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Higher Order Implicit Scheme for Nonlinear Time-Dependent Convection-Diffusion-Reaction Equation

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Abstract

A mathematical model comprising of nonlinear reaction, diffusion, and convection mechanisms seen in natural and anthropogenic processes is numerically investigated here. It is proposed that a higher order numerical scheme of finite difference method be used in conjunction with an iterative approach in order to solve the nonlinear one dimensional convection-diffusion-reaction equation. To account for the wide variety of physical characteristics and boundary conditions, an iterative approach is presented that yields a reliable and precise solution every time. We examined the accuracy and operational efficiency of two distinct finite difference approaches. The efficiency of the system is determined by comparing the estimated results to the appropriate analytical solution by adhering to established norms. Coherence and convergence were analyzed for each approach. The simulation results demonstrate the efficacy and accuracy of these methods in solving nonlinear convection-diffusion-reaction equations. Convection-diffusion-reaction equation modeling is critical for employing the offered results in heat and mass transport processes.

Keywords

Finite Difference Method (FDM), Crank-Nicholson (CN), Fourth Order Implicit (FOI), Convection-Diffusion-Reaction (CDR)

1. Introduction

There are several kinds of partial differential equations that control mathematical models of mechanical, chemical, ecological, and environmental events.

Nonlinear convection-diffusion-reaction equations are of the kind

$$\phi_t + A\phi(\phi_x) = B\phi(\phi_{xx}) + C(\phi) \tag{1}$$

where unknown function is denoted by ϕ and variable coefficients represent the smooth functions. Numerous applications necessitate the modeling of convection-diffusion-reaction (CDR) equations that are time dependent. Common examples also include chemical reaction and electrophoresis separation phenomena simulations in flow fields. Modeling processes in chemistry, physics, engineering, ecology and biology typically use convection-diffusion-reaction equations. Using the convection-diffusion-reaction model, one can see how a chemical or biological species evolve over time. It is possible to represent these phenomena using a non-linear framework of advection, diffusion, and reaction equations that are time-dependent. Such processes require numerical algorithms capable of computing crisp layers while also preventing specious oscillations from occurring for reliable simulations.

Extensive study has been done on the numerical characteristics of simulating diffusion advection transport, and that research is currently ongoing. A large quantity of literature on advection diffusion transport has been produced as a result [1]. The convection-diffusion-reaction equation is frequently employed in the mathematical models used to analyze water pollution in lakes, waterways and rivers [2] [3] [4]. The equations of convection-diffusion-reaction emerge in the modeling of the process of cancer and tumor growth [5] [6] [7] [8] [9]. Fluid flow simulation in a non-inertial frame is yet another intriguing use of this technique. In order to model these phenomena, we use a convection-diffusive-reactive structure, with inertia represented in the convective term, viscous effects represented in the diffusion expression, and centripetal forces represented in the reaction term [10]. As a result of the strong gradients in the flow behavior, it is necessary to use a specific numerical treatment. The large percentage of classical systems features erroneous oscillations, resulting in a high level of numerical dispersion [11]-[16]. Identifying precise answers with a biological, physical, or chemical interpretation is crucial. For the solution of nonlinear partial differential equations, conventional approaches are inapplicable. There are several numerical methods that can be used to approximate the solution of nonlinear CDR equation.

A stabilized finite element method for solving systems of CDR equations based on the subgrid scale approach was developed by R. Codina in 1997 [17]. To handle unstable CDR problems using the finite element approach, A. Huerta *et al.* [18] introduced Galerkin least-squarres, streamline-upwind Petrov-Galerkin, and sub-grid scale solutions in 2002. A numerical investigation for the 1D and 2D steady state advection-diffusion-absorption equations using the stabilized finite element approach was presented by E. Onate [19] in the year 2005. In order to solve the advection diffusion response equation, J. A. Pudykiewicz [20] proposed a finite volume technique based on the notion of semidiscretization in the end of 2005. According to J. Kacur *et al.* [21] in 2009, the convection-diffusion-absorption problem can be approximated using the method of lines and interface modeling. Erik Burman and Miguel A. Fernandez [22] conducted research into semi-implicit and implicit time-stepping approaches for finite element approxima-

tions to time dependent CDR problems in the same year. Later, P. Nadukandi *et al.* [23] presented the formulation of Petrov-Galerkin scheme for the one-dimensional CDR problem based on the finite element method.

Hendrik Speleers (2012) *et al.* [24] investigated the approximate solution of the CDR problem using isogeometric analysis based on Powell-Sabin splines. In 2016, E. Onate *et al.* [25] used Galerkin scheme of finite element method for one dimensional advection diffusion reaction equation. Reproducing kernel particle scheme was discussed in 2017 by M. Gharib *et al.* [26] in order to solve the advection-diffusion-reaction problem. It was suggested in 2019 by F. Zhao *et al.* [27] that the convection, diffusion, and reaction equations on implicit fields be computationally solved using the radial basis function-generated finite differences approach. This meshless system relies on compactly supported radial basis functions. In 2019, U. Erdogan *et al.* [28] introduced a method that linearized first using Newton Iteration, and then discretized spatially and temporally in the second phase. To show that the nonlinear reaction component dampens the solution profile, A. Sing *et al.* (2019) [29] used an efficient and reliable finite difference approach to save computing time. For the CDR equation with anisotropic diffusion, N. Rauf *et al.* (2019) [30] employed a boundary element approach to evaluate the accuracy and consistency of the solutions.

The numerical solution of CDR equations was also examined by S. Singh *et al.* (2020) [31] using implicit explicit compact techniques. J. Lin [32] developed a meshless approach for solving linear and nonlinear advection-diffusion-reaction equations. To study the approximate solution of the CDR equation, Sengupta *et al.* [33] conducted a global spectral analysis in 2020. Shortly thereafter, using a one-sided Laplace transform and assuming constant diffusivity, velocity, and reactivity, Kim [34] was able to find the CDR equation's one-dimensional analytical solution. Later, A. Puigferrat [35] suggested a finite increment calculus scheme based on stabilized finite element method for advection-diffusion-absorption problems. To solve the nonlinear convection diffusion response equation in one dimension, Ali *et al.* [36] proposed a numerical technique based on a combination of Lucas and Fibonacci polynomials in 2021. Soon after, A. Jain [37] presented eigenvalue analysis for multilayer 1D convection diffusion reaction equation. Svetislav Savovi [38] investigated the numerical solution of the advection-diffusion-reaction equation describing the transport phenomenon at the end of the same year using unconditionally positive finite difference and the usual explicit finite difference schemes. Luis Blanco-Cocom and colleagues [39] published a mathematical model of a fuel cell in 2022 that represented the physical modeling of the fuel cell. Using a strategy that eliminated the artificial diffusion of the finite element method, they were able to numerically investigate the proposed CDR model.

2. Problem Statement

2.1. Governing Equation

For unsteady CDR problem in one dimension, a partial differential equation can

be stated as follows

$$u_t = uu_{xx} + 3uu_x + 2\left(u - u^2\right) \tag{2}$$

where $(x,t) \in \Gamma \times (0,T]$ with initial conditions $u(x,0) = u_0(x)$, $x \in \Gamma$. The Dirichlet boundary conditions are denoted the expression $u(a,t) = f_1(x,t)$, $u(b,t) = f_2(x,t)$.

Here $(x,t) \in \Gamma \times (0,T]$, $\Gamma = x : a \le x \le b$ is a domain in *R*, $(0,T]$ is the time interval. $h = dx$ and smooth functions are defined to u_0, f_1 and f_2.

2.2. Analytical Solution

The one dimensional non linear CDR Equation (2) has an analytical solution [40]

$$U(x,t) = 2\mathrm{e}^{2t}\sqrt{\mathrm{e}^{x} - \mathrm{e}^{-4x}} \tag{3}$$

The constraint element $h = dx$, the boundary conditions and the initial condition $u_0 = u(x,0) = 2\sqrt{\mathrm{e}^{x} - \mathrm{e}^{-4x}}$ are all taken from the analytical solution during the computations. Here $\Gamma \times T = \{(x,t) : 0 \le x \le 1, 0 < t \le T\}$.

3. Numerical Methods

A numerical solution to CDR equation in one dimension will be investigated in this part, using numerical techniques to examine at the domain Γ. In the beginning, we establish that the integer *S* that will be used to describe the space step size, $d_x = (b-a)/S$ in horizontal direction. Divide the interval $[a,b]$ into *S* equal sections with a width of d_x and equidistant from each other. Afterwards, draw a layout by connecting the points x_s using horizontal lines, with $x_s = a + c \cdot d_x$ for each $s = 0,1,2,\cdots,S$. Each action point inside the matrix is represented by x_s, where *s* is of $1,2,\cdots,S-1$. In this Equation (2), we use several computations to approximate the numerical layout of the problem. Here $t_n = nk$, where $n = 0,1,\cdots,NT$ and *t* is the time.

3.1. Crank-Nicolson Implicit Scheme

By using Crank-Nicholson technique to solve Equation (2) and integrating in a compact manner, we may obtain:

$$\left.\begin{aligned} u_t &= \frac{u_s^{n+1} - u_s^n}{k},\quad u = \frac{u_s^{n+1} + u_s^n}{2},\quad \delta_x u = \frac{u_{s+1}^{n+1} - u_{s-1}^{n+1} + u_{s+1}^n - u_{s-1}^n}{4h} \\ \delta_x^2 u &= \frac{u_{s+1}^{n+1} - 2u_s^{n+1} + u_{s-1}^{n+1} + u_{s+1}^n - 2u_s^n + u_{s-1}^n}{2h^2} \end{aligned}\right\}$$

Equation (2) may be solved for the second order implicit CN scheme by replacing the previous terms

$$\left.\begin{aligned} &u_s^{n+1} - u_s^n + Q_1\left(u_s^{n+1} + u_s^n\right)\left[\left(u_{s+1}^{n+1} - 2u_s^{n+1} + u_{s-1}^{n+1}\right) + \left(u_{s+1}^n - 2u_s^n + u_{s-1}^n\right)\right] \\ &+ Q_2\left(u_s^{n+1} + u_s^n\right)\left[\left(u_{s+1}^{n+1} - u_{s-1}^{n+1}\right) + \left(u_{s+1}^n - u_{s-1}^n\right)\right] - k\left(u_s^{n+1} + u_s^n\right) + Q_3\left(u_s^{n+1} + u_s^n\right)^2 = 0 \\ &\text{where } Q_1 = -\frac{k}{4h^2},\ Q_2 = -\frac{3k}{4h},\ Q_3 = \frac{k}{2} \end{aligned}\right\} \tag{4}$$

The implicit approach implies that the accuracy is of $O\left(k^2+h^2\right)$, our nomenclature also includes u_s and U_s for the numerical and analytical solutions of points $\left(x_s,t_n\right)$. The Von-Neuman stability research of method (4) is used to assess the stability of the 2nd order implicit method, which demonstrates the unconditional stability of the scheme. Despite that the results are positive, the system is currently tri-diagonal. However, because of the large iteration size, the inclining at the tiniest n segments missing from each direction amplifies, but various methods, strategies that can be used to deal with similar issues, are more difficult to implement because of the high transfer speed. Due to the huge amount of computations, another numerical technique is required to solve this problem. When dealing with the linear system, the iterative approach is used. The CN is time consuming to implement it.

3.2. Fourth Order Implicit Scheme

A compact integration strategy, such as fourth order implicit scheme, may be used to solve Equation (2), which allows us to get

$$\left.\begin{aligned} u_t &= \frac{u_s^{n+1}-u_s^n}{k}, \quad u=\frac{u_s^{n+1}+u_s^n}{2} \\ \delta_x u &= \frac{-u_{s+2}^{n+1}+8u_{s+1}^{n+1}-8u_{s-1}^{n+1}+u_{s-2}^{n+1}-u_{s+2}^n+8u_{s+1}^n-8u_{s-1}^n+u_{s-2}^n}{24h} \\ \delta_x^2 u &= \frac{-u_{s+2}^{n+1}+16u_{s+1}^{n+1}-30u_s^{n+1}+16u_{s-1}^{n+1}-u_{s-2}^{n+1}}{24h^2} \\ &\quad + \frac{-u_{s+2}^n+16u_{s+1}^n-30u_s^n+16u_{s-1}^n-u_{s-2}^n}{24h^2} \end{aligned}\right\}$$

Equation (2) may be solved for the fourth order implicit scheme by replacing the previous terms

$$\left.\begin{aligned} &u_s^{n+1}-u_s^n+P_1\left(u_s^{n+1}+u_s^n\right)\left[u_{s+2}^{n+1}+16u_{s+1}^{n+1}-30u_s^{n+1}+16u_{s-1}^{n+1}-u_{s-2}^{n+1}\right] \\ &+P_1\left(u_s^{n+1}+u_s^n\right)\left[u_{s+2}^n+16u_{s+1}^n-30u_s^n+16u_{s-1}^n-u_{s-2}^n\right] \\ &+P_2\left(u_s^{n+1}+u_s^n\right)\left[u_{s+2}^{n+1}+8u_{s+1}^{n+1}-8u_{s-1}^{n+1}+u_{s-2}^{n+1}\right] \\ &+P_2\left(u_s^{n+1}+u_s^n\right)\left[u_{s+2}^n+8u_{s+1}^n-8u_{s-1}^n+u_{s-2}^n\right]-k\left(u_s^{n+1}+u_s^n\right) \\ &\text{where } P_1=-\frac{k}{24h^2},\ P_2=-\frac{3k}{24h},\ P_3=\frac{k}{2} \end{aligned}\right\} \tag{5}$$

3.3. Algorithm 1

In order to develop a Newton iterative approach, we must first determine the Jacobian. The Jacobian matrix shrinks to a row vector $\nabla^{\mathrm{T}}g$ since all of the function's partial derivatives are in the same row for $g:R^n\to R$. This means that the Jacobian is the transpose of the function's slope, which is equivalent to $J_g=\nabla^{\mathrm{T}}g$.

$$F\left(H\right)=0 \tag{6}$$

where

$$\underline{H} \approx \left[u^{n+1}\right] = \left[H_1, H_2, \cdots, H_{2S-2}\right]^{\mathrm{T}} \tag{7}$$

$$\underline{u}^{n+1} = \left[u_1^{n+1}, u_2^{n+1}, \cdots, u_{S-1}^{n+1}\right]^{\mathrm{T}} \tag{8}$$

$\underline{H} = \left[H_1, H_2, \cdots, H_{2S-2}\right]^{\mathrm{T}}$ where $H_1, H_2, \cdots, H_{2S-2}$ are nonlinear equations. Newton's iterative approach can be applied by using following steps

1) Set an initial approximation of $u(0)$ as starting point

2) Up till the point of convergence for $k = 0$

- Determination of linear system $C\left(u^k\right)\Delta u^k = -W\left(u^k\right)$
- Set $u^{k+1} = u^k + \Delta u^k$

An analytically computed Jacobian is $C\left(u^k\right)$, and the corrective variable is u^k. The starting estimate in the iteration process is the solution from the previous step. Every time step is terminated when $W\left(u^k\right)$

$$z = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_{s-1} \end{pmatrix} \approx u^{n+1} = \begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ u_3^{n+1} \\ \vdots \\ u_{s-1}^{n+1} \end{pmatrix}$$

$$u_S^{n+1} = u_S^n = \beta$$

For First Iteration

$$\frac{\partial g_1}{\partial z_1} = 1 + Q_1\left[u_2^{n+1} - 2u_1^{n+1} + u_0^{n+1} + u_2^n - 2u_1^n + u_0^n - 2u_1^{n+1} - 2u_1^n\right] + Q_2\left[u_2^{n+1} - u_0^{n+1} + u_2^n - u_0^n\right] + 2Q_3\left[u_1^{n+1} + u_1^n\right] - k$$

$$\frac{\partial g_1}{\partial z_2} = Q_1\left[u_1^{n+1} + u_1^n\right] + Q_2\left[u_1^{n+1} + u_1^n\right]$$

For Intermediate Iterations

$$g\left(u_{s-1}^{n+1}, u_s^{n+1}, u_{s+1}^{n+1}\right) = u_s^{n+1} - u_s^n + Q_1\left(u_s^{n+1} + u_s^n\right)\left[u_{s+1}^{n+1} - 2u_s^{n+1} + u_{s-1}^{n+1} + u_{s+1}^n - 2u_s^n + u_{s-1}^n\right] + Q_2\left(u_s^{n+1} + u_s^n\right)\left[u_{s+1}^{n+1} - u_{s-1}^{n+1} + u_{s+1}^n - u_{s-1}^n\right] - k\left(u_s^{n+1} + u_s^n\right) + Q_3\left(u_s^{n+1} + u_s^n\right)^2$$

$$\frac{\partial g_1}{\partial z_{s-1}} = Q_1\left[u_1^{n+1} + u_1^n\right] - Q_2\left[u_1^{n+1} + u_1^n\right]$$

$$\frac{\partial g_1}{\partial z_s} = 1 + Q_2\left[u_{s+1}^{n+1} - u_{s-1}^{n+1} + u_{s+1}^n - u_{s-1}^n\right] + 2Q_3\left[u_s^{n+1} + u_s^n\right] - k + Q_1\left[u_{s+1}^{n+1} - 2u_s^{n+1} + u_{s-1}^{n+1} + u_{s+1}^n - 2u_s^n + u_{s-1}^n - 2u_s^{n+1} - 2u_s^n\right]$$

$$\frac{\partial g_1}{\partial z_{s+1}} = Q_1\left[u_s^{n+1} + u_s^n\right] + Q_2\left[u_s^{n+1} + u_s^n\right]$$

For Final Iteration

$$g\left(u_{s-2}^{n+1}, u_{s-1}^{n+1}, \beta\right) = u_{s-1}^{n+1} - u_{s-1}^n + Q_1\left(u_{s-1}^{n+1} + u_{s-1}^n\right)\left[u_s^{n+1} - 2u_{s-1}^{n+1} + u_{s-2}^{n+1} + u_s^n - 2u_{s-1}^n + u_{s-2}^n\right]$$

$$+Q_2\left(u_{s-1}^{n+1}+u_{s-1}^{n}\right)\left[u_{s}^{n+1}-u_{s-2}^{n+1}+u_{s}^{n}-u_{s-2}^{n}\right]-k\left(u_{s-1}^{n+1}+u_{s-1}^{n}\right)+Q_3\left(u_{s-1}^{n+1}+u_{s-1}^{n}\right)^2$$

$$\frac{\partial g_1}{\partial z_{s-2}}=Q_1\left[u_{s-1}^{n+1}+u_{s-1}^{n}\right]-Q_2\left[u_{s-1}^{n+1}+u_{s-1}^{n}\right]$$

$$\frac{\partial g_1}{\partial z_{s-1}}=1+Q_1\left[u_{s}^{n+1}-2u_{s-1}^{n+1}+u_{s-2}^{n+1}+u_{s}^{n}-2u_{s-1}^{n}+u_{s-2}^{n}-2u_{s-1}^{n+1}-2u_{s-1}^{n}\right]$$
$$+Q_2\left[u_{s}^{n+1}-u_{s-2}^{n+1}+u_{s}^{n}-u_{s-2}^{n}\right]+2Q_3\left[u_{s-1}^{n+1}+u_{s-1}^{n}\right]-k$$

3.4. Algorithm 2

It is evident that the structure is tridiagonal and that the Thomas technique can be applied to address it. In general, the following is how a tridiagonal system is written. Tridiagonal system can be expressed in the following ways

$$c_s x_{s-1}+c_s x_{s-1}+d_s x_s+e_s x_{s+1} \quad \text{where } c_1=c_s=0$$

A matrix vector representation of the above system is possible

$$Au=b$$

where A is a coefficient matrix There is a column vector on the right. Our primary objective is to discover the u vector.

$$A=\begin{bmatrix}\beta_1 & \gamma_1 & 0 & 0 & 0 & \cdots 0\\ \alpha_2 & \beta_2 & \gamma_2 & 0 & 0 & \cdots 0\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\ \cdots & \cdots & \cdots & \alpha_{n-1} & \beta_{n-1} & \gamma_{n-1}\\ \cdots & \cdots & \cdots & \cdots & \alpha_n & \beta_n\end{bmatrix}$$

$$\underline{u}=\left[u_1,u_2,\cdots,u_s\right]^{\mathrm{T}} \tag{9}$$

$$\underline{b}=\left[b_1,b_2,\cdots,b_s\right]^{\mathrm{T}} \tag{10}$$

The implementation of the Thomas algorithm is demonstrated in the results by equating both sides of the $Au=S$ equation.

4. Error Norms

The precision and consistency of the methods is studied in terms of error norms specifically L_2 and L_∞ which can be expressed as:

$$RMSError=\sqrt{\frac{\sum_{p,q=1}^{L}\left(U_{p,q}-u_{p,q}\right)^2}{L\times L}} \tag{11}$$

$$L_\infty=\max_{1\le p\le P}\sum_{q=1}^{P}\left|\left(U_{p.q}-u_{p,q}\right)\right| \tag{12}$$

$$L_2=\sqrt{\rho\left(U_{p,q}-u_{p,q}\right)^t\left(U_{p,q}-u_{p,q}\right)} \tag{13}$$

where $u(x,y,t)$ and $U(x,y,t)$ represents the numerical and exact solutions

at the grid point $\left(x_p, y_q, t_n\right)$. In this method $\rho\left(U_{p,q} - u_{p,q}\right) = \max\left(\lambda\right)$ and λ is an eigen value of $\left(U_{p,q} - u_{p,q}\right)$ respectively.

5. Results and Discussion

In several application areas, such as electromagnetics, biomathematics, precise modelling of electric signals and water modeling takes more time. To calculate numerical derivatives effectively, we utilized a short step size along the grid line. MATLAB algorithms for the 1D nonlinear CDR Equation (2) were also constructed.

In this section, we examined two numerical finite difference algorithms. The fact that implicit schemes are always unconditionally stable, both of them are implicitly stated. Table 1 shows numerical findings that are compared to analytic results by modifying typical locations at time step size 0.01. Additionally, in Table 1, the error is reported as a measure of second order precision. Table 2 indicates that utilizing the fourth order implicit scheme, greater precision may be attained by stating approximate and analytic results at distinct locations. In the next two tables, the *RMS*, L_2, and L_{infnty} norms are provided. The error estimation of the CN scheme is shown in Table 3 and Table 4, respectively, for partition size of 100 and 200. Similarly, the behavior of the fourth order implicit scheme in terms of error estimates across partition sizes of 100 and 200, respectively, is explained in the Table 5 and Table 6.

Table 1. Analysis of CN scheme at 50 partition size and $t = 1$ for unknown $u\left(s,t\right)$.

Solution Comparison			
x	*U-Exact*	*u-CN*	Error
1.90	3.8210e1	3.8201e1	9.0e−3
2.98	6.5572e1	6.5538e1	3.40e−3
4.42	1.3471e2	1.3452e2	1.90e−3
6.94	4.7492e2	4.7334e2	1.58e−2
9.64	1.8320e3	1.8211e3	1.09e−2

Table 2. Analysis of fourth order scheme at 100 partition size, $h = 0.04$ and $t = 1$ for unknown $u\left(s,t\right)$.

Solution Comparison			
x	*U-Exact*	*u*-4th *Order*	Error
1.44	0.303493e2	0.303842e2	1.1e−5
2.08	0.418098e2	0.417973e2	1.25e−4
3.08	0.689338e2	0.689227e2	1.113e−4
4.04	1.114022e2	1.114008e2	1.391e−5
4.84	1.661925e2	1.661813e2	1.12e−4

Table 3. Calculating error norms of CN at different time for unknown $u(s,t)$.

Error estimation at 100 partition size and time step size = 0.001			
t	L_2-*CN*	L_∞-*CN*	*RMS-CN*
0.1	1.67e−3	2.67e−4	1.31e−3
0.5	2.67e−2	8.98e−3	1.66e−2
1	3.30e−2	5.10e−3	2.40e−2
1.5	5.12e−2	8.60e−2	3.30e−2
2	1.10e−1	7.03e−2	1.04e−1

Table 4. Calculating error norms of CN at different time for unknown $u(s,t)$.

Error estimation at partition size 200			
t	L_2-*CN*	L_∞-*CN*	*RMS-CN*
2	1.4142e−2	3.1307e−2	1.3136e−2
1.5	1.1224e−2	2.6091e−3	1.083e−2
1	6.3552e−3	8.3815e−4	4.3273e−3
0.5	3.0250e−3	4.6615e−4	2.0104e−3
0.1	5.6743e−4	2.1330e−5	3.6011e−4

Table 5. Calculating error norms of 4th order implicit scheme at different time for unknown $u(s,t)$.

Error estimation at 100 partition size			
t	L_2-4th *Order*	L_∞-4th *Order*	*RMS*-4th *Order*
0.1	5.2004e−4	1.4011e−5	2.1439e−4
0.5	7.6840e−4	9.0213e−4	3.8301e−4
1	1.2032e−3	2.2713e−4	1.0037e−3
1.5	3.5204e−2	1.7251e−3	2.8113e−2
2	3.1298e−1	2.4102e−2	1.9805e−1

Table 6. Calculating error norms of 4th order implicit scheme at different time for unknown $u(s,t)$.

Error estimation at 200 partition size			
t	L_2-4th *Order*	L_∞-4th *Order*	*RMS*-4th *Order*
2	2.8284e−2	6.0371e−2	1.1216e−2
1.5	2.005e−2	1.1955e−3	1.0167e−2
1	4.2102e−3	2.2050e−4	3.1153e−3
0.5	5.4394e−4	3.5737e−5	2.9945e−4
0.1	2.8284e−5	1.0038e−6	2.8312e−5

Finally, we investigated the accuracy of fourth order implicit scheme that were implemented on Equation (2). We employed norms in this investigation by modifying the space and time step sizes. Using different time step sizes, we may derive an error estimate as shown in Table 7. In this case, it suggests that precision improves when the step size is shrunk. Consequently, the accuracy of fourth order implicit scheme is discussed by varying the space step size in Table 8. It is evident from Table 7 and Table 8 that reducing the step size, whether it be in space or time, leads to higher accuracy in our calculation.

As shown in Figure 1, when the second order CN implicit scheme is used to the CDR problem, the numerical results are approaching to the analytical findings when the partition size is 50 and the k is 0.01. Despite the fact that the results are near, still substantial improvement is possible, as seen by Figure 1. Figure 2 shows that the results appear to be better with 75 partition size and t=1 as compared to Figure 1. Fourth order implicit scheme outperforms the second order CN approach for Equation (2) as demonstrated in Figure 3 and Figure 4, when compared to the two preceding figures.

Figure 5 indicates that decreasing the time step size of second order CN system can enhance the precision of the scheme, but that doing so is computationally intensive. Figure 6 shows a comparison of second and fourth order implicit methods for a 100 partition size and k = 0.0001. It illustrates that the numerical findings obtained from proposed methods are highly comparable to the obtained exact ones. It demonstrates that for very tiny time step sizes, both strategies can produce results, albeit at the expense of a significant increase in computational

Table 7. Calculating error norms of CN at different time step size for unknown $u(s,t)$.

Error estimation at grid size = 100			
k	L_2	L_∞	*RMS*
0.1	6.3692e−2	9.3550e−3	2.2067e−2
0.5	4.3210e−3	6.6382e−3	3.9477e−3
0.05	3.1400e−3	4.9956e−4	2.9033e−3
0.005	2.6369e−3	1.2032e−4	1.0386e−3
0.0005	5.9426e−4	2.4330e−5	4.0217e−4

Table 8. Calculating error norms of 4th order implicit scheme at different space step size for unknown $u(s,t)$.

Error estimation at 50 partition size and time = 0.1			
h	L_2-4th *Order*	L_∞-4th *Order*	*RMS*-4th *Order*
0.1	7.7141e−3	5.0023e−4	7.3214e−3
0.09	4.0391e−3	1.5259e−3	3.0391e−3
0.06	2.3321e−3	2.6234e−4	1.3781e−3
0.001	6.0121e−4	3.3210e−5	5.3312e−4

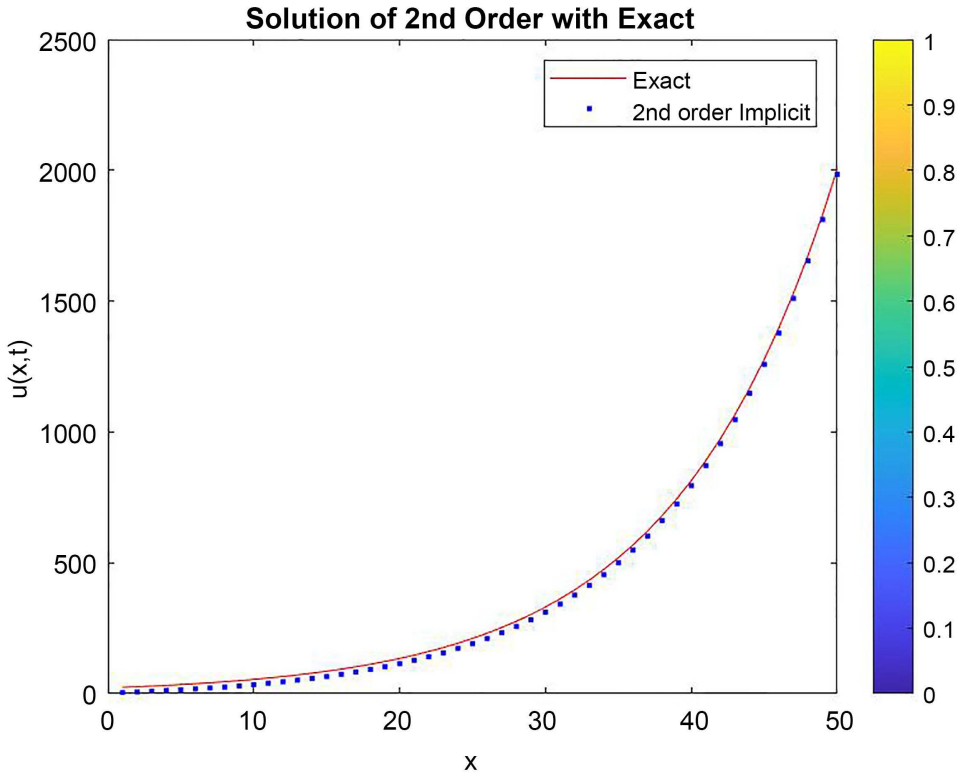

Figure 1. Exact and approximate results of second order CN scheme at 50 partition size and $k = 0.01$.

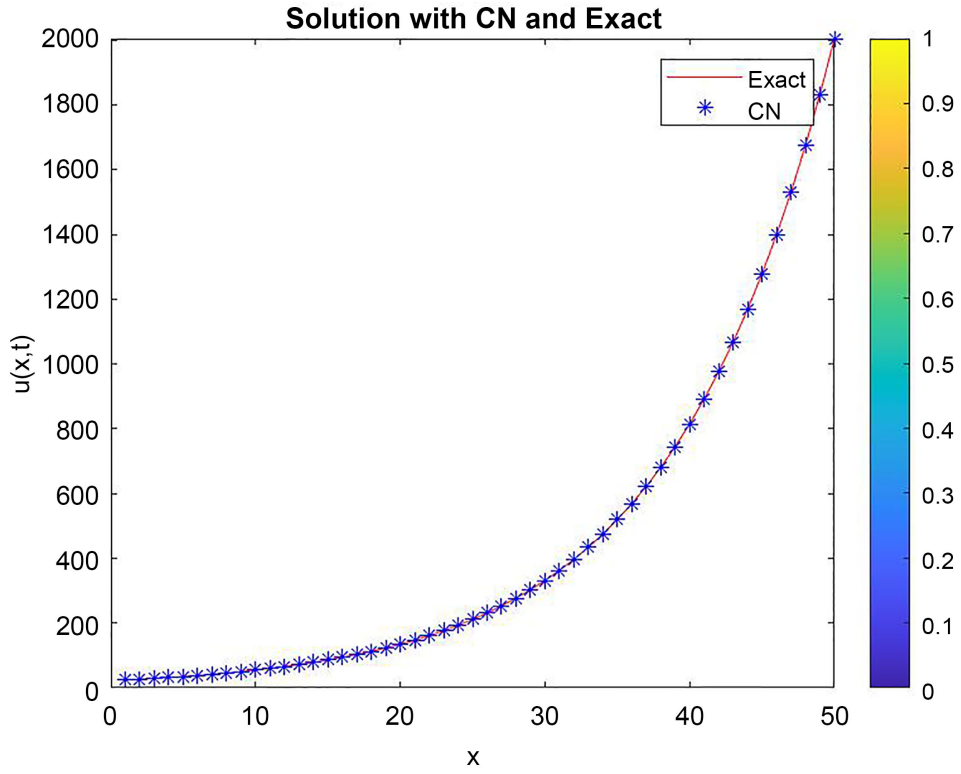

Figure 2. Exact and approximate results of second order CN scheme at 75 partition size and time = 1.

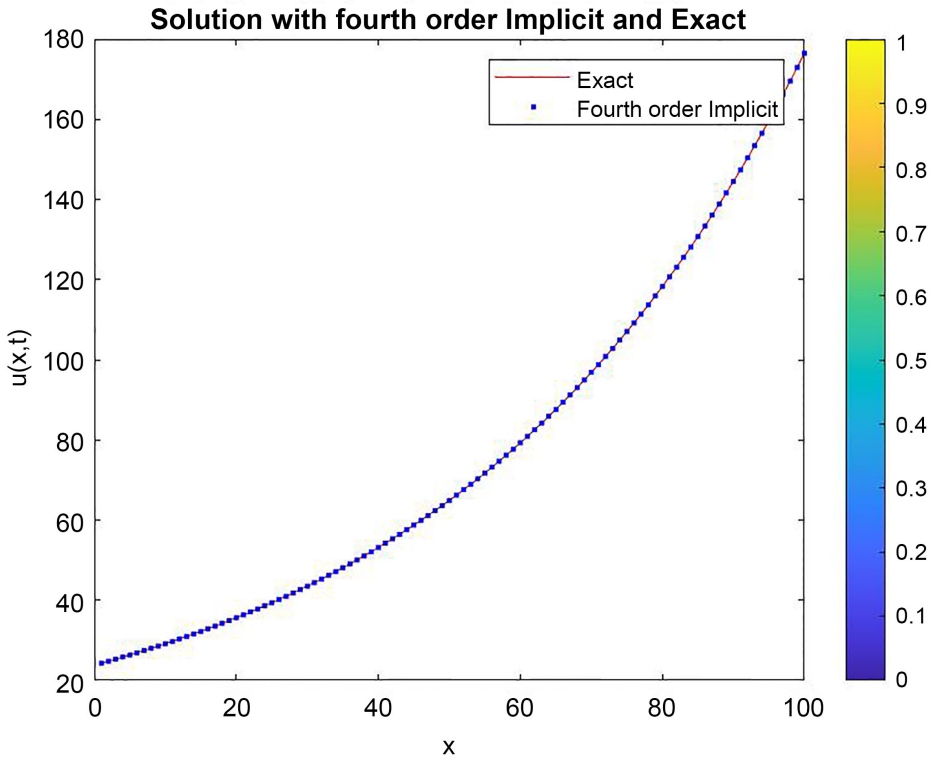

Figure 3. Exact and approximate results of fourth order implicit scheme at 100 partition size, time = 1 and $h = 0.04$.

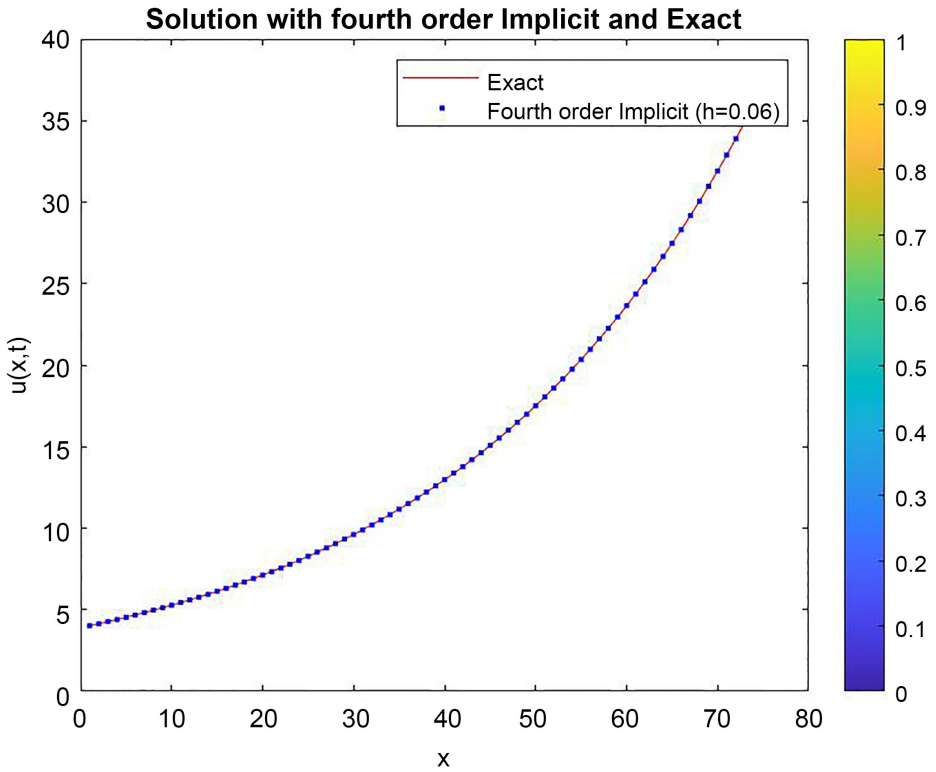

Figure 4. Exact and approximate results of fourth order implicit scheme at 75 partition size, time = 0.1 and $h = 0.06$.

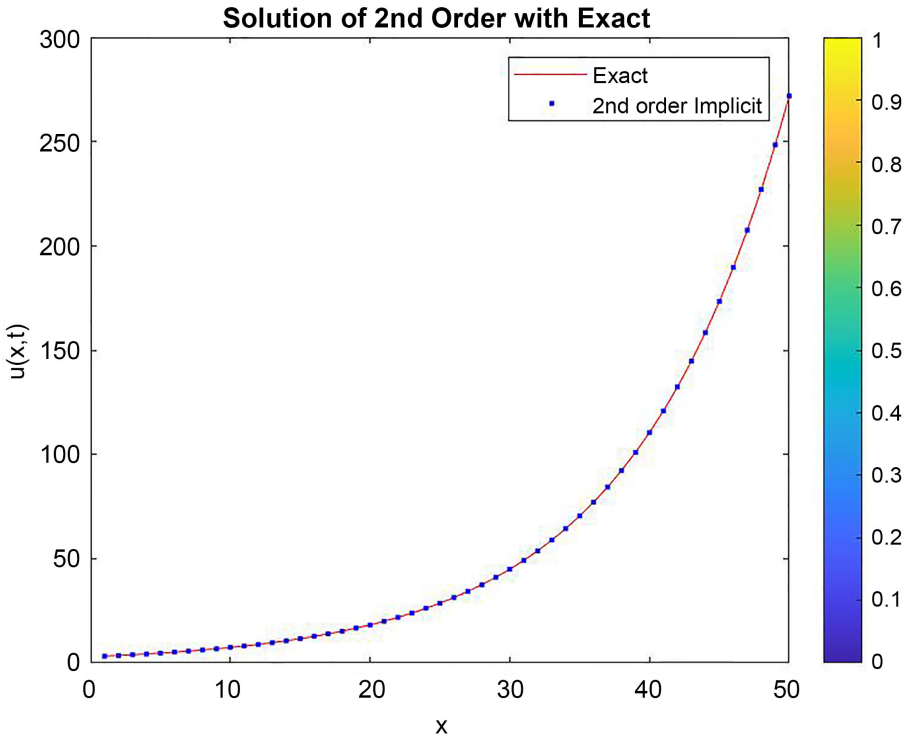

Figure 5. Exact and approximate results of second order CN scheme at 50 partition size and $k = 0.0001$.

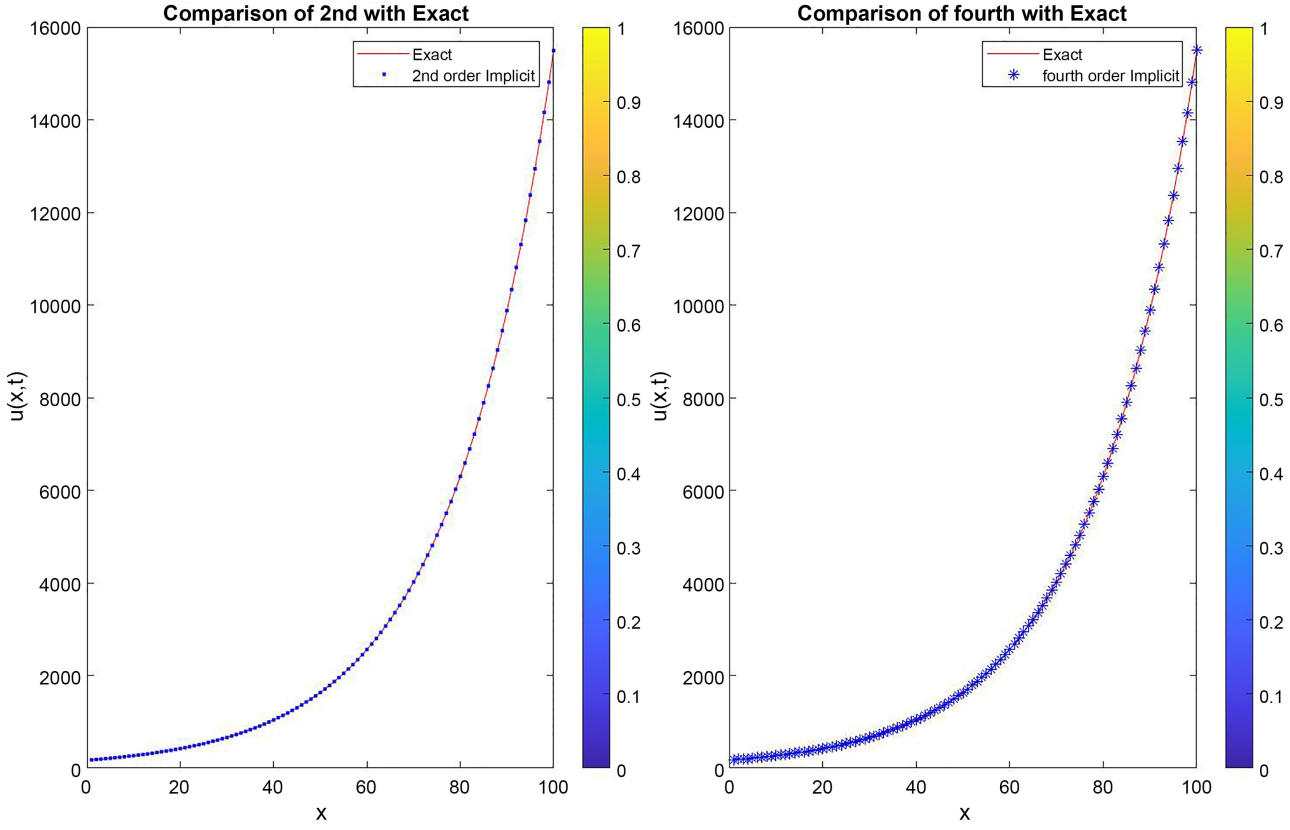

Figure 6. Comparison of fourth order and second order implicit schemes at 100 partition size and $k = 0.0001$.

cost while dealing with CN. As a result, for the one-dimensional nonlinear convection-diffusion-reaction equation, the fourth order implicit method provides better approximate results since it achieves higher accuracy while converging quickly and requiring less computational complexity.

6. Conclusion

Two distinct numerical methods are compared for solving partial differential equations with nonlinear reaction, convection, and diffusion terms: a Crank-Nicolson second order and a fourth order implicit finite-difference scheme. A thorough examination of the theoretical formulations of the suggested schemes was conducted. The effectiveness, accuracy, and stability of the two schemes are demonstrated by a compelling example. We have demonstrated that, even though the Crack-Nicolson method assures the existence of a solution for any step size, this technique is less precise. The accuracy study of the schemes has revealed that the application of high-order implicit algorithm yields substantially better results to those obtained using the traditional Crank-Nicolson approach. The error norms converged to zero when the partition size was increased, or the step size was decreased. Similar mathematical problems in biological, physical sciences, and technology might be addressed with the proposed scheme. This study may be further refined by comparing the efficiency and accuracy of currently utilized schemes with the finite volume schemes to determine the most appropriate scheme for the CDR equation.

Declarations

Conflicts of Interest

The authors state that they have no conflicts of interest to disclose in relation to the current study.

Authors Contribution

All authors contributed equally.

References

[1] Hossain, Md.A. (1999) Modeling Advective-Dispersive Transport with Reaction: An Accurate Explicit Finite Difference Model. *Applied Mathematics and Computation*, **102**, 101-108. https://doi.org/10.1016/S0096-3003(98)10036-X

[2] Simon, T. and Koya, P.R. (2016) Numerical Simulation of System of Time-Dependent Advection-Diffusion-Reaction Equations Describing River Pollution. *International Journal of Scientific Progress and Research*, **30**, 94-106. https://doi.org/10.9790/5728-1303023036

[3] Kachiashvili, K., Gordeziani, D., Lazarov, R. and Melikdzhanian. D. (2007) Modeling and Simulation of Pollutants Transport in Rivers. *Applied Mathematical Modeling*, **31**, 1371-1396. https://doi.org/10.1016/j.apm.2006.02.015

[4] Samalerk, P. and Pochai, N. (2018) Numerical Simulation of a One-Dimensional Water-Quality Model in a Stream Using a Saulyev Technique with Quadratic Interpolated

Initial-Boundary Conditions. *Abstract and Applied Analysis*, **2018**, Article ID: 1926519. https://doi.org/10.1155/2018/1926519

[5] Hillen, T. and Painter, K.J. (2009) A User's Guide to PDE Models for Chemotaxis. *Mathematical Biology*, **58**, Article No. 183. https://doi.org/10.1007/s00285-008-0201-3

[6] Di Costanzo, E., Ingangi, V., Angelini, C., Carfora, M.F., Carriero, M.V. and Natalini, R. (2016) A Macroscopic Mathematical Model for Cell Migration Assays Using a Real-Time Cell Analysis. *PLoS One*, **11**, e0162553. https://doi.org/10.1371/journal.pone.0162553

[7] Meghdadi, N., Soltani, M., Niroomand-Oscuii, H. and Yamani, N. (2020) Personalized Image-Based Tumor Growth Prediction in a Convection-Diffusion-Reaction Model. *Acta Neurologica Belgica*, **120**, 49-57. https://doi.org/10.1007/s13760-018-0973-1

[8] Alt, W. (1980) Biased Random Walk Models for Chemotaxis and Related Diffusion Approximations. *Journal of Mathematical Biology*, **9**, 147-177. https://doi.org/10.1007/BF00275919

[9] Sarra, S.A. (2012) A Local Radial Basis Function Method for Advection-Diffusion-Reaction Equations on Complexly Shaped Domains. *Applied Mathematics and Computation*, **218**, 9853-9865. https://doi.org/10.1016/j.amc.2012.03.062

[10] Idelsohn, S., Nigro, N., Storti, M. and Buscaglia, G. (1996) A Petrov-Galerkin Formulation for Advection-Reaction-Diffusion Problems. *Computer Methods in Applied Mechanics and Engineering*, **136**, 27-46. https://doi.org/10.1016/0045-7825(96)01008-0

[11] Principe, J. and Codina, R. (2010) On the Stabilization Parameter in the Subgrid Scale Approximation of Scalar Convection-Diffusion-Reaction Equations on Distorted Meshes. *Computer Methods in Applied Mechanics and Engineering*, **199**, 1386-1402. https://doi.org/10.1016/j.cma.2009.08.011

[12] Wang, H. and Liu, J. (2006) A Semi-Implicit Finite-Difference Approach for Two-Dimensional Coupled Burgers Equations. *SIAM Journal on Scientific Computing*, **23**, 1418-1438. https://doi.org/10.1137/S1064827500376181

[13] Kurganov, A., and Tadmor, E. (2000) New High-Resolution Central Schemes for Nonlinear Conservation Laws and Convection-Diffusion Equations. *Journal of Computational Physics*, **160**, 241-282. https://doi.org/10.1006/jcph.2000.6459

[14] Malatip, A., Wansophark, N. and Dechaumphai, P. (2006) Combined Streamline Upwind Petrov Galerkin Method and Segregated Finite Element Algorithm for Conjugate Heat Transfer Problems. *Journal of Mechanical Science and Technology*, **20**, 1741-1752. https://doi.org/10.1007/BF02916278

[15] Leveque, R.J. (2005) Finite Volume Methods for Hyperbolic Problems. 3rd Edition, Cambridge University Press, Cambridge.

[16] Phongthanapanich, S. and Dechaumphai, P. (2009) Combined Finite Volume and Finite Element Method for Convection-Diffusion-Reaction Equation. *Journal of Mechanical Science and Technology*, **23**, 790-801. https://doi.org/10.1007/s12206-008-1204-0

[17] Codina, R. (2000) On Stabilized Finite Element Methods for Linear Systems of Convection-Diffusion-Reaction Equations. *Computer Methods in Applied Mechanics and Engineering*, **188**, 61-82. https://doi.org/10.1016/S0045-7825(00)00177-8

[18] Huerta, A., Roig, B. and Donea, J. (2002) Time-Accurate Solution of Stabilized Convection-Diffusion-Reaction Equations: II—Accuracy Analysis and Examples. *Communications in Numerical Methods in Engineering*, **18**, 575-584.

https://doi.org/10.1002/cnm.518

[19] Oñate, E., Miquel, J. and Zárate, F. (2007) Stabilized Solution of the Multidimensional Advection-Diffusion-Absorption Equation Using Linear Finite Elements. *Computers & Fluids*, **36**, 92-112. https://doi.org/10.1016/j.compfluid.2005.07.003

[20] Pudykiewicz, J.A. (2006) Numerical Solution of the Reaction-Advection-Diffusion Equation on the Sphere. *Journal of Computational Physics*, **213**, 358-390. https://doi.org/10.1016/j.jcp.2005.08.021

[21] Kacur, J., Malengier, B. and Trojakov, E. (2010) Numerical Modelling of Convection-Diffusion-Adsorption Problems in 1D Using Dynamical Discretization. *Chemical Engineering Science*, **65**, 2301-2309. https://doi.org/10.1016/j.ces.2009.09.020

[22] Burman, E. and Fernández, M.A. (2009) Finite Element Methods with Symmetric Stabilization for the Transient Convection-Diffusion-Reaction Equation. *Computer Methods in Applied Mechanics and Engineering*, **198**, 2508-2519. https://doi.org/10.1016/j.cma.2009.02.011

[23] Nadukandi, P., Oñate, E. and Garcia, J. (2010) A High-Resolution Petrov-Galerkin Method for the 1D Convection-Diffusion-Reaction Problem. *Computer Methods in Applied Mechanics and Engineering*, **199**, 525-546. https://doi.org/10.1016/j.cma.2009.10.009

[24] Speleers, H., Manni, C., Pelosi, F. and Sampoli, M.L. (2012) Isogeometric Analysis with Powell-Sabin Splines for Advection-Diffusion-Reaction Problems. *Computer Methods in Applied Mechanics and Engineering*, **221-222**, 132-148. https://doi.org/10.1016/j.cma.2012.02.009

[25] Oñate, E., Miquel, J. and Nadukandi, P. (2016) An Accurate FIC-FEM Formulation for the 1D Advection-Diffusion-Reaction Equation. *Computer Methods in Applied Mechanics and Engineering*, **298**, 373-406. https://doi.org/10.1016/j.cma.2015.09.022

[26] Gharib, M., Khezri, M., Foster, S.J. and Castel, A. (2017) Application of the Meshless Generalised RKPM to the Transient Advection-Diffusion-Reaction Equation. *Computers & Structures*, **193**, 172-186. https://doi.org/10.1016/j.compstruc.2017.08.007

[27] Zhao, F., Li, J., Xiao, X. and Feng, X. (2019) The Characteristic RBF-FD Method for the Convection-Diffusion-Reaction Equation on Implicit Surfaces. *Numerical Heat Transfer*, *Part A*: *Applications*, **75**, 548-559. https://doi.org/10.1080/10407782.2019.1608771

[28] Erdogan, U., Sari, M. and Kocak, H. (2019) Efficient Numerical Treatment of Nonlinearities in the Advection-Diffusion-Reaction Equations. *International Journal of Numerical Methods for Heat & Fluid Flow*, **29**, 132-145. https://doi.org/10.1108/HFF-05-2017-0198

[29] Singh, A., Das, S., Ong, S.H. and Jafari, H. (2019) Numerical Solution of Nonlinear Reaction-Advection-Diffusion Equation. *Journal of Computational and Nonlinear Dynamics*, **14**, 041003. https://doi.org/10.1115/1.4042687

[30] Rauf, N., Halide, H., Haddade, A., Suriamihardja, D.A. and Azis, M.I. (2019) A Numerical Study on the Effect of the Material's Anisotropy in Diffusion Convection Reaction Problems. *Journal of Physics*: *Conference Series*, **1341**, 082014. https://doi.org/10.1088/1742-6596/1341/8/082014

[31] Singh, S., Bansal, D., Kaur, G. and Sircar, S. (2020) Implicit-Explicit-Compact Methods for Advection Diffusion Reaction Equations. *Computers & Fluids*, **212**, 104709. https://doi.org/10.1016/j.compfluid.2020.104709

[32] Lin, J., Xu, Y. and Zhang, Y. (2020) Simulation of Linear and Nonlinear Advec-

tion-Diffusion-Reaction Problems by a Novel Localized Scheme. *Applied Mathematics Letters*, **99**, 106005. https://doi.org/10.1016/j.aml.2019.106005

[33] Sengupta, S., Sengupta, T.K., Puttam, J.K. and Vajjala, K.S. (2020) Global Spectral Analysis for Convection-Diffusion-Reaction Equation in One and Two-Dimensions: Effects of Numerical Anti-Diffusion and Dispersion. *Journal of Computational Physics*, **408**, 109310. https://doi.org/10.1016/j.jcp.2020.109310

[34] Kim, A.S. (2020) Complete Analytic Solutions for Convection-Diffusion-Reaction Source Equations without Using an Inverse Laplace Transform. *Scientific Reports*, **10**, Article No. 8040. https://doi.org/10.1038/s41598-020-63982-w

[35] Puigferrat, A., de-Pouplana, I. and Oñate, E. (2020) FIC-FEM Formulation for the Multidimensional Transient Advection-Diffusion-Absorption Equation. *Computer Methods in Applied Mechanics and Engineering*, **365**, 112984. https://doi.org/10.1016/j.cma.2020.112984

[36] Ali, I., Haq, S., Nisar, K.S. and Arifeen, S.U. (2021) Numerical Study of 1D and 2D Advection-Diffusion-Reaction Equations Using Lucas and Fibonacci Polynomials. *Arabian Journal of Mathematics*, **10**, 513-526. https://doi.org/10.1007/s40065-021-00330-4

[37] Jain, A., Zhou, L. and Parhizi, M. (2021) Multilayer One-Dimensional Convection-Diffusion-Reaction (CDR) Problem: Analytical Solution and Imaginary Eigenvalue Analysis. *International Journal of Heat and Mass Transfer*, **177**, 121465. https://doi.org/10.1016/j.ijheatmasstransfer.2021.121465

[38] Savović, S., Drljača, B. and Djordjevich, A. (2021) A Comparative Study of Two Different Finite Difference Methods for Solving Advection-Diffusion Reaction Equation for Modeling Exponential Traveling Wave in Heat and Mass Transfer Processes. *Ricerche di Matematica*, 1-8. https://doi.org/10.1007/s11587-021-00665-2

[39] Blanco-Cocom, L., Botello-Rionda, S., Ordoñez, L.C. and Valdez, S.I. (2022) A Reaction-Convection-Diffusion Model for PEM Fuel Cells. *Finite Elements in Analysis and Design*, **201**, 103703. https://doi.org/10.1016/j.finel.2021.103703

[40] Shidfar, A., Babaei, A., Molabahrami, A. and Alinejadmofrad, M. (2011) Approximate Analytical Solutions of the Nonlinear Reaction-Diffusion-Convection Problems. *Mathematical and Computer Modelling*, **53**, 261-268. https://doi.org/10.1016/j.mcm.2010.08.014