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The use of the Sinc-collocation method for solving steady-state concentrations of carbon dioxide absorbed into phenyl glycidyl ether

Fatemeh Zabihi
Department of Applied Mathematics, Faculty of Mathematical Science, University of Kashan, Kashan, 87317-51167, Iran.

Abstract

In this paper, the Sinc-collocation method is applied to solve a system of coupled nonlinear differential equations that report the chemical reaction of carbon dioxide CO_2 and phenyl glycidyl ether in solution. The model has Dirichlet and Neumann boundary conditions. The given scheme has transformed this problem into some algebraic equations. The approach is quite simple to handle and the new numerical solutions are compared with some known solutions, which shows that the new technique is accurate and efficient.

Keywords. Sinc functions, Collocation method, Carbon dioxide, Phenyl glycidyl ether, Boundary value problem.
2010 Mathematics Subject Classification. 65L10, 34B15.

1. Introduction

Various important physical, chemical, mechanical, and biological phenomena in nature are described mathematically using linear or non-linear differential equations. For example, in chemistry, we have used a system of nonlinear ordinary differential equations to describe the reaction between carbon dioxide and phenyl glycerol ether. A dual model of nonlinear differential equations for the solution of CO_2 and PGE concentration in steady-state is given in [12] as

$$\frac{d^2u}{d\xi^2} = \frac{\alpha_1 u(\xi)v(\xi)}{1+\beta_1 u(\xi)+\beta_2 v(\xi)}, \tag{1.1}$$

$$\frac{d^2v}{d\xi^2} = \frac{\alpha_2 u(\xi)v(\xi)}{1+\beta_1 u(\xi)+\beta_2 v(\xi)}, \tag{1.2}$$

with boundary conditions of Dirichlet and Neumann types:

$$u(0)=1,\ u(1)=\kappa,\ v'(0)=0,\ v(1)=1, \tag{1.3}$$

where $u(\xi)$ and $v(\xi)$ represent the dimensionless concentrations of CO_2 and PGE, respectively. Also $\alpha_i, \beta_i : i=1,2$ are numerical constants, ξ represents the dimensionless distance measured from the center and κ represents the dimensionless concentration of CO_2 on the surface of the catalyst.

Carbon dioxide is obtained from the chemical combination of two oxygen atoms and one carbon atom. Carbon dioxide is present in the Earth's atmosphere, but it has a low concentration and is considered a greenhouse gas. Today, we see the optimal use of carbon dioxide gas in oil recycling, welding, fire re-extinguishers, air guns, and coffee decaffeination. Recently, due to the dangers of greenhouse gases in the earth's atmosphere, some authors have investigated methods of chemical stabilization of carbon dioxide. The reaction between CO_2 and phenyl glycidyl ether (PGE) in solution is one of these chemical stabilizations. The chemical reaction between carbon dioxide solutions and PGE using The TEACPMS41 catalyst has been reviewed by Park et al in [3, 4].

A solution to this problem is found in very few numerical analysis articles. Authors in [5, 7] have used the Adomin decomposition method to solve this problem. In [14], the residual method is applied to solve this problem. The

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Corresponding author. Email: zabihi@kashanu.ac.ir.

variational iteration method was used by Al-Jawari and Radhi in [2] to solve the problem (1.1-1.3). In addition, these authors and Raham presented another iterative method in [1]. Singha and Wazwaz obtained approximate numerical solutions via the optimal homotopy analysis method [12]. Recently, Zabihi in [23] solved these coupled equations by the Chebyshev finite difference method.
This problem belongs to the category of second-order differential equations that can be solved by different numerical methods [15–22]. A new method has been used in this article, which is completely different from the method used by the author for this problem in [23]. The combination of the collocation method and the Sinc method is our plan to obtain the numerical solution to this problem. Concepts and general definitions of Sinc function approximation can be found in [6, 13]. We have seen the use of the Sinc method in the last few decades to solve various problems, including Troesch's problem [8], Blasius equation [9], nonlinear two-point boundary value problems arising in chemical reactor theory [10] and the coupled model of concentrations of oxygen and carbon substrate within a microbial floc particle [11].
The rest of this paper is organized as follows: In the next section, the Sinc function method and its features are reviewed. We apply the Sinc-collocation method to solve the studied system in section 3. In section 4, the numerical solutions for the problem (1.1)-(1.3) with the proposed scheme are presented. Also, by comparing the new results with the results in the literature, we show the correctness of our results. Finally, in section 5, we finish the study with conclusions.

2. Sinc function approximation

In this section, some of the basic definitions of Sinc functions that are necessary for our further development are provided. A Sinc function for $\xi \in \mathbb{R}$ is a function of form the books [6, 13]:

$$Sinc(\xi) = \begin{cases} \frac{\sin(\pi\xi)}{\pi\xi}, \ \xi \neq 0, \\ 1, \ \xi = 0. \end{cases}$$

The translated Sinc functions for $h > 0$, and $k \in \mathbb{Z}$ with evenly spaced points are defined by

$$S(k,h)(\xi) \equiv Sinc(\frac{\xi - kh}{h}) = \begin{cases} \frac{\sin[\frac{\pi}{h}(\xi - kh)]}{\frac{\pi}{h}(\xi - kh)}, \ \xi \neq kh, \\ 1, \ \xi = kh. \end{cases} \tag{2.1}$$

For a function of $f(\xi)$ in the set of real numbers and for $h > 0$, the following estimate is called Cardinal Whitaker expansion of f whenever this series converges:

$$C(f,h)(\xi) = \sum_{k=-\infty}^{\infty} f(kh) Sinc(\frac{\xi - kh}{h}).$$

In [6], many features of the Whittaker cardinal expansion have been published. Stenger states in [13] that the function f defined in the above relation is an analytic function on D_E which is defined as follows. If $\mathbb{C}$ is the set of complex numbers, for a certain $d > 0$, we define

$$D_E = \{z \in \mathbb{C} : |arg(\frac{z}{1-z})| < d \leq \frac{\pi}{2}\},$$

and let $\phi(z) = \ln(\frac{z}{1-z})$ be the conformal map of a simply connected region D_E onto the infinite strip

$$D_S = \{z \in \mathbb{C} : |Im(z)| < d \leq 2\}.$$

Let us introduce the temporary symbol $S(k,h)(\phi(\xi))$ for $S(k,h)o\phi(\xi)$ because the problem (1.1)-(1.3) in the interval $[0,1]$ is defined, so we use the Sinc function transferred to this interval and let

$$S_k(\xi) \equiv S(k,h)o\phi(\xi) = Sinc(\frac{\phi(\xi) - kh}{h}), \tag{2.2}$$

and the rang of $\psi = \phi^{-1}$ on $\mathbb{R}$ is $(0,1)$. The Sinc points grid corresponding to uniform nodes $\{kh\}_{k=-\infty}^{\infty}$ in the set of real numbers $\mathbb{R}$ is defined as follows

$$\xi_k = \psi(kh) = \frac{e^{kh}}{1+e^{kh}}, \ k \in \mathbb{Z}. \tag{2.3}$$

Now, we recall the following definition and theorem for our purpose.

Definition 2.1. Suppose that the set $M(D_E)$ contains all the analytic functions f in D_E that apply in the following conditions:

$$\lim_{\tau\to\pm\infty} \int_{\psi(\tau+L)} |f(z)dz| \to 0,$$

$$N(F) = \int_{\partial D_E} |f(z)dz| < 0,$$

where $L = \{iy : |y| < d \leq \frac{\pi}{2}\}$ and ∂D_E is the boundary of D_E.

The following result was proved in [13].

Theorem 2.2. *Assume that $\phi' f \in M(D_E)$ then for all $\xi \in \Gamma$, we have*

$$|f(\xi) - \sum_{j=-\infty}^{\infty} f(\xi_j)S_j(\xi)| \leq \frac{N(f\phi')}{2\pi d \sinh(\frac{\pi d}{h})} \leq \frac{2N(f\phi')}{\pi d} e^{\frac{-\pi d}{h}}.$$

Furthermore, if there exist positive constants C and α such that $|f(\xi)| \leq Ce^{-\alpha|\phi(\xi)|}, \xi \in \Gamma$, and if the selection $h = \sqrt{\frac{\pi d}{\alpha N}} \leq \frac{2\pi d}{\ln 2}$ is made, then

$$|f(\xi) - \sum_{j=-N}^{N} f(\xi_j)S_j(\xi)| \leq C_2\sqrt{N}e^{-\sqrt{\pi d\alpha N}}, \ \xi \in \Gamma,$$

so that C_2 depends only on α, d and f.

The above theorem shows the convergence rate of exponential order for the Sinc numerical method [6, 13]. Furthermore, the derivatives of Sinc basis functions can be approximated at the nodes as [6, 13]:

$$\delta_{k,j}^{(0)} = [S(k,h)o\phi(\xi)]|_{\xi=\xi_j} = \begin{cases} 1, \ k=j, \\ 0, \ k \neq j, \end{cases} \tag{2.4}$$

$$\delta_{k,j}^{(1)} = \frac{d}{d\phi}[S(k,h)o\phi(\xi)]|_{\xi=\xi_j} = \frac{1}{h}\begin{cases} 0, \ k=j, \\ \frac{(-1)^{j-k}}{j-k}, \ k \neq j, \end{cases} \tag{2.5}$$

$$\delta_{k,j}^{(2)} = \frac{d^2}{d\phi^2}[S(k,h)o\phi(\xi)]|_{\xi=\xi_j} = \frac{1}{h^2}\begin{cases} \frac{-\pi^2}{3}, \ k=j, \\ \frac{-2(-1)^{j-k}}{(j-k)^2}, \ k \neq j. \end{cases} \tag{2.6}$$

3. Solving Equations (1.1)-(1.3) by Sinc method

For the boundary conditions in (1.3), it can be seen that the Sinc basis functions $S_k(\xi)$ do not have a derivative when ξ tends to 0, therefore, we change the Sinc basis functions as $\frac{S_k(\xi)}{\phi'(\xi)}$. Here, we have that the first-order derivative of these modified Sinc basis functions is equal to zero when ξ approaches zero. Also, for the approximate solutions based on the Sinc basic functions to apply to other boundary conditions in (1.3), we define the following boundary basis functions, which are cubic polynomials. These polynomials are obtained by Hermite interpolation [10] at points 0 and 1, which are defined by

$$\mu_0(\xi) = \xi(1-\xi)^2, \ \mu_1(\xi) = (2\xi+1)(1-\xi)^2, \tag{3.1}$$

$$\mu_2(\xi) = (3-2\xi)\xi^2,\ \ \mu_3(\xi) = \xi^2(1-\xi), \tag{3.2}$$

By applying the Sinc-collocation method, we approximate $u(\xi)$ and $v(\xi)$ as

$$u_N(\xi) = U_N(\xi) + p(\xi),\ \ v_N(\xi) = V_N(\xi) + q(\xi), \tag{3.3}$$

where

$$U_N(\xi) = \sum_{k=-N}^{N} a_k \frac{S_k(\xi)}{\phi'(\xi)} = \xi(1-\xi)\sum_{k=-N}^{N} a_k S_k(\xi), \tag{3.4}$$

and

$$V_N(\xi) = \sum_{k=-N}^{N} b_k \frac{S_k(\xi)}{\phi'(\xi)} = \xi(1-\xi)\sum_{k=-N}^{N} b_k S_k(\xi). \tag{3.5}$$

In addition, $p(\xi)$ and $q(\xi)$ are chosen as linear combinations of $\mu_j(\xi) : j = 0,1,2,3$ in (3.1)-(3.2). In order for $u_N(\xi)$ and $v_N(\xi)$ to apply in boundary condition (1.3), the boundary parts of $p(\xi)$ and $q(\xi)$ are written in the following forms:

$$p(\xi) = a_{N-1}\mu_0(\xi) + \mu_1(\xi) + \kappa\mu_2(\xi) + a_{N+1}\mu_3(\xi), \tag{3.6}$$

$$q(\xi) = b_{N-1}\mu_1(\xi) + \mu_2(\xi) + b_{N+1}\mu_3(\xi). \tag{3.7}$$

In Eqs. (3.6) and (3.7), $a_{N-1}, a_{N+1}, b_{N-1}, b_{N+1}$ are coefficients to be determined. By collocating Eqs. (1.1) and (1.2) at the sinc points

$$\xi_j = \frac{e^{jh}}{1+e^{jh}},\ \ j = -N-1, ..., N+1, \tag{3.8}$$

we get the $4N+6$ coefficients $\{a_k\}_{k=-N}^{N}$ and $\{b_k\}_{k=-N}^{N}$. By placing points $\xi_j, j = -N-1, ..., N+1$ in Eqs. (3.4) and (3.5) and using Eq. (2.4), we have

$$\begin{cases} U_N(\xi_j) = \frac{a_j}{\phi'(\xi_j)},\ V_N(\xi_j) = \frac{b_j}{\phi'(\xi_j)},\ j = -N, ..., N, \\ U_N(\xi_j) = V_N(\xi_j) = 0,\ j = -N-1, N+1. \end{cases}$$

In addition, using Eqs. (2.4)- (2.6) and (3.4), we get

$$\begin{aligned} U_N(\xi_j) &= \sum_{k=-N}^{N} a_k [\frac{S_k(\xi)}{\phi'(\xi)}]_{\xi=\xi_j} = \sum_{k=-N}^{N} a_k [(\frac{-\phi''(\xi)}{\phi'(\xi)^2})S_k(\xi) + \frac{d}{d\phi}S_k(\xi)]_{\xi=\xi_j} \\ &= \sum_{k=-N}^{N} a_k [(\frac{-\phi''(\xi_j)}{\phi'(\xi_j)^2})\delta_{kj}^{(0)} + \delta_{kj}^{(1)}]. \end{aligned}$$

In a similar way, we get

$$V_N(\xi_j) = \sum_{k=-N}^{N} b_k [(\frac{-\phi''(\xi_j)}{\phi'(\xi_j)^2})\delta_{kj}^{(0)} + \delta_{kj}^{(1)}].$$

By using Eqs. (2.4)- (2.6), (3.4) and (3.5) , the formulas for the second derivative of $\frac{S_k(\xi)}{\phi'(\xi)}$ are

$$U_N''(\xi_j) = \sum_{k=-N}^{N} a_k \{(\frac{2\phi''(\xi_j)^2 - \phi'''(\xi_j)\phi'(\xi_j)}{\phi'(\xi_j)^3})\delta_{kj}^{(0)} - (\frac{\phi''(\xi_j)}{\phi'(\xi_j)})\delta_{kj}^{(1)} + \phi'(\xi_j)\delta_{kj}^{(2)}\},$$

Table 1. Results for $u(\xi)$ and $v(\xi)$.

ξ	u_{OHAM}	$u_{Sinc(N=8)}$	v_{OHAM}	$v_{Sinc(N=8)}$
0.1	0.9428972	0.9429145	0.8415794	0.8419224
0.2	0.8875699	0.8875998	0.8469568	0.8472826
0.3	0.8339414	0.8339840	0.8557293	0.8560406
0.4	0.7819371	0.7819910	0.8677478	0.86804435
0.5	0.7314845	0.7315460	0.8828670	0.88314391
0.6	0.6825121	0.6825758	0.9009442	0.9011930
0.7	0.6349490	0.6350083	0.9218381	0.92204782
0.8	0.5887240	0.5887719	0.9454074	0.9455646
0.9	0.5437652	0.5437939	0.9715097	0.9715983

$$V_N''(\xi_j) = \sum_{k=-N}^{N} b_k \{ (\frac{2\phi''(\xi_j)^2 - \phi'''(\xi_j)\phi'(\xi_j)}{\phi'(\xi_j)^3}) \delta_{kj}^{(0)} - (\frac{\phi''(\xi_j)}{\phi'(\xi_j)}) \delta_{kj}^{(1)} + \phi'(\xi_j) \delta_{kj}^{(2)} \}.$$

Now, in order to solve problem (1.1)-(1.3), we insert the equations obtained above and the equations in (3.3) into Eqs. (1.1)-(1.2) and obtain

$$U_N''(\xi_j) + p''(\xi_j) = \alpha_1 F(U_N(\xi_j) + p(\xi_j), V_N(\xi_j) + q(\xi_j)), \tag{3.9}$$

$$V_N''(\xi_j) + q''(\xi_j) = \alpha_2 F(U_N(\xi_j) + p(\xi_j), V_N(\xi_j) + q(\xi_j)). \tag{3.10}$$

where

$$F(x, y) = \frac{xy}{1 + \beta_1 x + \beta_2 y}.$$

Eqs. (3.9) and (3.10) produce $4N+6$ nonlinear algebraic equations that can be used to obtain the unknown coefficients a_k and $b_k, (k = -N-1, ..., N+1)$ with Newton's method. Subsequently $u_N(\xi)$ and $v_N(\xi)$ can be calculated via Eq. (3.3) by the maple's fsolve command.

4. Numerical simulations

In this section, we put fixed values instead of parameters $\alpha_1, \alpha_2, \beta_1, \beta_2$ and κ of Eqs. (1.1)-(1.3) and report the approximate solutions obtained from the Sinc-collocation method. Also, we presented all the results using $\alpha = 1$ and $d = \frac{\pi}{2}$ which yield $h = \frac{\pi}{\sqrt{2N}}$ according to Theorem 1. We approximate $u(\xi) \simeq u_N(\xi)$, $v(\xi) \simeq v_N(\xi)$ as defined in Eq. (3.3) with substituing (3.4), (3.5), (3.6) and (3.7). Then by placing $u_N(\xi)$ and $v_N(\xi)$ in Eqs. (1.1) and (1.2), equations (3.9) and (3.10) are obtained. Now, by placing the points introduced in relation (3.8) in these equations, we get a system of algebraic equations.
We define the following residual error functions to evaluate the accuracy of approximate solutions

$$Res_{1,N}(\xi) = \frac{d^2 u_N}{d\xi^2} - \frac{\alpha_1 u_N(\xi) v_N(\xi)}{1 + \beta_1 u_N(\xi) + \beta_2 v_N(\xi)}, \tag{4.1}$$

$$Res_{2,N}(\xi) = \frac{d^2 v_N}{d\xi^2} - \frac{\alpha_2 u_N(\xi) v_N(\xi)}{1 + \beta_1 u_N(\xi) + \beta_2 v_N(\xi)}. \tag{4.2}$$

We assign $\alpha_1 = 1, \alpha_2 = 2, \beta_1 = 1, \beta_2 = 3, \kappa = \frac{1}{2}$ and then compare the approximate solutions of the Sinc-collocation method for N equal to 8 with the optimal homotopy analysis method [12] in Table 1 and Figure 1. In addition, graphs of residual error functions for $N = 8$ and other similar parameters are drawn in Figure 2.

Now, for $N = 8$, the effect of the parameters $\alpha_1, \alpha_2, \beta_1, \beta_2$ and κ on the approximate solutions is investigated. In Figure 3, we present the effect of κ on $u_N(\xi)$ when $\alpha_1 = 1, \alpha_2 = 1, \beta_1 = 1, \beta_2 = 3$. We have also presented the behavior

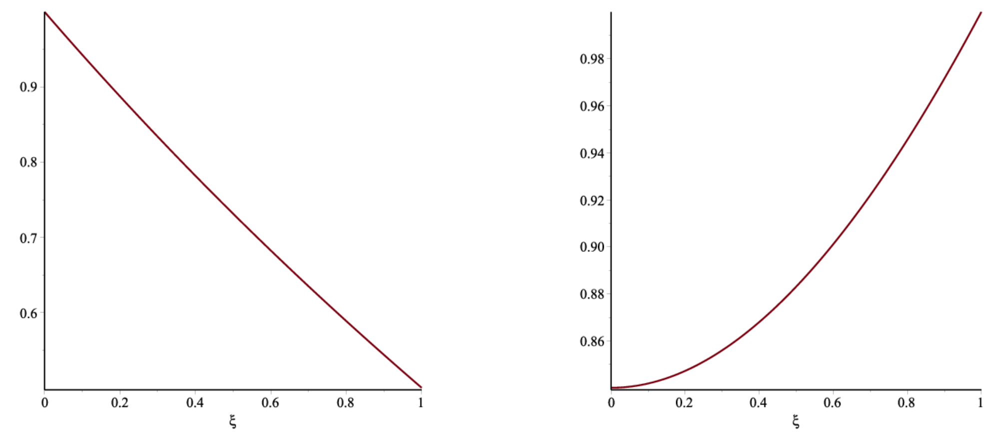

FIGURE 1. Plotting the approximate solutions $u_8(\xi)$ on the left side and $v_8(\xi)$ on the right side with $\alpha_1 = 1, \alpha_2 = 2, \beta_1 = 1, \beta_2 = 3, \kappa = \frac{1}{2}$.

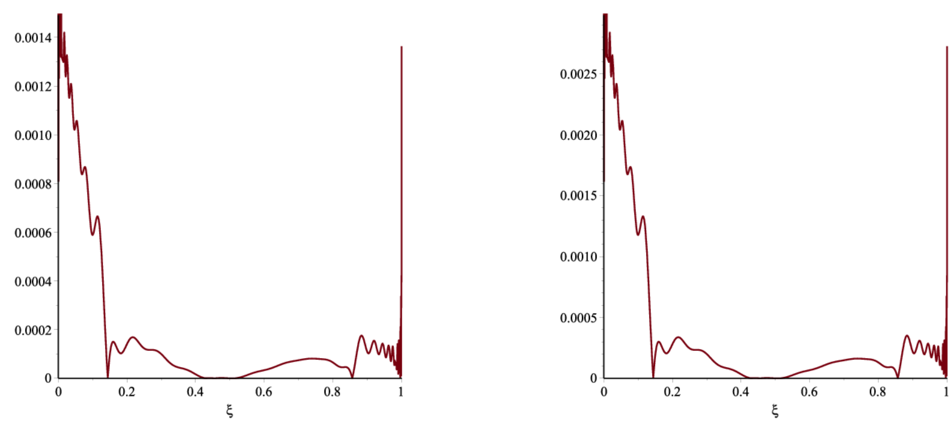

FIGURE 2. Plotting the approximate residual error functions $|Res_{1,8}(\xi)|$ on the left and $|Res_{2,8}(\xi)|$ on the right in $\alpha_1 = 1, \alpha_2 = 2, \beta_1 = 1, \beta_2 = 3, \kappa = \frac{1}{2}$.

of β_1 in $u_N(\xi)$ for $\alpha_1 = 1, \alpha_2 = 1, \beta_2 = 0.001$ and $\kappa = 0.1$ in Figure 4 .
The effect of β_2 on $u_N(\xi)$ when $\alpha_1 = 3, \alpha_2 = 1, \beta_1 = 1, \kappa = 0.1$ is shown in Figure 5. Also, Figure 6 shows the effect of α_2 on $v_N(\xi)$ when $\alpha_1 = 1, \beta_1 = 100, \beta_2 = 10$ and $\kappa = 0.1$. From Figure 7, we can see that the accuracy of the approximate solution $v_N(\xi)$ decreases with the increase of α_1. It is worth noting here that the images in Figures 3-6 are almost identical to the Figures obtained in [7, 14].

5. Conclusion

In this article, the Sinc-collocation scheme is used to solve the equations related to the solutions of stable concentrations of carbon dioxide absorbed in phenyl calicidyl ether. With the help of the properties of this method, we reduce the governing equations of this reaction to algebraic equations. In addition, the effects of different values of parameters $\alpha_1, \alpha_2, \beta_1, \beta_2$ and κ on the problem are also investigated. It can be seen that the approximate solutions obtained from the sinc-collocation method have a very good agreement with the approximate solutions obtained from

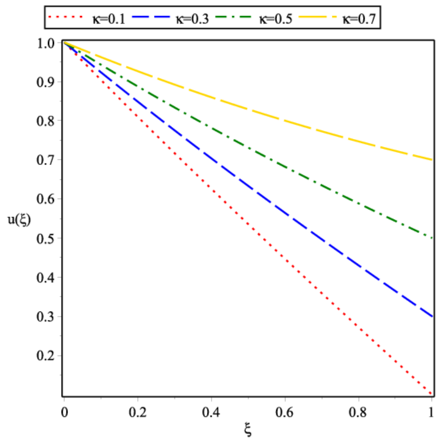

FIGURE 3. Graph for $u(\xi)$ of presented scheme with $\alpha_1 = 1, \alpha_2 = 1, \beta_1 = 1, \beta_2 = 3$ and different values of κ.

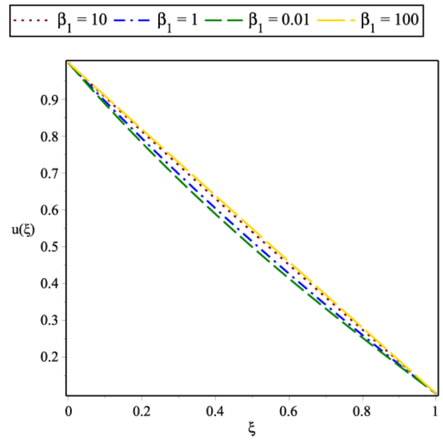

FIGURE 4. Graph for $u(\xi)$ of presented scheme with $\alpha_1 = 1, \alpha_2 = 1, \beta_2 = 0.001, \kappa = 0.1$ and different values of β_1.

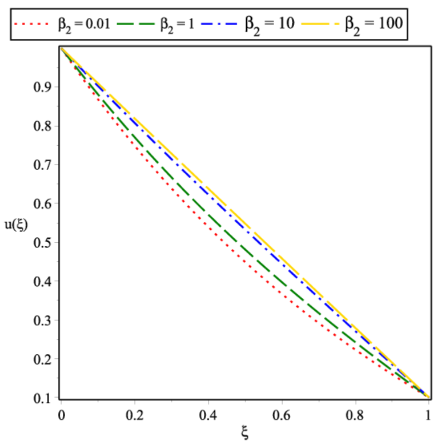

FIGURE 5. Graph for $u(\xi)$ of presented scheme with $\alpha_1 = 3, \alpha_2 = 1, \beta_1 = 1, \kappa = 0.1$ and different values of β_2.

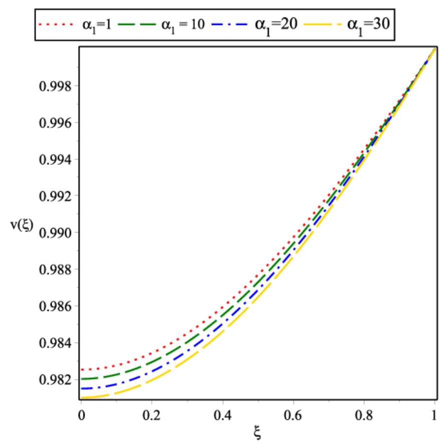

FIGURE 6. Graph for $v(\xi)$ of presented scheme with $\alpha_2 = 1, \beta_1 = 10, \beta_2 = 10, \kappa = 0.1$ and different values of α_1.

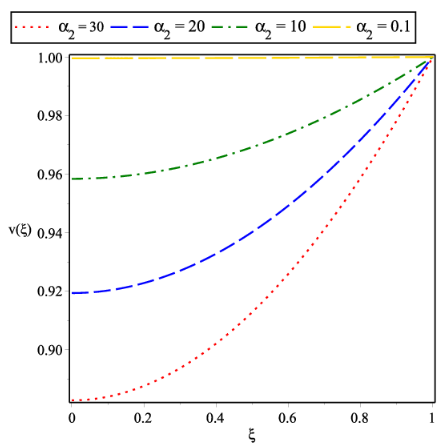

FIGURE 7. Graph for $v(\xi)$ of presented scheme with $\alpha_1 = 1, \beta_1 = 100, \beta_2 = 10, \kappa = 0.1$ and different values of α_2.

other numerical methods such as Adomian decomposition method [7], optimal homotopy analysis method [12] and residual method [14].

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