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AN ITERATIVE METHOD FOR CALCULATING CARBON DIOXIDE ABSORBED INTO PHENYL GLYCIDYL ETHER

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Abstract. In this paper, the system of two coupled nonlinear ordinary differential equations is solved by using an iterative method (DJM) which represent the condensations of carbon dioxide (CO_2) and phenyl glycidyl ether (PGE). There are two types of boundary conditions in this system are Dirichlet type and the other is a mixed set of Neumann and Dirichlet type. The solution obtained by DJM is an approximate solution with rapid convergence. The results are compare with the other results obtained by variation iteration method (VIM) and Adomian decomposition method (ADM), detects that the numerical solution obtained by DJM is equal to solution obtained by VIM and converge faster than Adomian's method. All our calculations obtained from using the software Mathematica®9.

Keywords: Carbon dioxide, Phenyl glycidyl ether, Iterative method, Approximate solution, Maximal error remainder.

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1. Introduction

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The components of carbon dioxide can be illustrated as one carbon atom and two oxgen atoms [1]. One of important gasses in nature is a carbon dioxide, where it enters in many areas in our lives such as, the powering of pneumatic systems in robots, used in fire extinguishers, removing caffeine from coffee, the manufacturing of carbonated soft drinks, ... etc [1,2]. The adomian decomposition method (ADM) was used for the simple steady-state condensations of CO_2 and PGE and obtained the approximate analytical form and it is presented in [1]. The solution of chemical absorption of carbon dioxide (CO_2) into phenyl glycidyl ether(PGE) containing power a catalyst THA-CP-MS41in inhomogeneous systems has been investigated by park et al.[3]and Choe et al.[4]. Moreover, the variation iteration method (VIM) was applied on this system [5]. The varsha Daftardar and Hossein Jafari in 2006 were first suggested the iterative method namely (DJM)[6]. It is possible to apply the DJM on many differential and integral equations, linear and nonlinear equations, algebraic equations and systems of ordinary differential equations, and fractional equations, ... ect [6]. It is easy task to find the exact solution for many of nonlinear problems by using the DJM[6]. The DJM was applied on fractional partial differential in [7] and the Laplace equations in [8]. The DJM is simple to understand and easy to implement using computer packages and yields better results than the existing Adomiam decomposition method (ADM), Homotopy perturbation method (HPM)or Variational iteration method(VIM)[9]. The DJM when apply to solve nonlinear ordinary differential equations don't need to the Adomian polynomial to calculate the nonlinear terms, while the ADM takes a long time to compute each component in the solution because the nonlinear terms are represented by the Adomian's polynomial in each equations in the system [10,11].

In this work, the DJM will be applied to get an approximate solution for system of two coupled nonlinear ordinary differential equations which represent the condensation of carbon dioxide (CO2) and phenyl glycidyl ether.

This paper has been ordered as follows: In section two, the steady-state concentrations of carbon dioxide absorbed into phenyl glycidyl ether is introduced. In section three, an Iterative Method is introduced and discussed. In section four, solving the system of steady-state concentrations of CO2 and PGE by the DJM will be given. In section five, numerical simulation and will be followed the conclusion in section six.

2. Steady-State Concentrations of Carbon Dioxide Absorbed into Phenyl Glycidyl Ether

The system of two nonlinear differential equations represents the steady-state condensations of two chemicals carbon dioxide CO2 and PGE is given in [1, 5, 12, 13] this system can be represented by:

$$u^{''}(x) = \frac{\alpha_1 u(x) v(x)}{1+\beta_1 u(x) + \beta_2 v(x)} \tag{1}$$

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

and the boundary conditions are :

$$u(0) = 1, \qquad v'(0) = 0,$$

$$u(1) = k, \qquad v(1) = 1.$$

Where $\alpha_1, \alpha_2, \beta_1$ and β_2 are the parameters of normalized system and u(x) is the condensation of CO2, v(x) is the condensation of PGE and x is the ”dimensionless distance ” from the center, k is the condensation of CO2 at the surface catalyst [13].

This system solved by the Adomian decomposition method (ADM) where it was calculated acceptable approximate results with the statement of the maximal error and the amount of the accuracy [1, 13] after converted into system of two coupled integral equations and take the advantage of the given boundary conditions with this problem. However, due to the nonlinear terms, the Adomian polynomials is calculated which required more calculations and time [5], and the Variation iteration method (VIM) was used to solve this system of equations such that it was implemented to get an approximate solution with statement of the maximal error remainder and the measure of accuracy [5], this method provides the approximations by using the correction functional requiring the lagrange's multiplayer. In this work, we will solve this system of this two coupled nonlinear ordinary differential equations (ODEs) directly by using DJM more details of DJM can be found in [6–9, 14].

The equations (1)and (2) can be written as :

$$u^{''}(x) = -\beta_1 u(x) u^{''}(x) - \beta_2 v(x) u^{''}(x) + \alpha_1 u(x) v(x) \tag{3}$$

$$v^{''}(x) = -\beta_1 u(x) v''(x) - \beta_2 v(x) v''(x) + \alpha_2 u(x) v(x) \tag{4}$$

Eqs. (3),(4) will be solved by using DJM.

3. An iterative method (DJM)

Let us consider the following general functional equation [6]:

$$u = N(u) + f \tag{5}$$

Where f is a known function and N is a nonlinear operator.

The series form of the solution u of the Eq. (5) is follow by:

$$u = \sum_{i=0}^{\infty} u_i \tag{6}$$

The nonlinear operator N can be decomposed as

$$N\left(\sum_{i=0}^{\infty} u_i\right) = N(u_0) + [N\left(\sum_{j=0}^{i} u_j\right) - N\left(\sum_{j=0}^{i-1} u_j\right)] \tag{7}$$

From Eqs. (6) and (7), the Eq.(5) is equivalent to

$$\sum_{i=0}^{\infty} u_i = f + N(u_0) + \sum_{i=1}^{\infty} [N\left(\sum_{j=0}^{i} u_j\right) - N\left(\sum_{j=0}^{i-1} u_j\right)] \tag{8}$$

We defined the recurrence relation:

$$u_0 = f$$

$$u_1 = N(u_0)$$

$$u_{m+1} = N(u_0 + u_1 + \cdots + u_m) - N(u_0 + u_1 + \cdots + u_{m-1}),\ m = 1, 2, 3, \ldots.. \tag{9}$$

Then

$$(u_0 + u_1 + \cdots + u_{m-1}) = N(u_0 + u_1 + \cdots + u_m),\ m = 1, 2, 3, \ldots\ldots \tag{10}$$

then

$$u = f + \sum_{i=0}^{\infty} u_i \tag{11}$$

4. Solving the system of steady-state condensation of CO2 and PGE by the DJM

Let us rewrite equations (3) and (4) as :

$$u^{''}(x) = -\beta_1 u(x) u^{''}(x) - \beta_2 v(x) u^{''}(x) + \alpha_1 u(x) v(x) \tag{12}$$

$$v^{''}(x) = -\beta_1 u(x) v''(x) - \beta_2 v(x) v''(x) + \alpha_2 u(x) v(x) \tag{13}$$

with the boundary conditions

$$u(0) = 1, \qquad v'(0) = 0,$$

$$u(1) = k, \qquad v(1) = 1.$$

By integrating both sides of the Eqs. (12) and (13) twice, the following equations will be obtained:

$$u(x) = 1 + xu'(0) + \int_0^x \int_0^x [-\beta_1 u(t) u''(t) - \beta_2 v(t) u''(t) + \alpha_1 u(t) v(t)] dt dt, \tag{14}$$

$$v(x) = v(0) + \int_0^x \int_0^x \left[-\beta_1 u(t) v''(t) - \beta_2 v(t) v''(t) + \alpha_2 u(t) v(t)\right] dt dt. \tag{15}$$

Let

$$1 + xu'(0) = x, \text{ and } v(0) = x. \tag{16}$$

from Eq.(16) we get

$$u(x) = x + \int_0^x \int_0^x [-\beta_1 u(t) u''(t) - \beta_2 v(t) u''(t) + \alpha_1 u(t) v(t)] dt dt, \tag{17}$$

$$v(x) = x + \int_0^x \int_0^x \left[-\beta_1 u(t) v''(t) - \beta_2 v(t) v''(t) + \alpha_2 u(t) v(t)\right] dt dt. \tag{18}$$

By rewriting Eqs. (17), (18) in nonlinear operator form as

$$u(x) = x + N_1(u,v) \tag{19}$$

$$v(x) = x + N_2(u,v) \tag{20}$$

where the nonlinear operators N_1, N_2 are

$$N_1(u,v) = \int_0^x \int_0^x [-\beta_1 u(t) u''(t) - \beta_2 v(t) u''(t) + \alpha_1 u(t) v(t)] dt dt, \tag{21}$$

$$N_2(u,v) = \int_0^x \int_0^x \left[-\beta_1 u(t) v''(t) - \beta_2 v(t) v''(t) + \alpha_2 u(t) v(t)\right] dt dt. \tag{22}$$

The solution u and v have the series form

$$u = \sum_{i=0}^{\infty} u_i, \quad v = \sum_{i=0}^{\infty} v_i \tag{23}$$

by Eq. (23) the nonlinear operator N_1, N_2 can be decomposed as

$$N_1(u,v) = N_1(u_0,v_0) + \sum_{i=1}^{\infty} [N_1\left(\sum_{j=0}^{i} u_j, \sum_{j=0}^{i} v_j\right) - N_1\left(\sum_{j=0}^{i-1} u_j, \sum_{j=0}^{i-1} v_j\right)] \tag{24}$$

$$N_2(u,v) = N_2(u_0,v_0) + \sum_{i=1}^{\infty} [N_2\left(\sum_{j=0}^{i} u_j, \sum_{j=0}^{i} v_j\right) - N_2\left(\sum_{j=0}^{i-1} u_j, \sum_{j=0}^{i-1} v_j\right)] \tag{25}$$

and the Eqs. (19), (20) are equivalent to

$$\sum_{i=0}^{\infty} u_i = x + N_1(u_0,v_0) + \sum_{i=1}^{\infty} [N_1\left(\sum_{j=0}^{i} u_j, \sum_{j=0}^{i} v_j\right) - N_1\left(\sum_{j=0}^{i-1} u_j, \sum_{j=0}^{i-1} v_j\right)] \tag{26}$$

$$\sum_{i=0}^{\infty} v_i = x + N_2(u_0,v_0) + \sum_{i=1}^{\infty} [N_2\left(\sum_{j=0}^{i} u_j, \sum_{j=0}^{i} v_j\right) - N_2\left(\sum_{j=0}^{i-1} u_j, \sum_{j=0}^{i-1} v_j\right)] \tag{27}$$

the initial approximations have been taken : $u_0(x) = \frac{x}{m}$, $v_0(x) = \frac{x}{m}$, with $m = 1$.

The following approximations are achieved

$$u_0(x) = x,$$

$$v_0(x) = x,$$

$$u_1 = N_1(u_0,v_0) = \int_0^x \int_0^x \left[-\beta_1 u_0(t)\, u_0''(t) - \beta_2 v_0(t)\, u_0''(t) + \alpha_1 u_0(t)\, v_0(t)\right] dtdt = \frac{x^4\alpha_1}{12}$$

$$v_1 = N_2(u_0,v_0) = \int_0^x \int_0^x \left[-\beta_1 u_0(t)\, v_0''(t) - \beta_2 v_0(t)\, v_0''(t) + \alpha_2 u_0(t)\, v_0(t)\right] dtdt = \frac{x^4\alpha_2}{12}$$

$$u_2 = \int_0^x \int_0^x [-\beta_1(u_0+u_1)(u_0+u_1)'' - \beta_2(v_0+v_1)(u_0+u_1)'' + \alpha_1(u_0+u_1)(v_0+v_1)]dtdt - u_1$$

$$= \frac{1}{504}x^7\alpha_1^2 + \frac{1}{504}x^7\alpha_1\alpha_2 + \frac{x^{10}\alpha_1^2\alpha_2}{12960} - \frac{1}{20}x^5\alpha_1\beta_1 - \frac{1}{672}x^8\alpha_1^2\beta_1 - \frac{1}{20}x^5\alpha_1\beta_2 - \frac{1}{672}x^8\alpha_1\alpha_2\beta_2,$$

$$v_2 = \int_0^x \int_0^x [-\beta_1(u_0+u_1)(v_0+v_1)'' - \beta_2(v_0+v_1)(v_0+v_1)'' + \alpha_2(u_0+u_1)(v_0+v_1)]dtdt - v_1$$

$$= \frac{1}{504}x^7\alpha_1\alpha_2 + \frac{1}{504}x^7\alpha_2^2 + \frac{x^{10}\alpha_1\alpha_2^2}{12960} - \frac{1}{20}x^5\alpha_2\beta_1 - \frac{1}{672}x^8\alpha_1\alpha_2\beta_1 - \frac{1}{20}x^5\alpha_2\beta_2 - \frac{1}{672}x^8\alpha_2^2\beta_2,$$

and so on continue , we will obtain successive approximations of $u_n(x)$ and $v_n(x)$ but for brevity not listed. Our calculation are obtained by Mathematica® 9.

For a study the accuracy of the achieved approximate solution, relevance functions of the error remainder will be [1, 5]

$$ER_{1,n} = u_n''(x) + \beta_1 u_n(x)\, u_n''(x) + \beta_2 v_n(x)\, u_n''(x) - \alpha_1 u_n(x)\, v_n(x) \quad (28)$$

$$ER_{2,n} = v_n''(x) + \beta_1 u_n(x)\, v_n''(x) + \beta_2 v_n(x)\, v_n''(x) - \alpha_2 u_n(x)\, v_n(x) \quad (29)$$

and the maximal error remainder parameters are

$$MER_{1,n} = \max_{0\le x\le 1} |ER_{1,n}| \ , \qquad MER_{2,n} = \max_{0\le x\le 1} |ER_{2,n}| \quad (30)$$

5. Numerical simulations:

We taking the values of the parameters will be equaled to: $\alpha_1 = 1$, $\alpha_2 = 2$, $\beta_1 = 1$, $\beta_2 = 3$ and $k = 0.5$ as existed in[1, 5] to calculate the approximate solutions, the error remainder and the maximal error remainder. The values of $MER_{1,n}$ and $MER_{2,n}$ which are obtained by DJM are compared with those resulted by ADM and VIM [1, 5] in the tables below. It can observe that the maximal error remainder values obtained from the DJM are equal to those obtained from VIM and least of those obtained from ADM and it is better accuracy, where the values of n is increasing from 1 to 4.

Table.1: Comparison between the ADM and the VIM and DJM of MER$_{1,n}$

n	**MER$_{1,n}$ by the ADM**	**MER$_{1,n}$ by the VIM**	**MER$_{1,n}$ by the DJM**
1	0.2	0.003	0.003
2	0.0888889	0.00159895	0.00159895
3	0.00888889	0.00063952	0.00063952
4	0.00099943	0.0002558	0.0002558

Table.2: Comparison between the ADM and the VIM and DJM of MER$_{2,n}$

n	**MER$_{2,n}$ by the ADM**	**MER$_{2,n}$ by the VIM**	**MER$_{2,n}$ by the DJM**
1	0.4	0.00799617	0.00799617
2	0.177778	0.0031979	0.0031979
3	0.0177778	0.00127904	0.00127904
4	0.00099943	0.000511601	0.000511601

We show below the analysis of the error remainders for both $MER_{1,n}$ and $MER_{2,n}$ in the Figs. 1and 2 respectively, it can be clearly seen that the points are lay on a straight lines which mean exponential rate of convergence is achieved.

It is important to mention here, by increasing denominator of the initial approximations ($\frac{x}{m}$) for u and v (i.e. $m > 1$) the accuracy will be increasing and the error will be degreasing, furthermore, from tables 3, 4 and Figs. 3 and 4 we can observe that when increasing the iteration (n from 1 to 5) we obtain a better accuracy. Tables 3 and 4 show the maximal error remainders are decreases when the values of m is increases for both u_n (x)and v_n(x).

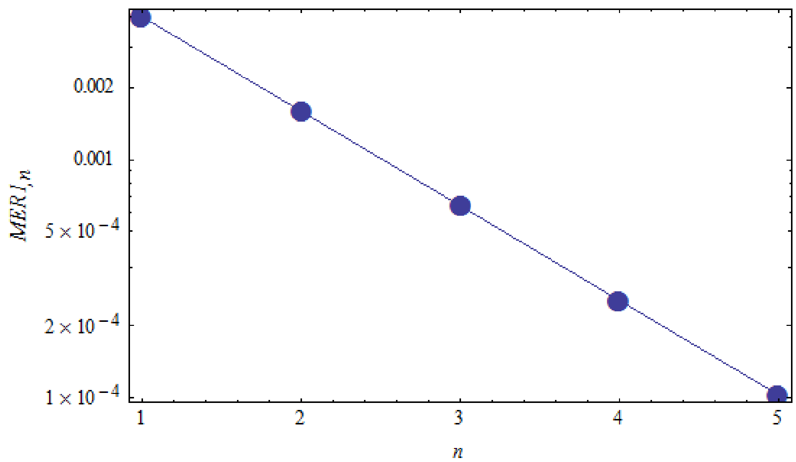

FIGURE 1. Logarithmic plots of $MER_{1,n}$ versus n is 1 through 5 and $m = 1$.

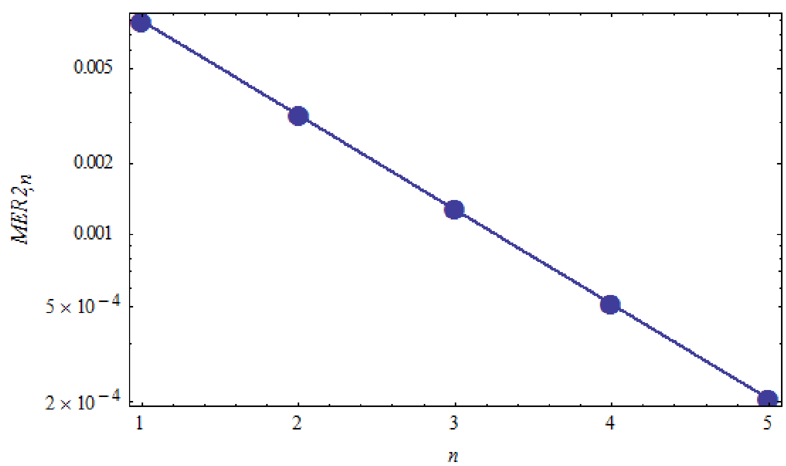

FIGURE 2. Logarithmic plots of $MER_{2,n}$ versus n is 1 through 5 and $m = 1$.

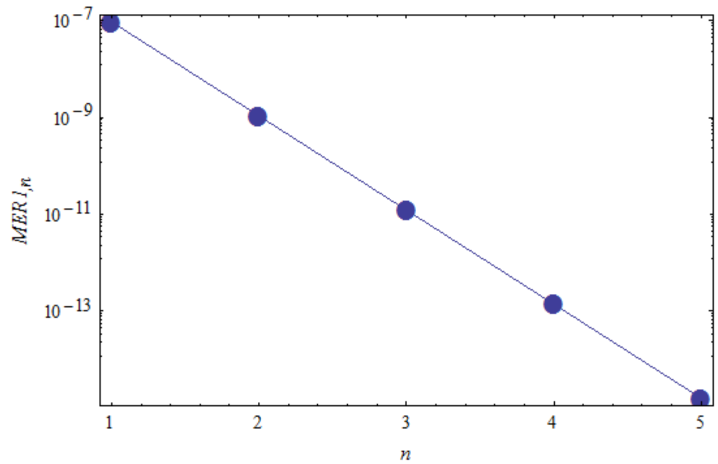

FIGURE 3. Logarithmic plots of $MER_{1,n}$ versus n is 1 through 5 and $m = 35$.

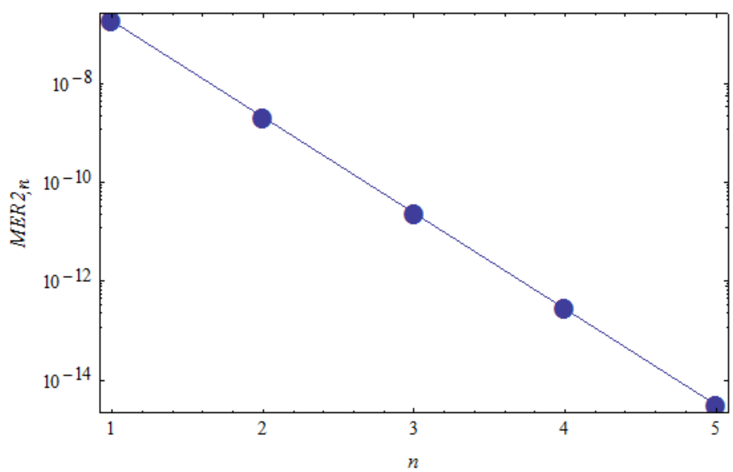

FIGURE 4. Logarithmic plots of $MER_{2,n}$ versus n is 1 through 5 and $m = 35$.

Table.3: the maximal error remainder:$MER_{1,n}$ by DJM with $n = 1,\ldots,5$ and x divide by m

n / **m**	**1**	**2**	**3**	**4**	**5**
1	0.0039981	0.0015989	0.0006395	0.0002558	0.0001023
5	0.0001481	0.0000197	2.63094×10^{-6}	3.50749×10^{-7}	4.67628×10^{-8}
10	3.99756×10^{-6}	1.59846×10^{-7}	6.39237×10^{-9}	2.55654×10^{-10}	1.0225×10^{-11}
15	1.18446×10^{-6}	3.15741×10^{-8}	8.41777×10^{-10}	2.24437×10^{-11}	5.98424×10^{-13}
20	4.99691×10^{-7}	9.99019×10^{-9}	1.99756×10^{-10}	3.99444×10^{-12}	7.98788×10^{-14}
25	2.55841×10^{-7}	4.09197×10^{-9}	6.54556×10^{-11}	1.04711×10^{-12}	1.67516×10^{-14}
30	1.48056×10^{-7}	1.97336×10^{-9}	2.6305×10^{-11}	3.50673×10^{-13}	4.67505×10^{-15}
35	9.32365×10^{-8}	1.06517×10^{-9}	1.21704×10^{-11}	1.39066×10^{-13}	1.58912×10^{-15}
40	6.24612×10^{-8}	6.24381×10^{-10}	6.24228×10^{-12}	6.24119×10^{-14}	6.24037×10^{-16}
45	4.38685×10^{-8}	3.89798×10^{-10}	3.46402×10^{-12}	3.07859×10^{-14}	2.73618×10^{-16}
50	3.19801×10^{-8}	2.55746×10^{-10}	2.04546×10^{-12}	1.63609×10^{-14}	1.3087×10^{-16}

Table.4: the maximal error remainder: $MER_{2,n}$ by the DJM with $n = 1,\ldots,5$ and x divide by m

n / **m**	**1**	**2**	**3**	**4**	**5**
1	0.0079962	0.0031979	0.001279	0.0005116	0.0002046
5	0.0002961	0.0000395	5.26188×10^{-6}	7.01499×10^{-7}	9.35257×10^{-8}
10	7.99512×10^{-6}	3.19692×10^{-7}	1.27847×10^{-8}	5.11307×10^{-10}	2.04499×10^{-11}
15	2.36891×10^{-6}	6.31483×10^{-8}	1.68355×10^{-9}	4.48873×10^{-11}	1.19685×10^{-12}
20	9.99382×10^{-7}	1.99804×10^{-8}	3.99512×10^{-10}	7.98888×10^{-12}	1.59758×10^{-13}
25	5.11683×10^{-7}	8.18393×10^{-9}	1.30911×10^{-10}	2.09422×10^{-12}	3.35033×10^{-14}
30	2.96113×10^{-7}	3.94672×10^{-9}	5.26101×10^{-11}	7.01347×10^{-13}	9.35009×10^{-15}
35	1.86473×10^{-7}	2.13034×10^{-9}	2.43407×10^{-11}	2.78132×10^{-13}	3.17824×10^{-15}
40	1.24922×10^{-7}	1.24876×10^{-9}	1.24846×10^{-11}	1.24824×10^{-13}	1.24807×10^{-15}
45	8.77369×10^{-8}	7.79595×10^{-10}	6.92803×10^{-12}	6.15718×10^{-14}	5.47236×10^{-16}
50	6.39602×10^{-8}	5.11492×10^{-10}	4.09093×10^{-12}	3.27217×10^{-14}	2.6174×10^{-16}

6. Conclusion

In this paper, we successfully applied an iterative method (DJM) to calculate the concentration of carbon dioxide absorbed into phenyl glycidyl ether. The solutions obtained by DJM was reliable and efficient. Unlike the results obtained by ADM where the ADM was used Adomian's polynomials to calculate the nonlinear terms. The numerical solution obtained by the DJM is faster than the results obtained by Adomian's method. From figures and tables it has been shown that when the number of iterations are increased the maximal error remainders were decreased.

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