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Chebyshev Finite Difference Method for Steady-State Concentrations of Carbon Dioxide Absorbed Into Phenyl Glycidyl Ether

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Abstract

In this work, we present the Chebyshev finite difference method for solving the nonlinear coupled boundary value system that report the concentrations of carbon dioxide CO_2 and phenyl glycidyl ether in solution. This method is based on Chebyshev ploynomials approximation and finite difference method. The equations of this problem with boundary conditions can be reduced to a system of algebraic equations. We solve this system and compare the new solutions with some well-known results which show the new scheme is accurate and efficient.

1 Introduction

In practical life, different phenomena in chemistry, mechanics, biology, physics, chemical engineering and fluid dynamics are descripted by using linear or nonlinear differential equations. In chemistry for example, a system of nonlinear ordinary differential equations presented for chemical kinetics problem of carbon dioxide CO_2 and phenyl glycidyl ether. A coupled model of nonlinear differential equations for the steady-state concentrations of CO_2 and PGE is given in [15] as

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

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

$$u(0) = 1, \quad u(1) = k, \qquad v'(0) = 0, \quad v(1) = 1. \tag{3}$$

Here $u(x)$ and $v(x)$ are show the dimensionless concentrations of CO_2 and PGE, respectively. The constants $\alpha_i, \beta_i : i = 1, 2$ are some constants, x denote the dimensionless distance as measured from the center, and the dimensionless concentration of CO_2 at the surface of the catalyst is denoted by k.

Carbon dioxide is a chemical compound made of one carbon and two oxygen atoms. Carbon dioxide is coverd at a low concentration in the Earth's atmosphere and acts as a greenhouse gas. Also, carbon dioxide gas is used in welding, fire extinguishers, airguns, oil recovery and decaffeination of coffee. Recently, many authors studied about carbon dioxide chemical fixation becuse the danger posed by global warming. One of these chemical fixations is the reaction between CO_2 and phenyl glycidyl ether (PGE) in solution.

Park et al have investigated the chemical reaction between carbon dioxide and PGE solutions with using TEA-CP-MS41 catalyst in [4, 5]. The literature of numerical analysis includes a little of the solutions for this problem. In [7, 10], authors applied the Adomian decomposition method to solved this system model and boundary conditions (1-3). AL-Jawary and Radhi in [2] used the variational iteration method for calculating the solutions of this problem. Also, the iterative method is presented by AL-Jawary et al. in [1]. Recently, authors in [15,16] solved this coupled equation and Lane-Emden equation by optimal homotopy analysis method [16].

In this paper, a different method is used. Our plan is to use Chebyshev finite difference method to obtain numerical solution of the problem (1-3). In this method, we reduced the problem to a set of algebraic equations by expanding $u(t)$ in terms of Chebyshev polynomials with unknown coefficients and used the Chebyshev-Gauss-Lobatto points for the interpolation points [8]. This method can obtain a better solutions than the finite difference and finite elements methods [3, 11, 12] because the approximation of the derivatives is defined over the whole domain. Chebyshev finite difference method has been widely applied to solve many problems in physics and engineering. This method has been used to obtain numerical solutions of the system arising in wastewater treatment plants [13], the problem of the steady flow in a porous half space [14], boundary value problems [8] and laminar flow [9].

The residual part of this paper is systematized as follows: In the next section, Chebyshev finite difference method and its properties is reviewed. In section 3, we apply Chebyshev finite difference method on the studied system. Numerical results for three cases of problem (1-3) with this method are given in section 4. Also, we have compared the new results with existing results in the literature to show how accurate our results are. Finally, we conclude the study in section 5.

2 Chebyshev finite difference method

The first kind of Chebyshev polynomials of degree n for $\xi \in [-1,1]$ are usually given by this formula

$$T_n(\xi) = \cos(n \arccos(\xi)),$$

and satisfies in the following recurrence relation

$$T_0(\xi) = 1, \quad T_0(\xi) = \xi,$$

$$T_{n+1}(\xi) = 2\ \xi\ T_n(\xi) - T_{n-1}(\xi), \quad n = 1, 2, ...$$

Futhermore, we consider the famous Chebyshev-Gauss-Lobatto nodes with

$$\xi_i = \cos(\frac{i\pi}{N}), \quad i = 0, 1, 2, ..., N.$$

In fact, all points $\xi_N = -1 < \xi_{N-1} < ... < \xi_1 < \xi_0 = 1$ are obtained of $(1-\xi^2)T_n'(\xi) = 0$, where $T_n'(\xi)$ is the first derivative of $T_n(\xi)$. The approximation of Chebyshev finite difference method is introduced in [6] of the function $u(\xi)$,

$$u_N(\xi) = \sum_{n=0}^{N} {}''a_n T_n(\xi), \quad a_n = \frac{2}{N}\sum_{j=0}^{N} {}''u(\xi_j)T_n(\xi_j), \tag{4}$$

where, the definition of the symbol $\sum''$ is a summation with both the first and last terms divided into two. Also, Elbarbary in [8] denoted the first and second derivatives for the function $u(\xi)$ at the point ξ_k with

$$u_N^{(k)}(\xi_i) = \sum_{j=0}^{N} d_{i,j}^{(k)} u(\xi_j), \quad k = 1, 2.$$

Here, $d_{i,j}^{(1)}$ and $d_{i,j}^{(2)}$ for $i, j = 0, 1, ..., N$, are obtained by

$$d_{i,j}^{(1)} = \frac{4\theta_j}{N} \sum_{n=0}^{N} \sum_{m=0,(n+m)\ odd}^{n-1} \frac{n\theta_n}{c_m} T_n(\xi_j)T_m(\xi_i),$$

$$d_{i,j}^{(2)} = \frac{2\theta_j}{N} \sum_{n=0}^{N} \sum_{m=0,(n+m)\ even}^{n-2} \frac{n(n^2-m^2)\theta_n}{c_m} T_n(\xi_j)T_m(\xi_i), \tag{5}$$

with $\theta_0 = \theta_N = \frac{1}{2}$, $\theta_n = 1$ for $n = 1, 2, ..., N-1$, and $c_0 = 2, c_m = 1$, for $m = 1, 2, ..., N$.

3 Numerical procedure

In this section, we apply the Chebyshev finite difference (ChFD) method to obtain solutions of Eqs. (1) and (2) with boundary conditions (3). The domain of this problem is $0 \leq x \leq 1$. The map $\xi = 2x - 1$ is also found to be of the interval $[0, 1]$ into the interval $[-1, 1]$ and the Eqs. (1-3) are transformed into an equivalent equations

$$4u''(\xi) = \frac{\alpha_1 u(\xi)v(\xi)}{1 + \beta_1 u(\xi) + \beta_2 v(\xi)}, \tag{6}$$

$$4v''(\xi) = \frac{\alpha_2 u(\xi)v(\xi)}{1 + \beta_1 u(\xi) + \beta_2 v(\xi)}, \tag{7}$$

$$u(-1) = 0,\ u(1) = k,\ v'(-1) = 0,\ v(1) = 1. \tag{8}$$

Now using Eq. (4) to approximate $u(\xi)$ and $v(\xi)$ as

$$u_N(\xi) = \sum_{n=0}^{N}{}'' \lambda_n T_n(\xi), \quad v_N(\xi) = \sum_{n=0}^{N}{}'' \mu_n T_n(\xi), \tag{9}$$

where

$$\lambda_n = \frac{2}{N} \sum_{n=0}^{N}{}'' u(\xi_j) T_n(\xi_j), \quad \mu_n = \frac{2}{N} \sum_{n=0}^{N}{}'' v(\xi_j) T_n(\xi_j),$$

Substituting Eq. (9) into Eqs. (6)-(7) and putting $\xi = \xi_i, i = 1, ...N - 1$ that are the Gauss-Lobatto points, we have

$$\sum_{j=0}^{N} 4d_{i,j}^{(2)} u(\xi_j) = \frac{\alpha_1 u(\xi_j)v(\xi_j)}{1 + \beta_1 u(\xi_j) + \beta_2 v(\xi_j)}, \tag{10}$$

$$\sum_{j=0}^{N} 4d_{i,j}^{(2)} v(\xi_j) = \frac{\alpha_2 u(\xi_j)v(\xi_j)}{1 + \beta_1 u(\xi_j) + \beta_2 v(\xi_j)}, \tag{11}$$

where $d_{i,j}^{(2)}$ is given in Eq. (5). We get $\xi = \xi_0, \xi_N$ in the the boundary conditions (8) and the following result is obtained

$$u(\xi_N) = 0,\ u(\xi_0) = k,\ \sum_{j=0}^{N} d_{i,j}^{(1)} v(\xi_j) = 0,\ v(\xi_0) = 1. \tag{12}$$

Eqs. (10), (11) and (12) are a system of $2N + 2$ nonlinear equations which can be solved numerically for the unknown parameters $u(\xi_i)$ and $v(\xi_i)$ for $i = 0, ..., N$ by Newton's method. Consequently $u_N(\xi)$ and $v_N(\xi)$ given in Eq. (9) can be calculated instead of $u(x)$ and $v(x)$, respectively.

4 Results and discussion

Here, we fix the parameters $\alpha_1, \alpha_2, \beta_1, \beta_2$ and k in Eqs. (1-3) and calculate the approximate solutions by applying the Chebyshev finite difference method. We introduce the error remainder functions in order to evaluate the accuracy of our approximate solutions

$$Res_{1,N}(x) = \frac{d^2u}{dx^2} - \frac{\alpha_1 u(x)v(x)}{1+\beta_1 u(x)+\beta_2 v(x)}, \tag{13}$$

$$Res_{2,N}(x) = \frac{d^2v}{dx^2} - \frac{\alpha_2 u(x)v(x)}{1+\beta_1 u(x)+\beta_2 v(x)}, \tag{14}$$

and the maximal error remainder parameters

$$MRes_{1,N} = \max_{0\le x\le 1} |Res_{1,N}(x)|, \quad MRes_{2,N} = \max_{0\le x\le 1} |Res_{2,N}(x)|. \tag{15}$$

Now, we consider the following three cases for the problem variables:

Case 1: $\alpha_1 = 1, \alpha_2 = 2, \beta_1 = 1, \beta_2 = 3, k = \frac{1}{2}$.

In Figure 1, the numerical solutions $u_N(x)$ and $v_N(x)$ are plotted with $N = 12$ for this case. Also, in Figure 4, the graphs of $Res_{1,N}(x)$ and $Res_{2,N}(x)$ are plotted with $N = 12$ for case 1. To make a comparison, in Table 1, we compare the parameters $MRes_{1,N}$ and $MRes_{2,N}$, with different values of N, together with the results obtained by using the Adomian decomposition method (ADM) and the Duan-Rach modified recursion scheme given in [7] and the optimal homotopy analysis method (OHAM) in [14] for case 1.

Case 2: $\alpha_1 = 1, \alpha_2 = 2, \beta_1 = 2, \beta_2 = 4, k = 2$.

In Figure 2, the numerical solutions $u_N(x)$ and $v_N(x)$ are plotted with $N = 12$ for case 2. Also, in Figure 5, the graphs of $Res_{1,N}(x)$ and $Res_{2,N}(x)$ are plotted with $N = 12$ for case 2. To make a comparison, in Table 2, we compare the parameters $MRes_{1,N}$ and $MRes_{2,N}$, for different values of N, together with the results obtained of ADM and OHAM for case 2.

Case 3: $\alpha_1 = 2, \alpha_2 = 3, \beta_1 = 1, \beta_2 = 3, k = 3$.

In Figure 3, the numerical solutions $u_N(x)$ and $v_N(x)$ are plotted with $N = 12$ for case 3. Also, in Figure 6, the graphs of $Res_{1,N}(x)$ and $Res_{2,N}(x)$ are plotted with $N = 12$ for case 3. To make a comparison, in Table 3, we compare the parameters $MRes_{1,N}$ and $MRes_{2,N}$, with different values of N, together with the result obtained of ADM and OHAM for case 3.

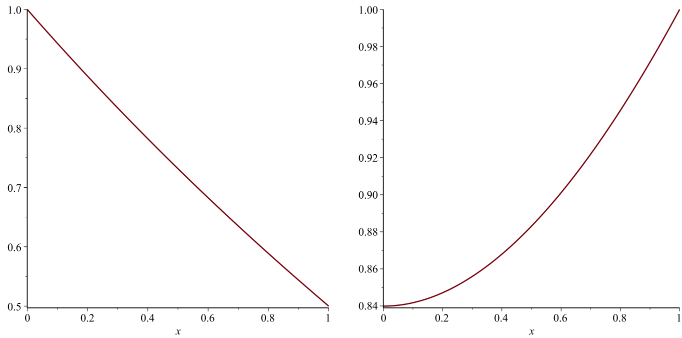

Figure 1. Plot of the numerical solutions $u_{12}(x)$ (left) and $v_{12}(x)$ (right) for case 1.

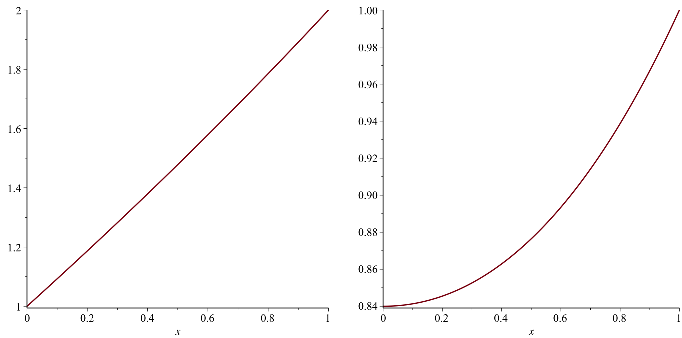

Figure 2. Plot of the numerical solutions $u_{12}(x)$ (left) and $v_{12}(x)$ (right) for case 2.

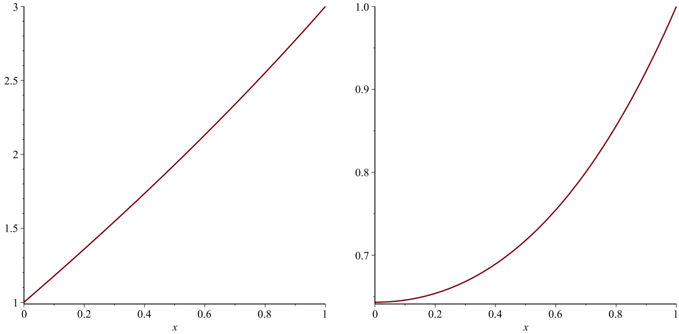

Figure 3. Plot of the numerical solutions $u_{12}(x)$ (left) and $v_{12}(x)$ (right) for case 3.

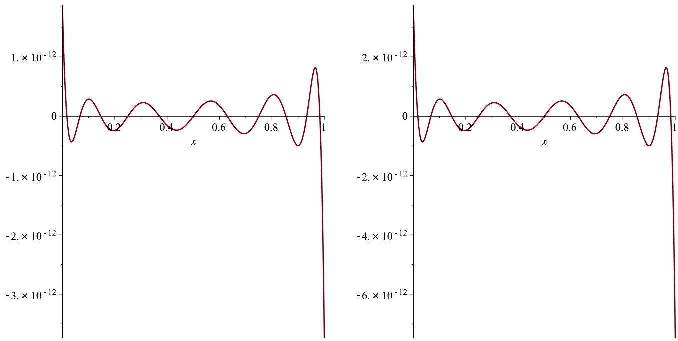

Figure 4. Plot of error remainder $Res_{1,12}(x)$ (left) and $Res_{2,12}(x)$ (right) for case 1.

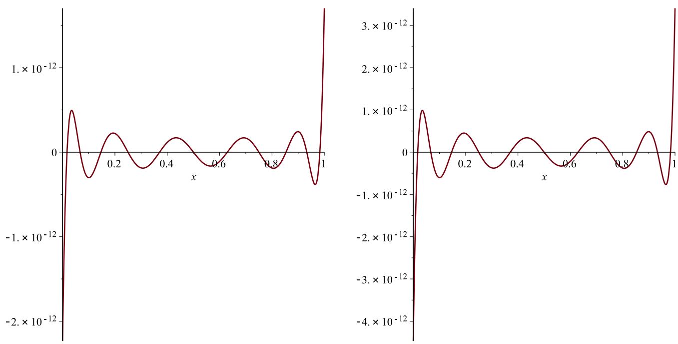

Figure 5. Plot of error remainder $Res_{1,12}(x)$ (left) and $Res_{2,12}(x)$ (right) for case 2.

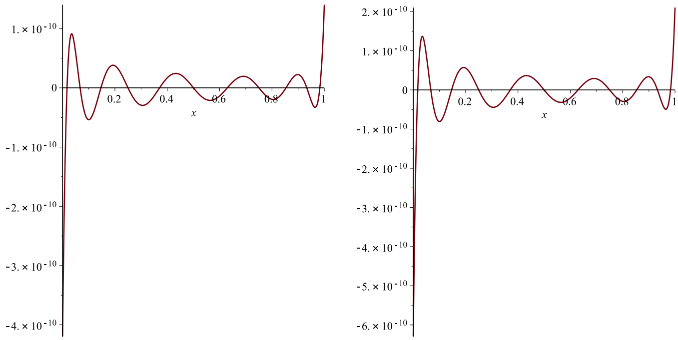

Figure 6. Plot of error remainder $Res_{1,12}(x)$ (left) and $Res_{2,12}(x)$ (right) for case 3.

Table 1. The OHAM, ADM and ChFD maximal error remainders for case 1.

x	u_{OHAM}	v_{OHAM}	u_{ADM}	v_{ADM}	u_{ChFD}	v_{ChFD}
0	$2.85E-04$	$3.15E-04$	$6.42E-04$	$6.31E-04$	$6.51E-04$	$1.30E-03$
0.2	$9.38E-05$	$4.90E-05$	$3.21E-05$	$9.80E-05$	$1.04E-04$	$2.08E-04$
0.4	$4.27E-04$	$4.08E-04$	$5.85E-04$	$8.17E-04$	$1.07E-04$	$2.14E-04$
0.6	$7.10E-04$	$7.54E-04$	$1.23E-03$	$1.50E-03$	$1.00E-04$	$2.00E-04$
0.8	$8.43E-04$	$9.81E-04$	$1.74E-03$	$1.96E-03$	$8.51E-05$	$1.70E-04$
1	$6.32E-04$	$8.88E-04$	$1.76E-03$	$1.77E-03$	$4.68E-04$	$9.37E-04$

Table 2. The OHAM, ADM and ChFD maximal error remainders for case 2.

x	u_{OHAM}	v_{OHAM}	u_{ADM}	v_{ADM}	u_{ChFD}	v_{ChFD}
0	$3.44E-05$	$2.90E-04$	$1.40E-04$	$5.80E-04$	$9.11E-04$	$1.82E-03$
0.2	$1.31E-04$	$1.53E-04$	$5.23E-04$	$3.06E-04$	$1.50E-04$	$3.01E-04$
0.4	$3.88E-04$	$4.40E-04$	$1.17E-03$	$8.80E-04$	$1.61E-04$	$3.23E-04$
0.6	$4.16E-04$	$1.45E-03$	$1.18E-03$	$2.90E-03$	$1.57E-04$	$3.15E-04$
0.8	$1.11E-04$	$3.41E-03$	$5.94E-06$	$6.83E-03$	$1.40E-04$	$2.80E-04$
1	$1.44E-03$	$6.47E-03$	$2.72E-03$	$1.29E-02$	$8.10E-04$	$1.62E-03$

Table 3. The OHAM, ADM and ChFD maximal error remainders for case 3.

x	u_{OHAM}	v_{OHAM}	u_{ADM}	v_{ADM}	u_{ChFD}	v_{ChFD}
0	$2.41E-03$	$4.81E-03$	$8.19E-04$	$7.22E-03$	$1.11E-02$	$1.66E-02$
0.2	$1.07E-02$	$1.70E-03$	$1.24E-02$	$2.55E-03$	$1.81E-03$	$2.72E-03$
0.4	$1.59E-02$	$4.13E-03$	$1.87E-02$	$6.20E-03$	$1.92E-03$	$2.89E-03$
0.6	$1.34E-02$	$1.57E-02$	$1.30E-02$	$2.36E-02$	$1.85E-03$	$2.78E-03$
0.8	$1.77E-04$	$3.87E-02$	$9.28E-03$	$5.80E-02$	$1.62E-03$	$2.43E-03$
1	$2.63E-02$	$7.31E-02$	$4.98E-02$	$1.09E-01$	$9.22E-03$	$1.38E-02$

5 Conclusion

In this article, the Chebyshev finite difference scheme is used to make an approximation solutions of steady-state concentrations of carbon dioxide absorbed into phenyl glycidyl ether. Properties of the Chebyshev finite difference method are helped to reduce this reaction formulas to a system of algebraic equations. The numerical solutions obtained by the Chebyshev finite difference method are in good agreement with the numerical results obtained in [7, 14], and to show that this method has good convergence and effectiveness.

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