of Cray machine. After that, there was a lot of improvement of the time domain computation, which has made it a novel one for application in practical problems. This has motivated the authors to apply the method to solve the nonlinear problem under prescribed initial and boundary conditions. The implementation of FDM here ensures positivity of the solution and thus numerical stability of the computation.

In the present endeavor, a sincere attempt has been taken to find the numerical solution of the one-dimensional nonlinear reaction–advection–diffusion equation with initial-boundary conditions using FDM. The considered problem is first converted into algebraic equations using finite difference approximation and then algebraic equations are solved for different grid points. The obtained results are depicted graphically for conservative as well as nonconservative systems for different particular cases. To validate the accuracy and efficiency of the considered method, the results obtained are compared with the existing analytical solution for the conservative system [7]. After successful validation, the authors have been motivated to apply the proposed method to solve the considered nonlinear problem for the nonconservative cases and the results obtained are displayed graphically.

In Sec. 2, the construction and implementation of the FDM are given. The stability analysis of the proposed mathematical model is discussed in Sec. 3. Section 4 presents the explicit solution. Section 5 gives the results with discussion and a comparison of the numerical results and existing analytical results. Section 6 concludes.

2 Construction and Implementation of the Method

Difference approximations may be constructed in various ways, among which Taylor's formula is probably the simplest one to serve our present purposes. First, the region is discretized into finite grids as shown in Fig. 1. Now, consider the space–time region such that space $x \in [0, L]$ discretized by dividing the length of the intervals into M equal subintervals of length h and then the time t is discretized with time spacing $k > 0$ such that $t_{j+1} = t_j + k$ with $t_0 = 0$. The partial derivatives in the PDEs at each grid

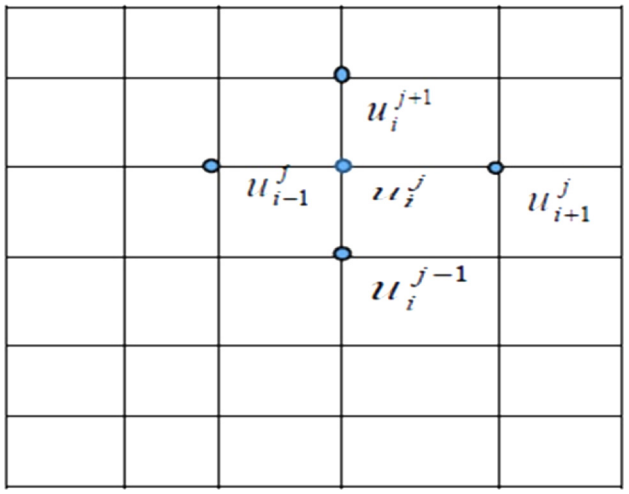

Fig. 1 A partition of the (x, t)-plane into uniform cells of size $h \times k$

point are approximated from neighboring values by using Taylor's theorem [15]. Next, the values of dependent variables at each and every internal grid points are calculated using the given initial and boundary conditions; FDM requires more grid points to achieve reasonable accuracy.

2.1 Finite Difference Approximation of Derivatives. In the finite difference approximation, the following notations are used: h is the spatial step, k is the time-step, $x_i = a + ih$, $i = 0,1, 2, \ldots, M$ points are the coordinate of the mesh and $M = (b - a)/h$, $t_j = jk, j = 0, 1, 2,\ldots, N, N = T/k$ are used. The values of the solution $u(x, t)$ at these grid points are given by $u(x_i, t_j) \simeq u_i^j$, where u_i^j the numerical estimate of the exact value of $u(x, t)$ at the point (x_i, t_j). The forward space and time difference schemes are

$$\frac{\partial u}{\partial x}(x_i, t_j) \simeq \frac{u_{i+1}^j - u_i^j}{h} \tag{2}$$

$$\frac{\partial u}{\partial t}(x_i, t_j) \simeq \frac{u_i^{j+1} - u_i^j}{k} \tag{3}$$

and the backward difference schemes for space and time are given by

$$\frac{\partial u}{\partial x}(x_i, t_j) \simeq \frac{u_i^j - u_{i-1}^j}{h} \tag{4}$$

$$\frac{\partial u}{\partial t}(x_i, t_j) \simeq \frac{u_i^j - u_i^{j-1}}{k} \tag{5}$$

Forward and backward difference approximations are first-order accuracy in x and t.

Another finite difference approximation of second-order accuracy, which is central difference scheme given by the relations

$$\frac{\partial u}{\partial x}(x_i, t_j) \simeq \frac{u_{i+1}^j - u_{i-1}^j}{2h} \tag{6}$$

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_j) \simeq \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{h^2} \tag{7}$$

One can also approximate higher order derivative to finite difference approximation [16].

3 Stability Analysis of the Problem

Let us consider the one-dimensional advection-diffusion equation with nonlinear reaction term as

$$\frac{\partial u(x,t)}{\partial t} = D\,\frac{\partial^2 u(x,t)}{\partial x^2} - V\,\frac{\partial u(x,t)}{\partial x} - \lambda\, u(x,t)\,(1 - u(x,t)) \tag{8}$$

To find the accuracy of the FDM for Eq. (8), let us apply an explicit scheme in the equation to get the truncation error as

$$\begin{aligned} E_i^j = {} & \frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{k} \\ & - D\frac{u(x_{i+1}, t_j) - 2\,u(x_i, t_j) + u(x_{i-1}, t_j)}{h^2} \\ & + V\frac{u(x_{i+1}, t_j) - u(x_i, t_j)}{h} + \lambda u\,(1 - u) \end{aligned} \tag{9}$$

The Taylor's series expansion of each term for the above equation given as

$$\frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{k} = \frac{\partial u}{\partial t} + \mathrm{O}(k)$$

$$\frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j)}{h^2} = \frac{\partial^2 u}{\partial x^2} + \mathrm{O}(h^2)$$

and

$$\frac{u(x_{i+1}, t_j) - u(x_i, t_j)}{h} = \frac{\partial u}{\partial x} + \mathrm{O}(h)$$

Substituting the above values in Eq. (9), we have

$$\begin{aligned} E_i^j = {} & \left(\frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2} + V\frac{\partial u}{\partial x} + \lambda u(1 - u)\right) \\ & + \mathrm{O}(k) + V.\,\mathrm{O}(h) + D.\,\mathrm{O}(h^2) \end{aligned} \tag{10}$$

The principal part of the truncation error goes to zero as per Eq. (8). In this method, Eq. (10) shows the second-order accuracy in space and first-order accuracy in time, that is $\mathrm{O}(h^2, k)$ for reaction–diffusion-equation and first-order accuracy in space and time, that is $\mathrm{O}(h, k)$ for RADE.

Next, we consider Von-Neumann method to investigate the stability of the proposed method. Using FDM, the RADE can be written as

$$\begin{aligned} u_i^{j+1} = {} & u_i^j + \frac{D\,k}{h^2}\left(u_{i+1}^j - 2\,u_i^j + u_{i-1}^j\right) - \frac{V\,k}{h}\left(u_{i+1}^j - u_i^j\right) \\ & - k\,\lambda\,u_i^j\left(1 - u_i^j\right) \end{aligned} \tag{11}$$

Since the method is applicable to the linear scheme, the nonlinear term $u_i^j(1 - u_i^j)$ is linearized [17,18] by taking $u_i^j = \tau$ (a constant value) so that Eq. (11) can be rewritten as

$$\begin{aligned} u_i^{j+1} = {} & u_i^j + \psi\,(u_{i+1}^j - 2\,u_i^j + u_{i-1}^j) - \sigma\,(u_{i+1}^j - u_i^j) \\ & - k\,\lambda\,u_i^j(1 - \tau) \end{aligned} \tag{12}$$

where mesh ratio parameter $\psi = Dk/h^2$, Courant number $\sigma = Vk/h$, and τ is the local constant.

Defining the error by U_i^j as $U_i^j = \xi^j e^{\boldsymbol{i}\,(i\beta h)}$, where $\boldsymbol{i} = \sqrt{-1}$ substituting in the above Eq. (12), we get the simplified form of the equation as

$$\xi = 1 - k\lambda(1-\tau) - 4\psi \sin^2\left(\frac{\beta h}{2}\right) - 2\sigma \sin^2\left(\frac{\beta h}{2}\right) + i\sigma \sin(\beta h) \tag{13}$$

whose magnitude is defined as

$$|\xi| = \sqrt{\left(1-k\lambda(1-\tau)-4\psi\sin^2\left(\frac{\beta h}{2}\right)-2\sigma\sin^2\left(\frac{\beta h}{2}\right)\right)^2 + \sigma^2\sin^2(\beta h)}$$

The Von-Neumann stability condition is given [18] as $|\xi| \le 1$, we get

$$0 \le \left(1 - k\lambda(1-\tau) - 4\psi \sin^2\left(\frac{\beta h}{2}\right) - 2\sigma \sin^2\left(\frac{\beta h}{2}\right)\right)^2 + \sigma^2 \sin^2(\beta h) \le 1 \tag{14}$$

If we choose local constant $\tau = 0$, max $(\sin^2(\beta h/2)) = 1$, and min $(\sin^2(\beta h)) = 0$, then we have

$$(1 - k\lambda - 4\psi - 2\sigma)^2 \le 1$$

i.e., $-(k\lambda/2) \le (2\psi + \sigma) \le ((2 - k\lambda)/2)$

If $V = 0$, i.e., for the case of reaction–diffusion equation, the range of mess ratio parameter becomes $-(k\lambda/4) \le \psi \le ((2 - k\lambda)/4)$.

Considering the stability sizes of mess ratios of the above two cases, it may be concluded that the finite difference method provides conditionally stability for the considered problem.

4 Solution of the Problem

In this section, an endeavor has been taken to find the numerical solution of one-dimensional advection–diffusion Eq. (8) with nonlinear reaction term under the initial condition

$$u(x, 0) = 0, \quad 0 \le x \le L \tag{15}$$

and boundary conditions as

$$u(0, t) = u_0, \quad t > 0 \tag{16}$$

$$\frac{\partial u\ (L, t)}{\partial x} = 0, \quad t > 0 \tag{17}$$

In this problem, first let us replace the region over which the independent variables in the differential equation are defined by a finite grid of the points and then replace the derivatives and its supplementary conditions given in the initial-boundary conditions (15)–(17) by finite difference approximations. Forward finite difference approximation for first-order time and space derivatives and central difference approximation for second-order space derivative have been used in Eq. (8).

After some mathematical calculations, we get the following system of algebraic equations as:

$$u_i^{j+1} = \alpha.\, u_{i-1}^j + \beta.\, u_i^j + \eta.\, u_{i+1}^j + \mu.\, (u_i^j)^2, \quad i = 1, 2, \ldots, M, j = 0, 1, 2, \ldots, N-1 \tag{18}$$

where $\alpha = Dk/h^2$, $\beta = (1 - (2Dk/h^2) + (Vk/h) - \lambda k)$, $\eta = ((Dk/h^2) - (Vk/h))$ and $\mu = \lambda k$.

The initial and boundary conditions are discretized as

$$u_i^0 = 0, \quad i = 0, 1, 2, \ldots, M \tag{19}$$

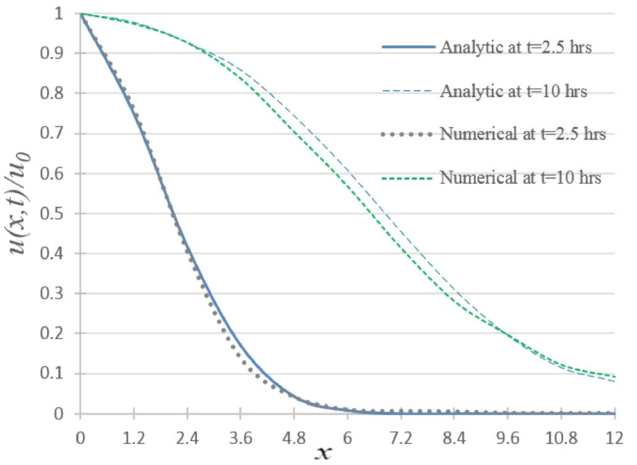

Fig. 2 Comparison between analytical and numerical results at $t = 2.5$, 10 when $\lambda = 0$

$$u_0^j = u_0, \quad u_M^j = u_{M-1}^j, \quad j = 1, 2, 3, \ldots, N \tag{20}$$

Nonlinear algebraic equations are solved by computation for different node points. The graphs between normalized concentration and column length for different time predict the physical significance of the nonlinear solute transport system.

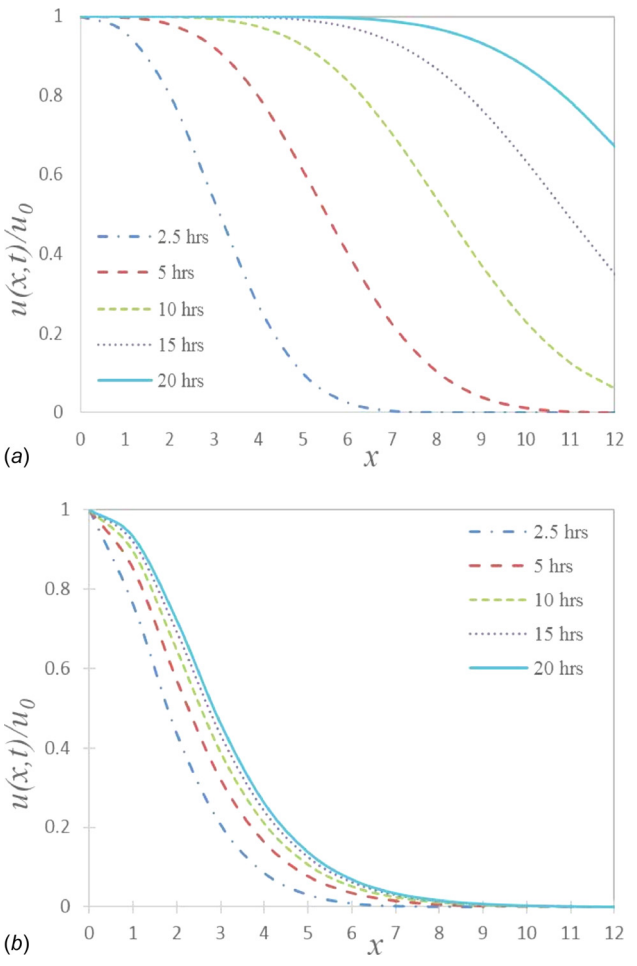

Fig. 3 (*a*) Plots of $u(x, t)/u_0$ versus x at $t = 2.5$, 5, 10, 15, 20, $D = 0.6$ and $V = 0.6$ when $\lambda = 0$ and (*b*) plots of $u(x, t)/u_0$ versus x at $t = 2.5$, 5, 10, 15, 20, $D = 0.6$ and $V = 0.6$ when $\lambda \ne 0$

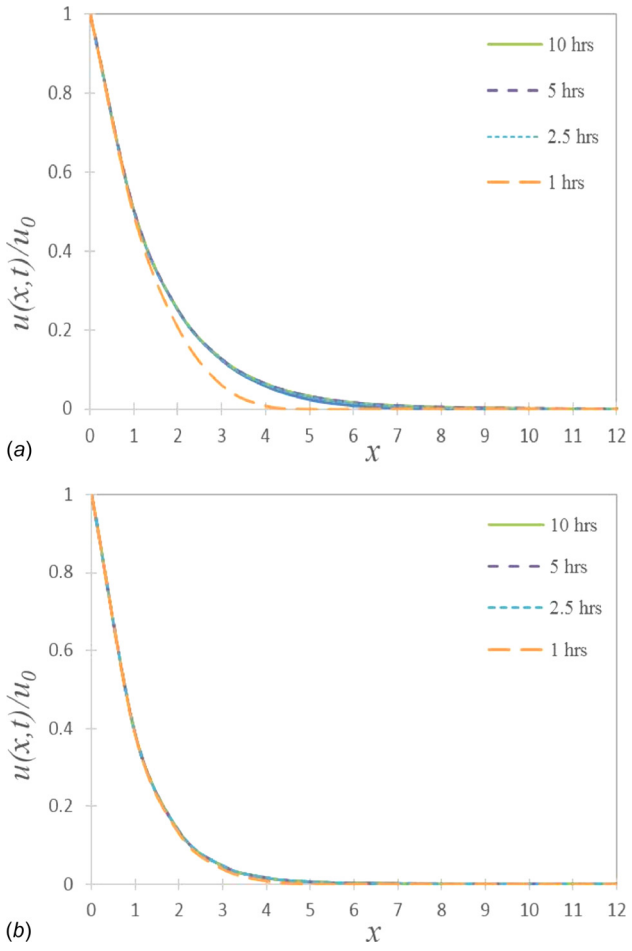

Fig. 4 (*a*) Plots of $u(x,t)/u_0$ versus x at $t = 1, 2.5, 5, 10$, $D = 0.6$ and $V = 0$ when $\lambda = 0$ and (*b*) plots of $u(x,t)/u_0$ versus x at $t = 1, 2.5, 5, 10$, $D = 0.6$ and $V = 0$ when $\lambda \neq 0$

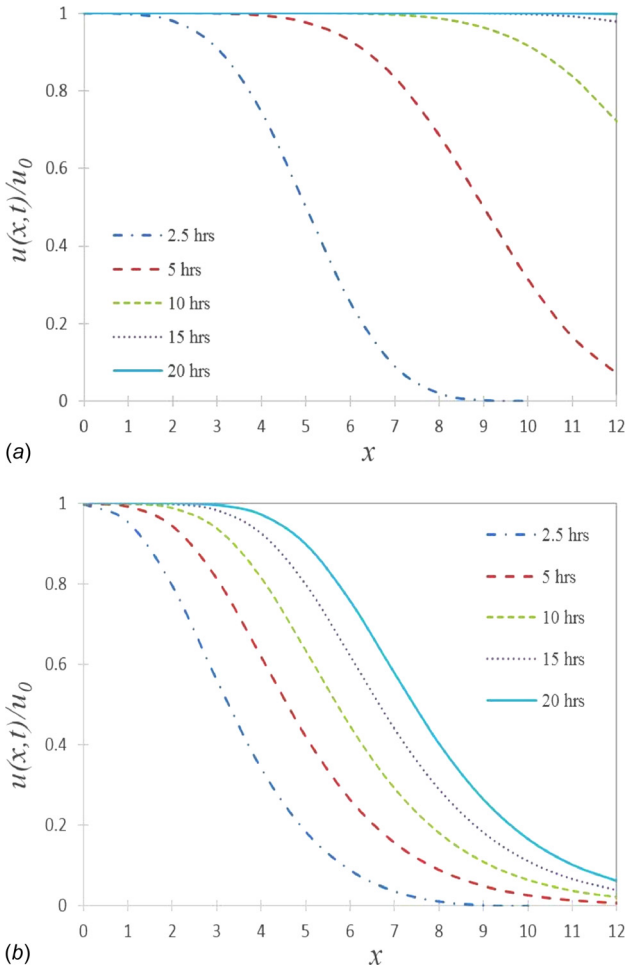

Fig. 5 (*a*) Plots of $u(x,t)/u_0$ versus x at $t = 2.5, 5, 10, 15, 20$, $D = 1$ and $V = 1$ when $\lambda = 0$ and (*b*) plots of $u(x,t)/u_0$ versus x at $t = 2.5, 5, 10, 15, 20$, $D = 1$ and $V = 1$ when $\lambda \neq 0$

5 Results and Discussion

In the present section, a drive has been taken to find the numerical solution of normalized solute concentration $u(x,t)/u_0$ for different particular cases, which are depicted through Figs. 2–5. During numerical computation, the values of the parameters are taken as $D = 0.6$ in.^{2}/h, $V = 0.6$ in/h and $\lambda = 0.6$ (for nonconservative system). To validate the considered method, a comparison of the numerical results with the existing analytical result [7] for $t = 2.5$ h and $t = 10$ h is shown through Fig. 2 for the conservative system ($\lambda = 0$). From the figure, it is clear that the numerical results are quite similar to the existing analytical results, which exhibits that our proposed method is effective and reliable.

Figure 3(*a*) shows the movement of normalized solute concentration in the finite length column in the conservative system for different $t = 2.5, 5, 10, 15, 20$. It is found from the figure that the solute covers more length in the soil column as time increases. Also, the slopes of the graphs are becoming flattered with time due to the prior existence of solute concentration in the column. Figure 3(*b*) shows the movement of solute concentration in the finite length column with effects of the sink term that is for the nonconservative system at various time levels $t = 2.5, 5, 10, 15, 20$. The nature of the graphs is similar to the previous one. Figure 3(*b*) depicts that the movement of solute concentration is less compared to a conservative system, due to the effect of the sink term ($\lambda > 0$).

The effect of the reaction term on the solution profile in the absence of the advection term $V = 0$ is displayed through Figs. 4(*a*) and 4(*b*). Figure 4(*a*) shows that in the absence of advection for the conservative case, the input concentration initially moves with time and after a certain time period it would stabilize, that is, there is no movement of concentration. It is also clear from Fig. 4(*b*) that the movement of solute is slow for the nonconservative system as compared to a conservative system, due to the presence of the sink term.

The effect of the reaction term, the solution profile for longitudinal dispersion, and advection–diffusion process ($D = 1.0$ in.^{2}/h, $V = 1.0$ in./h) are expressed through Figs. 5(*a*) and 5(*b*). The nature of the graphs is similar to Figs. 4(*a*) and 4(*b*) for both conservative and nonconservative cases through the movements of solute increase in each case, that is, it covers more length in the column for different times considered previously, which is physically justified.

6 Conclusions

The goal of the present scientific contribution is the numerical solution of the advection–diffusion equation with nonlinear reaction term using the finite difference method. To validate the efficiency of the proposed method, a comparative study between the approximate solution and the existing analytical result of the considered problem for the conservative case is carried out through error analysis, which is displayed graphically. The main contribution is finding the damping effect on the solution profile due to the presence of the reaction term. The effect of reaction term on the solution of the diffusion process in the absence or presence of advection term is the key feature of the article. This effect of reaction term toward the damping of the solute

concentration, for different column lengths at various time levels in the absence or presence of advection term, was determined with little computational time by applying the efficient and powerful FDM. Another striking feature of the article is the study of conditional stability when the proposed method is applied to find the stability regions of the mess size parameters for conservative and nonconservative cases.

Acknowledgment

The authors are extending their heartfelt thanks to the revered reviewers for their constructive suggestions towards the improvement of the article. The present research work is carried out with the financial support provided by the Science & Engineering Research Board (SERB), Government of India vide their letter number SB/S4/MS: 840/13 dated 07.05.2015.

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