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NUMERICAL SOLUTION OF NON-CONSERVATIVE LINEAR TRANSPORT PROBLEMS

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Abstract. In this study, trigonometric cubic B-spline differential quadrature method is developed for a linear transport problems constructed on the advection-diffusion equation. The weighting coefficients used in the derivative approximations are determined by using the proposed algorithm. Following the space discretization of the advection-diffusion equation, the resultant ODE system is integrated in time by using Rosenbrock implicit method of order four. The accuracy and validity of the proposed method are indicated by solving some initial boundary value problems (IBVPs) representing fade out of an initial positive pulse. The error between the analytical and the numerical solutions is measured by using the discrete maximum norm.
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1. Introduction

Advection-diffusion (AD) equation of the form

$$\frac{\partial u(x,t)}{\partial t}+\alpha\frac{\partial u(x,t)}{\partial x}-\beta\frac{\partial^2 u(x,t)}{\partial x^2}=0 \tag{1}$$

is widely used for various transport phenomena in various fields. In the equation, $u = u(x,t)$, α and β are the substance concentration, flow velocity, and diffusion coefficient, respectively. The AD equation appeared to explain the unsteady heat transfer within the film by reducing the number of independent variables from three to two by a similarity transformation [1]. The same equation is used to express the transport for the solute based on the mass conservation for a particular choice of the sink term as a function of solute concentration [2].According to Chatwin and Allen [3], the AD equation (1) with constant β [4] holds when the velocity field is statistically steady, the cross-sectional area is independent of x and t, and the elapsed time is sufficiently large compared with the time taken for thorough mixing of the contaminant over the cross-section area [5].
Having some analytical solutions in some cases, the AD equation attracts many researchers studying on the numerical methods field to check the accuracy and the validity of the new methods. A problem with steady state solution is numerically solved by two unconditionally stable fourth order compact implicit difference methods [6]. Several problems constructed on a one-dimensional form with constant coefficients of the AD equation are

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considered in the study of Dehghan [7]. The solutions of some initial-boundary value problems are obtained by various finite difference techniques covering second-order, third-order and fourth-order upwind explicit, the weighted two-level explicit methods in that study. Some various explicit methods containing the upwind explicit, the Lax-Wendroff and the upwind, the Crank-Nicolson, the modified Siemieniuch-Gladwell type implicit algorithms are constructed for the solution of a particular problem [8]. The equation is integrated in time with the Crank-Nicolson implicit method. Karahan's numerical approach determined the solutions of some initial-boundary value problems by implicit spreadsheet simulations with BTCS, upwind and Crank-Nicolson techniques [9]. A third order upwind spreadsheet simulation scheme is designed for the solutions of the AD equation modeling environment contamination [10]. Some unconditionally stable Saulyev explicit finite difference methods are also implemented for the solutions of some problems for the AD equation [11]. A sixth-order compact finite difference method combined with Runge-Kutta time integration technique is applied for three initial-boundary value problems modeling various transport phenomena [15]. Some high order finite difference schemes are also implemented for the numerical solutions of some problems for the AD equation[16].

Three problems covering pure advection case for the AD equation are numerically solved by the Galerkin-finite element methods in the study [12]. In another comperative study, Thongmoon and McKibbin[13] simulated transport problems by using natural cubic spline method and some standart finite difference methods. The weighted residual least squares method based on cubic B-splines is proposed with its error analysis for solute transport processes problems governed by the AD equation [14]. Dag et al. [17] set up a finite elements technique based on least square approach to solve the AD equation numerically. In the algorithm, the authors used both linear and quadratic B-spline shape functions. A high accurate algorithm based on classical and extended polynomial cubic B-spline collocation method derived for the AD equation by Irk et al. [18]. The problems in that study contains pure advective conservative substance transport and advective-diffusive transport.

Kaya [19] integrated the one-dimensional AD equation by using the differential quadrature approach based on polynomials and solved two initial boundary value problems as example. He also compared his results with the explicit and the implicit finite difference methods to check the performance of his technique. Kaya and Gharehbaghi' s experimental study compared various methods from three different method classes, finite volume, differential quadrature and finite difference schemes [20]. Korkmaz and Dag developed two differential quadrature approaches based on polynomial type cubic B-spline functions for the solutions of some initial boundary value problems for the AD equation [21]. In a recent study, two variations of the differential quadrature method using quartic and quintic B-spline functions as basis are combined with some Runge-Kutta methods of higher orders to determine the solutions of some transport problems set up with AD equation [22]. A detailed eigenvalue based stability analysis of the proposed methods is also reported. Korkmaz and Akmaz [23] developed a new differential quadrature technique based on the non-polynomial exponential type B-splines to solve conservative and non-conservative transport problems modeled by the AD equation. Nazir et al. [24] has developed a collocation method based on trigonometric cubic B-spline functions to solve various IBVPs for the AD equation.

Some of the methods to solve the AD equation are summarized above. In the present study, we derive a new technique in the class of differential quadrature methods to solve two IBVPs for the AD equation. Since Bellman et al. [25] suggested, various forms of differential quadrature method have been developed and implemented for various problems arising in different fields[26, 27, 28, 29, 30]. Some of these variations are based on polynomial cubic, quartic and quintic B-splines or exponential B-splines [21, 22, 23, 31, 32, 33, 34, 35, 36]. Different from these variations, we determine the weighting coefficients required for the derivative approximations by a new basis function set, trigonometric cubic B-spline functions. We solve a Dirichlet type initial-boundary value problem for the AD equation without ignoring the diffusion term. The space discretization of the governing equation will be carried out by the trigonometric cubic B-spline differential quadrature method(T3BSDQ). Using the differential quadrature approximations for the space derivatives of the dependent variable the AD equation is reduced to an ordinary differential equation system of order one in time variable. Then, the resultant system will be integrated in time by using implicit Rosenbrock third-fourth order Runge-Kutta method with degree three interpolant. The initial boundary value problem for the AD equation is chosen of the form

$$\frac{\partial u(x,t)}{\partial t}+\alpha\frac{\partial u(x,t)}{\partial x}-\beta\frac{\partial^2 u(x,t)}{\partial x^2}=0, \qquad a\leq x\leq b, \tag{2}$$

subject to the initial condition

$$u(x,0)=f(x), \qquad a\leq x\leq b, \tag{3}$$

and boundary conditions

$$u(a,t)=g_1(t), \qquad u(b,t)=g_2(t), \tag{4}$$

where α and β are real constants.

2. Trigonometric cubic B-spline differential quadrature method(T3BSDQ)

Let us consider a uniform grid distribution P of the finite real domain $[a,b]$ defined as $P: a=x_1<x_2<\ldots<x_N=b$, $h=x_i-x_{i-1}, i=2,3,...,N$. In differential quadrature method, the rth order derivative of the function $u(x,t)$ with respect to x at the distinct point x_i is approximated by the weighted functional values at each grid in the whole domain. The mathematical notation of the approximation is

$$\left.\frac{\partial u^{(r)}(x,t)}{\partial x^{(r)}}\right|_{x=x_i}=\sum_{j=1}^{N}w_{ij}^{(r)}u(x_j,t), \quad i=1,2,\ldots,N, \tag{5}$$

where $w_{ij}^{(r)}$ are weighting coefficients of rth order derivative approximation for fixed t [25]. In this study, we choose the test functions as the trigonometric cubic B-splines given in [37] as

$$C_i(x)=\frac{1}{\theta}\begin{cases}\omega^3(x_{i-2}) & , \quad [x_{i-2},x_{i-1}]\\ \omega(x_{i-2})(\omega(x_{i-2})\phi(x_i)+\omega(x_{i-1})\phi(x_{i+1}))+\phi(x_{i+2})\omega^2(x_{i-1}) & , \quad [x_{i-1},x_i]\\ \omega(x_{i-2})\phi^2(x_{i+1})+\phi(x_{i+2})(\omega(x_{i-1})\phi(x_{i+1})+\omega(x_i)\phi(x_{i+2})) & , \quad [x_i,x_{i+1}]\\ \phi^3(x_{i+2}) & , \quad [x_{i+1},x_{i+2}]\\ 0 & , \quad \text{otherwise}\end{cases} \tag{6}$$

where

$$\omega(x_i)=\sin\frac{x-x_i}{2},$$
$$\phi(x_i)=\sin\frac{x_i-x}{2},$$
$$\theta=\sin\frac{h}{2}\sin h\sin\frac{3h}{2}$$

.

Like other cubic B-splines[18, 38, 39], the trigonometric cubic B-spline set $\{C_0(x), C_1(x), ..., C_{N+1}(x)\}$ forms a basis for the functions defined over the domain $[a, b]$ [40].

2.1. **Weighting coefficients of the first order derivative approximations.**

In order to determine the weighting coefficients $w_{ij}^{(1)}$ of the first order derivative approximation, each trigonometric cubic B-spline function is substituted into the derivative approximation (5) resulting the following linear equation system:

$$\begin{aligned}
w_{i,-1}^{(1)}C_0(x_{-1}) + w_{i,0}^{(1)}C_0(x_0) + w_{i,1}^{(1)}C_0(x_1) &= C_0'(x_i)\\
w_{i,0}^{(1)}C_1(x_0) + w_{i,1}^{(1)}C_1(x_1) + w_{i,2}^{(1)}C_1(x_2) &= C_1'(x_i)\\
&\vdots\\
w_{i,m-1}^{(1)}C_m(x_{m-1}) + w_{i,m}^{(1)}C_m(x_m) + w_{i,m+1}^{(1)}C_m(x_{m+1}) &= C_m'(x_i)\\
&\vdots\\
w_{i,N}^{(1)}C_{N+1}(x_N) + w_{i,N+1}^{(1)}C_{N+1}(x_{N+1}) + w_{i,N+2}^{(1)}C_{N+1}(x_{N+2}) &= C_{N+1}'(x_i)
\end{aligned}$$

This system contains $N+2$ equations and $N+4$ unknowns. It should be noted that even though the grid points $x_{-1}, x_0, x_{N+1}, x_{N+2}$ are not in the problem domain, the nodal values of B-splines at those points are used to determine the weighting coefficients. Adding two more equations

$$\begin{aligned}
w_{i,-1}^{(1)}C_0'(x_{-1}) + w_{i,0}^{(1)}C_0'(x_0) + w_{i,1}^{(1)}C_0'(x_1) &= C_0''(x_i)\\
w_{i,N}^{(1)}C_{N+1}'(x_N) + w_{i,N+1}^{(1)}C_{N+1}'(x_{N+1}) + w_{i,N+2}^{(1)}C_{N+1}'(x_{N+2}) &= C_{N+1}''(x_i)
\end{aligned}$$

to the system, the number of equations and unknowns becomes equal. In the matrix form, the resulting linear equation system can be written as

$$\begin{bmatrix}
C_0'(x_{-1}) & C_0'(x_0) & C_0'(x_1) & & & & \\
C_0(x_{-1}) & C_0(x_0) & C_0(x_1) & & & & \\
 & C_1(x_0) & C_1(x_1) & C_1(x_2) & & & \\
 & & C_2(x_1) & C_2(x_2) & C_2(x_3) & & \\
 & & \ddots & \ddots & \ddots & & \\
 & & & C_N(x_{N-1}) & C_N(x_N) & C_N(x_{N+1}) & \\
 & & & & C_{N+1}(x_N) & C_{N+1}(x_{N+1}) & C_{N+1}(x_{N+2})\\
 & & & & C_{N+1}'(x_N) & C_{N+1}'(x_{N+1}) & C_{N+1}'(x_{N+2})
\end{bmatrix}
\begin{bmatrix}
w_{i,-1}^{(1)}\\ w_{i,0}^{(1)}\\ \vdots\\ w_{i,N+1}^{(1)}\\ w_{i,N+2}^{(1)}
\end{bmatrix}
=
\begin{bmatrix}
C_0''(x_i)\\ C_0'(x_i)\\ C_1'(x_i)\\ \vdots\\ C_{N+1}'(x_i)\\ C_{N+1}''(x_i)
\end{bmatrix}$$

Solving the linear equation system above for each $i, i = 1, 2, ..., N$ the weighting coefficients of the first order derivative approximation $w_{ij}^{(1)}$ are determined.

2.2. **Weighting coefficients of the second order derivative approximations.**

In a similar way, the weighting coefficients $w_{ij}^{(2)}$ of the second order derivative approximation can be determined. Substituting all trigonometric cubic B-spline functions into differential quadrature approximation equation (5) gives a linear equation system with $N+2$ equations and $N+4$ unknowns,

$$
\begin{aligned}
w_{i,-1}^{(2)}C_0(x_{-1}) + w_{i,0}^{(2)}C_0(x_0) + w_{i,1}^{(2)}C_0(x_1) &= C_0''(x_i)\\
w_{i,0}^{(2)}C_1(x_0) + w_{i,1}^{(2)}C_1(x_1) + w_{i,2}^{(2)}C_1(x_2) &= C_1''(x_i)\\
&\vdots\\
w_{i,m-1}^{(2)}C_m(x_{m-1}) + w_{i,m}^{(2)}C_m(x_m) + w_{i,m+1}^{(2)}C_m(x_{m+1}) &= C_m''(x_i)\\
&\vdots\\
w_{i,N}^{(2)}C_{N+1}(x_N) + w_{i,N+1}^{(2)}C_{N+1}(x_{N+1}) + w_{i,N+2}^{(2)}C_{N+1}(x_{N+2}) &= C_{N+1}''(x_i)
\end{aligned}
$$

In this case, we choose two parameters as $w_{i,-1}^{(2)} = w_{i,N+2}^{(2)} = 0$ for the convenience and calculate the remaining weighting coefficients by solving the linear equation system

$$
\begin{bmatrix}
C_0(x_{-1}) & C_0(x_0) & C_0(x_1) & & & & \\
 & C_1(x_0) & C_1(x_1) & C_1(x_2) & & & \\
 & & C_2(x_1) & C_2(x_2) & C_2(x_3) & & \\
 & & \ddots & \ddots & \ddots & & \\
 & & & C_N(x_{N-1}) & C_N(x_N) & C_N(x_{N+1}) & \\
 & & & & C_{N+1}(x_N) & C_{N+1}(x_{N+1}) & C_{N+1}(x_{N+2})
\end{bmatrix}
\begin{bmatrix}
w_{i,0}^{(2)}\\ \vdots \\ w_{i,N+1}^{(2)}
\end{bmatrix}
=
\begin{bmatrix}
C_0''(x_i)\\ C_1''(x_i)\\ \vdots \\ C_{N+1}''(x_i)
\end{bmatrix}
$$

3. Discretization and Application of Boundary Conditions

When the differential quadrature approximates are substituted in to the AD equation (2) instead of the terms $\frac{\partial u(x,t)}{\partial x}$ and $\frac{\partial^2 u(x,t)}{\partial x^2}$, it reduces (in the nodal functional value form) to

$$
\left.\frac{\partial u(x,t)}{\partial t}\right|_{x=x_i} = -\alpha\sum_{j=1}^{N} w_{ij}^{(1)}u(x_j,t) + \beta\sum_{j=1}^{N} w_{ij}^{(2)}u(x_j,t) \tag{7}
$$

where $1 \le i \le N$ and the time variable t is assumed to be fixed. Application of the boundary condition given in (4) gives the ordinary differential equation system

$$
\begin{aligned}
\left.\frac{\partial u(x,t)}{\partial t}\right|_{x=x_i} &= -\alpha\sum_{j=2}^{N-1} w_{ij}^{(1)}u(x_j,t) + \beta\sum_{j=2}^{N-1} w_{ij}^{(2)}u(x_j,t)\\
&\quad + (-\alpha w_{i1}^{(1)} + \beta w_{i1}^{(2)})g_1(t) + (-\alpha w_{iN}^{(1)} + \beta w_{iN}^{(2)})g_2(t)
\end{aligned} \tag{8}
$$

Now, the ordinary differential equation system of the unknowns $u_2(t) = u(x_2,t)$, $u_3(t) = u(x_3,t)$, …, $u_{N-1}(t) = u(x_{N-1},t)$ can be integrated in time by using any algorithm. Due to its large stability region we prefer Rosenbrock' s implicit third-fourth order algorithm[41].

4. Test Problem 1

The initial boundary value problem demonstrating the fade out of an initial pulse is constructed with the initial condition

$$
u(x,0) = \exp\left(-\frac{(x-x_0)^2}{\beta}\right) \tag{9}
$$

and the homogeneous Dirichlet boundary conditions

$$
\begin{aligned}
u(0,t) &= 0\\
u(9,t) &= 0
\end{aligned} \tag{10}
$$

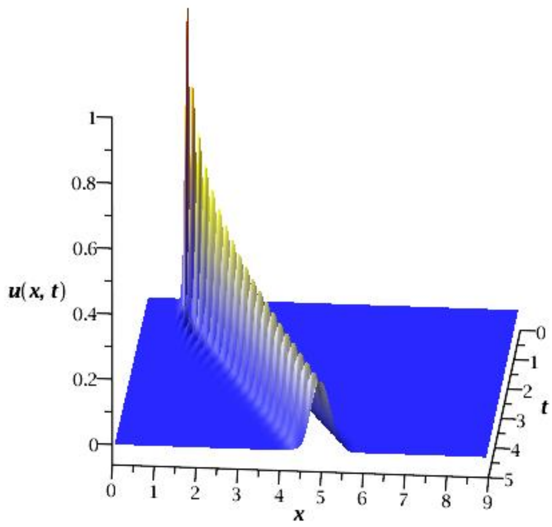

Figure 1. Fade out of an initial pulse simulation

at both ends of the problem interval $[0, 9]$. This problem models fade out of an initial pulse of unit height and centered at $x = x_0$ initially. The analytical solution of this problem is given by [42] as:

$$u(x,t) = \frac{1}{\sqrt{4t+1}} \exp\left(-\frac{(x - x_0 - \alpha t)^2}{\beta(4t+1)}\right) \tag{11}$$

The initial pulse moves along the horizontal axis with the velocity α. Due to effects of both advective and diffusive terms, the initial pulse fades out as it travels. In order to accomplish the simulation, the diffusion coefficient β, the velocity α and the initial peak position x_0 are fixed as 0.005, 0.8 and 1, respectively. The solution algorithm for the simulation of the motion is run till the terminating time $t = 5$. The simulation is plotted for $\Delta t = 0.25$ and $h = 0.05$ in Fig 1. The pulse travels to the right along the axis as its height decreases. The peak reaches to $x = 5$ at the end of the simulation as expected because of the constant speed $\alpha = 0.8$. In Fig 2, the maximum errors during the simulation is sketched. When examined, it can be concluded that the maximum error is decreasing as time goes owing to the fade out. This situation will keep till the pulse crashes to the right end of the domain. In order to see the effect of the choice of space step length in the method, we have tested the same algorithm for various values of h with a fixed time step length Δt. The maximum errors at the terminating time $t = 5$ are tabulated in Table 1 for various space step lengths. Even though, to reduce the space step length from 0.2 to 0.1 improves the accuracy of the results in decimal digits, the reduction of it to 0.05 does not provide such an improvement in results.

5. Test Problem 2

Another fade out problem for the AD equation is constructed with the initial condition

$$u(x,0) = exp(-\frac{(x - x_0)^2}{2\delta_0^2}) \tag{12}$$

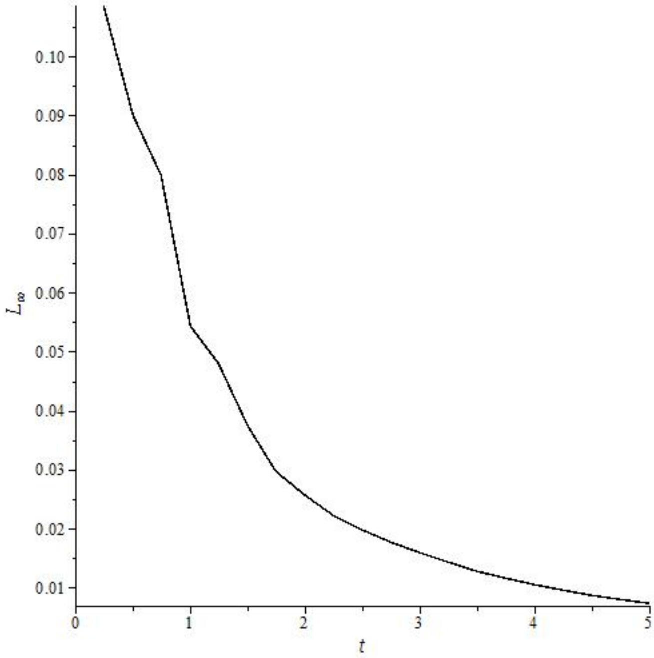

FIGURE 2. Maximum error-time graph for Problem 1

TABLE 1. Maximum errors

h	N	Δt	Maximum error
0.2	46	0.25	2.576×10^{-2}
0.1	91	0.25	7.841×10^{-3}
0.05	181	0.25	7.401×10^{-3}

where x_0 is the initial peak position. The homogeneous Dirichlet boundary data at both ends are used due to being compatible with the property $u(x,t) \to 0$ as $|x| \to 0$ of the analytical solution. This solution also represents a non-conservative fade out of an initial pulse of unit height as propagating to the right along the horizontal axis, Fig 3. The analytical solution of this problem is

$$u(x,t) = \left(\frac{\delta_0}{\delta_0^2 + 2\beta t}\right) exp\left(-\frac{(x - x_0 - \alpha t)^2}{2\delta^2}\right) \tag{13}$$

where $\delta^2 = \delta_0^2 + 2\beta t$[43]. The numerical solution of this problem is achieved by using the discretization parameters $h = 0.02$ and $\Delta t = 0.1$ in the finite problem interval $[0, 2]$. In order to reduce the boundary effect, the simulation is ended at the time $t = 1.0$. The numerical simulation of the problem is observed in a good accordance with the analytical solution and the results of the previous study [43]. The maximum error norm values are depicted in Fig 4. Parallel to the fade out of the initial pulse the error between the numerical solution and the analytical solution also decreases as time proceeds.

The effect of the number of the points used in the space discretization is also studied, Table 2. The number of points is chosen as 26 in the first experiment. Then, the maximum error is measured in three decimal digits. When the space step size is decreased half, the maximum error is determined in ten decimal digits at the simulation ending time. The increase of the number of points to 101 does not improve the results in decimal digits.

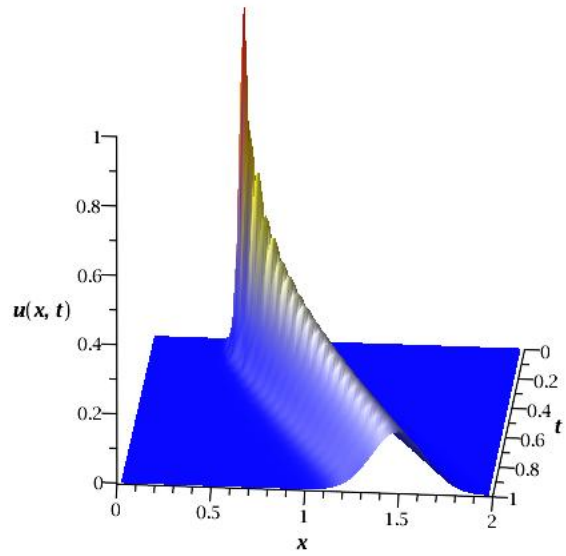

Figure 3. Fade out of an initial pulse of unit height

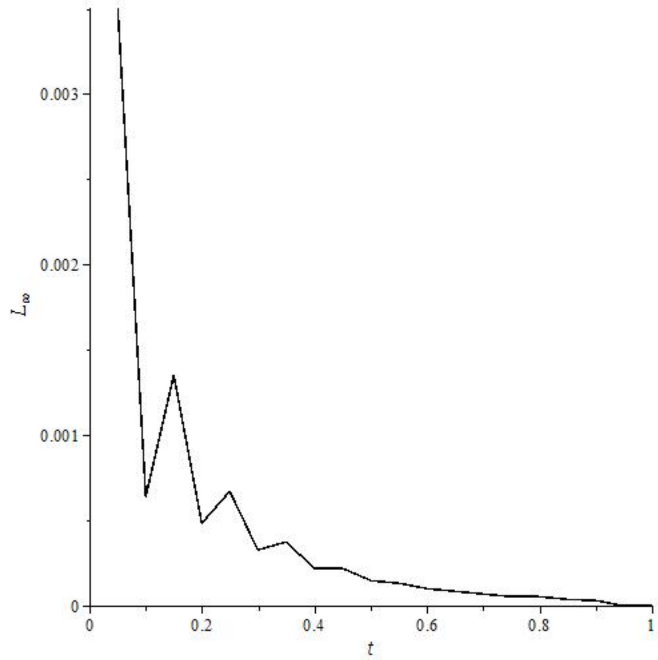

Figure 4. Maximum error-time graph for Problem 2

6. Conclusion

In the study, we derive a new differential quadrature technique to calculate the weighting coefficients in a semi-explicit form. Substituting trigonometric cubic B-spline into the fundamental differential quadrature approximation for each distinct point in the problem

TABLE 2. Maximum errors at various time for the Problem 2 at $t = 1$

h	N	Δt	Maximum error
0.08	26	0.1	2.872×10^{-3}
0.04	51	0.1	4.064×10^{-10}
0.02	101	0.1	4.905×10^{-10}

interval leads linear systems of equations with three-banded coefficient matrix. Solving this system, we determine the weighting coefficients of the derivative approximations at nodes. Substituting the space derivative approximations obtained by the differential quadrature method into the AD equation, we construct a system of ordinary differential equation of order one in time variable. Then, we integrate this system with respect to time variable by implicit third-fourth order Rosenbrock method due to its strong stability properties. In order to see the validity of the suggested algorithm, we solve some IBVPs for the AD equation. The simulation plots of the numerical results show that the results are in a good agreement with the analytical results. The plots indicating the maximum errors agree that the errors decrease as time goes due to accuracy, validity and stability of the method and the natures of the models. The implementation of the suggested algorithm can be extended to the other problems for the nonlinear equations and systems.

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