IOSR Journal of Mathematics (IOSR-JM)
e-ISSN: 2278-5728, p-ISSN: 2319-765X. Volume 11, Issue 6 Ver. 1 (Nov. - Dec. 2015), PP 99-105
www.iosrjournals.org

The variational iteration method for calculating carbon dioxide absorbed into phenyl glycidyl ether

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Abstract: *In this paper, the variational iteration method (VIM) is used to get an approximate solution for a system of two coupled nonlinear ordinary differential equations which represent the concentrations of carbon dioxide CO_2 and phenyl glycidyl ether. In this system there are boundary conditions of Dirichlet type and the other is a mixed set of Neumann and Dirichlet type. Our calculations evidenced by tables and figures for the analysis of the maximal error remainder values. The variational iteration method gives approximate solutions with fast convergence. Comparison with the results obtained by the Adomian decomposition method (ADM) reveals that the numerical solutions obtained by the VIM converge faster than those of Adomian's method. The software we used in our study of these calculations is Mathematica® 9.*

Keywords - *Variational iteration method, Lagrange multiplier, Carbon dioxide, Phenyl glycidyl ether*.

I. Introduction

Among the very important gases in nature is carbon dioxide CO_2 [1] where this gas is made up of only one carbon atom with two atoms of oxygen [2]. Carbon dioxide is considered an important factor in plant photosynthesis, in the powering of the pneumatic systems in robots used in extinguishing fires, carbonated soft drinks industry and remove the caffeine from coffee,... etc. [2,3,4]. Carbon dioxide considered a rich and cheap source of carbon. Benefits from carbon dioxide are considered an important development through the industry of most useful materials and the reduction of the threat posed by greenhouse effect.

The chemical absorption of carbon dioxide into phenyl glycidyl ether solution containing a catalyst THA-CP-MS41 in heterogeneous systems has been investigated by Park et al. [4] and Choe et al. [5]. Approximate analytical expression for the simple steady-state concentrations of CO_2 and PGE using the Adomian decomposition method is presented in [2]. However, the ADM required calculating the Adomian polynomials which needs more time and calculations.

In 1999, the Variational Iteration Method was first suggested by the Chinese mathematician Ji-Haun He [6, 7]. It can be applied to many differential and integral equations, linear and nonlinear, note that the finding of the exact solution for many of nonlinear problems is not easy task. In comparison to other methods used for solving the nonlinear differential equations [8], for example, Lie group method [9], homogeneous balance method [10], inverse scattering method [11], Adomian's decomposition method [12,13,14] and He's homotopy perturbation method (HPM) [15,16,17], the VIM is very effective, simple and does not require any restrictive assumptions for nonlinear terms.

The VIM has an advantage make us adopt in to calculate this system of nonlinear ordinary differential equations that is the VIM reduces the amount of calculations with survival maintain the higher accuracy in the solution.

He's VIM provides the approximations by using the correction functional requiring the Lagrange's multiplayer, while the ADM gives us components that are collected together to reach the solution and each component takes a long time to calculate it because of the terms of Adomian's polynomial which represent the nonlinear terms for both equations in the system [12,13]. The VIM does not need to calculate small parameters like as in the traditional perturbation methods, therefore the limitations of these methods has been eliminated. It is worth mentioning that this method is a modification for the general Lagrange multiplier method [18].

In this work, the VIM will be implemented to get an approximate solution for a system of two coupled nonlinear ordinary differential equations which represent the concentrations of carbon dioxide CO_2 and phenyl glycidyl ether.

This paper has been organized as follows. The steady-state concentrations of carbon dioxide absorbed into phenyl glycidyl ether solutions is given in details in section II. The variational iteration method is presented in section III. In section IV, solving the system of steady-state concentrations of CO_2 and PGE by the VIM will be given. Section V provides numerical simulation and the conclusion will be followed in section VI.

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

A system of two nonlinear differential equations represents the steady-state concentrations of two chemicals; carbon dioxide CO_2 and PGE is given in [2]. This system can be represented by [19]:

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

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

with the boundary conditions

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

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

Where, $u(x)$ is the concentration of CO_2, $v(x)$ is the concentration of PGE, α_1, α_2, β_1 and β_2 are the parameters of normalized system, x is the "dimensionless distance" from the center and k is the concentration of CO_2 at the surface catalyst [2].

This system of equations has been solved by the Adomian decomposition method [2,19] where it was calculated acceptable approximate results with the statement of the maximal error remainder and the amount of the accuracy [19], 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 are calculated which required more calculations and time.

In this work, we will solve this nonlinear system of these two coupled nonlinear ordinary differential equations [2,19] in a straightforward manner by using the Variational Iteration Method (VIM), details of the VIM can be found in [20-25].

Equations (1) and (2) can be written as:

$$u''(x)\big(1+\beta_1 u(x)+\beta_2 v(x)\big) = \alpha_1 u(x)v(x), \tag{3}$$

$$v''(x)\big(1+\beta_1 u(x)+\beta_2 v(x)\big) = \alpha_2 u(x)v(x). \tag{4}$$

The Eqs. (3),(4) will be solved by using the VIM.

III. The Variational Iteration Method:

According to the VIM [20-25], consider the following differential equation:

$$Lu + Nu = g(x), \tag{5}$$

where L is the linear operator, N is the nonlinear operator and $g(x)$ is the inhomogeneous term. The method employs the correction functional as follows:

$$u_{n+1}(x) = u_n(x) + \int_0^x \lambda(Lu_n(t) + N\tilde{u}_n(t) - g(t))\,dt, \tag{6}$$

where λ is the Lagrange multiplier [23, 24], which can be identified optimally via the variational theory [24], the subscript n represents the rank of the approximation u_n and $\tilde{u}_n$ is the restricted variation that is $\delta\tilde{u}_n = 0$. It is obvious now that the main steps of the He's variational iteration method require first the determination of the Lagrange multiplier λ(t) that will be identified optimally. Integration by parts is usually used for the selection of the Lagrange multiplier λ(t). In other words we can use

$$\int\lambda(t)u'_n(t)dt = \lambda(t)u_n(t) - \int\lambda'(t)u_n(t)dt,$$

$$\int\lambda(t)u''_n(t)dt = \lambda(t)u'_n(t) - \lambda'(t)u_n(t) + \int\lambda''(t)u_n(t)dt, \tag{7}$$

and so on. Having determined the Lagrange multiplier $\lambda(t)$, the successive approximations $u_{n+1}, n \geq 0$, of the solution u will be immediately obtained upon using any selective function u_0.

In general the exact solution can be obtained by

$$u(x) = \lim_{n\to\infty} u_n(x). \tag{8}$$

This method gives rapidly convergent successive approximations of the exact solution if such a solution exists, otherwise a few approximations can be used for numerical purposes. The VIM does not require restrictive conditions or specific assumptions as we have seen in other methods of other studies pertaining to the differential equations such as perturbation techniques.

IV. Solving the system of steady-state concentrations of CO_2 and PGE by the VIM:

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

$$u''(x)\big(1+\beta_1 u(x)+\beta_2 v(x)\big)-\alpha_1 u(x)v(x)=0, \tag{9}$$

$$v''(x)\big(1+\beta_1 u(x)+\beta_2 v(x)\big)-\alpha_2 u(x)v(x)=0, \tag{10}$$

with the boundary conditions

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

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

The correction functional for this system is given as

$$u_n(x)=u_{n+1}(x)+\int_0^x \lambda_1(t)(u''_n(t)(1+\beta_1 u_n(t)+\beta_2\, v_n(t))-\alpha_1 u_n(t)v_n(t))dt, \tag{11}$$

$$v_n(x)=v_{n+1}(x)+\int_0^x \lambda_1(t)(v''_n(t)(1+\beta_1 u_n(t)+\beta_2\, v_n(t))-\alpha_2 u_n(t)v_n(t))dt, \tag{12}$$

this yields the stationary conditions [27]

$$1-\lambda'_1|_{t=x}=0,\qquad \lambda_1|_{t=x}=0,\qquad \lambda''_1|_{t=x}=0, \tag{13}$$

$$1-\lambda'_2|_{t=x}=0,\qquad \lambda_2|_{t=x}=0,\qquad \lambda''_2|_{t=x}=0.$$

As a result, those will be obtained

$$\lambda_1(t)=\lambda_2(t)=t-x, \tag{14}$$

substitute Eq. (14) into Eqs. (11) and (12), gives the iterations formulas:

$$u_n(x)=u_{n+1}(x)+\int_0^x (t-x)(u''_n(t)(1+\beta_1 u_n(t)+\beta_2\, v_n(t))-\alpha_1 u_n(t)v_n(t))dt, \tag{15}$$

$$v_n(x)=v_{n+1}(x)+\int_0^x (t-x)(v''_n(t)(1+\beta_1 u_n(t)+\beta_2\, v_n(t))-\alpha_2 u_n(t)v_n(t))dt, n\geq 0, \tag{16}$$

the initial approximations have been taken: $u_0(x)=x^m$ and $v_0(x)=x^m$, with $m=1$.

The following approximations are achieved:

$u_0(x)=x,$

$v_0(x)=x,$

$$\begin{aligned}
u_1(x)&=x+\int_0^x (t-x)(u''_0(t)(1+\beta_1 u_0(t)+\beta_2\, v_0(t))-\alpha_1 u_0(t)v_0(t))dt\\
&=x+\frac{x^4\alpha_1}{12},\\
v_1(x)&=x+\int_0^x (t-x)(v''_0(t)(1+\beta_1 u_0(t)+\beta_2\, v_0(t))-\alpha_2 u_0(t)v_0(t))dt\\
&=x+\frac{x^4\alpha_2}{12},\\
u_2(x)&=x+\frac{x^4\alpha_1}{12}+\int_0^x (t-x)(u''_1(t)(1+\beta_1 u_1(t)+\beta_2\, v_1(t))-\alpha_1 u_1(t)v_1(t))dt\\
&=x+\frac{x^4\alpha_1}{12}+\frac{x^5\alpha_1(7x^5\alpha_1\alpha_2+180x^2(\alpha_1+\alpha_2)-4536(\beta_1+\beta_2)-135x^3(\alpha_1\beta_1+\alpha_2\beta_2))}{90720},\\
v_2(x)&=x+\frac{x^4\alpha_2}{12}+\int_0^x (t-x)(v''_1(t)(1+\beta_1 u_1(t)+\beta_2\, v_1(t))-\alpha_2 u_1(t)v_1(t))dt\\
&=x+\frac{x^4\alpha_1}{12}+\frac{x^5\alpha_1(7x^5\alpha_1\alpha_2+180x^2(\alpha_1+\alpha_2)-4536(\beta_1+\beta_2)-135x^3(\alpha_1\beta_1+\alpha_2\beta_2))}{90720}.
\end{aligned} \tag{17}$$

Thus we continue to obtain successive approximations of $u_n(x)$ and $v_n(x)$ but for brevity not listed. The calculations are obtained by using Mathematica 9.

In order to examine the accuracy of the achieved approximate solution, the convenience functions of the error remainder will be [19]:

$$ER_{1,n}(x)=u''_n(t)\big(1+\beta_1 u_n(t)+\beta_2\, v_n(t)\big)-\alpha_1 u_n(t)v_n(t), \tag{18}$$

$$ER_{2,n}(x)=v''_n(t)\big(1+\beta_1 u_n(t)+\beta_2\, v_n(t)\big)-\alpha_2 u_n(t)v_n(t), \tag{19}$$

and the maximal error remainder parameters are

$$MER_{1,n}=\max_{0\leq x\leq 1}\big|ER_{1,n}(x)\big|,\qquad MER_{2,n}=\max_{0\leq x\leq 1}\big|ER_{2,n}(x)\big|. \tag{20}$$

V. Numerical simulations:

The values of the parameters have been chosen: $\alpha_1 = 1, \alpha_2 = 2$, $\beta_1 = 1$, $\beta_2 = 3$ and $k = 0.5$ as in [19], then we calculate the error remainder with the maximal error remainder parameters and the approximate solutions. Below we have created both $MER_{1,n}$ and $MER_{2,n}$ as the values of n increase from 1 to 4 and in comparison with the Adomian decomposition method [19,12]. It can be seen that the maximal error remainder values of the VIM is the least of those obtained from the ADM. Therefore, better accuracy achieved for both $MER_{1,n}$ and $MER_{2,n}$:

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

n	$MER_{1,n}$ by the ADM[19]	$MER_{1,n}$ by the VIM
1	0.2	0.003
2	0.0888889	0.00159895
3	0.00888889	0.00063952
4	0.00099943	0.0002558

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

n	$MER_{2,n}$ by the ADM[19]	$MER_{2,n}$ by the VIM
1	0.4	0.00799617
2	0.177778	0.0031979
3	0.0177778	0.00127904
4	0.00099943	0.000511601

We insert below the Figs. 1 and 2, respectively, that show the analysis of the maximal error remainders for both $MER_{1,n}$ and $MER_{2,n}$, where the points are lay on a straight lines which mean we achieved exponential rate of convergence.

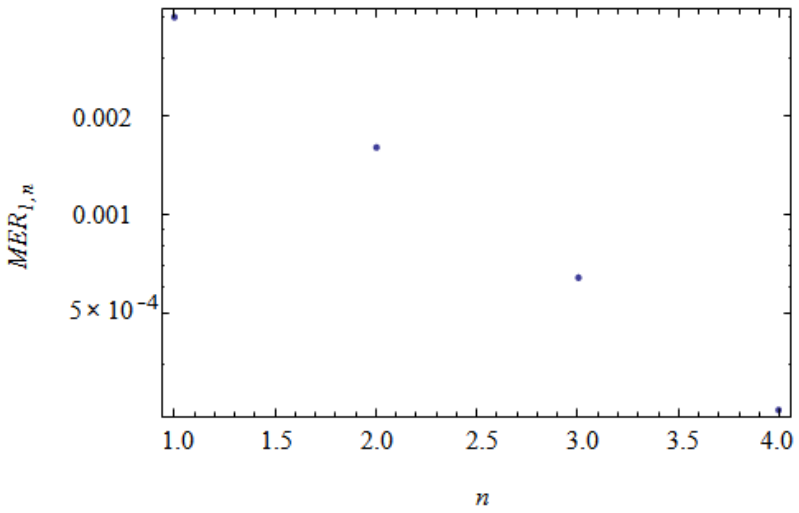

Fig.1: Logarithmic plots of $MER_{1,n}$ versus *n* is 1 through 4 and *m*=1

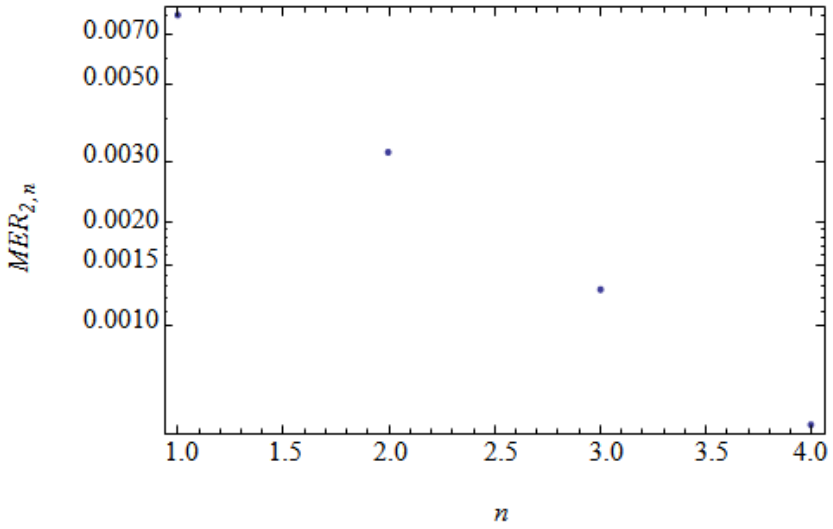

Fig.2: Logarithmic plots of $MER_{2,n}$ versus *n* is 1 through 4 and *m*=1

It is interesting to point out here, by increasing the power of the values of x (initial approximations) for both $u_n(x)$ and $v_n(x)$, the error decreases and the accuracy will be higher. Moreover, it can be seen clearly from tables 1, 2, Figs 1 and 2 that by increasing the iterations (*n* from 1 to 4) we achieved good accuracy as well.

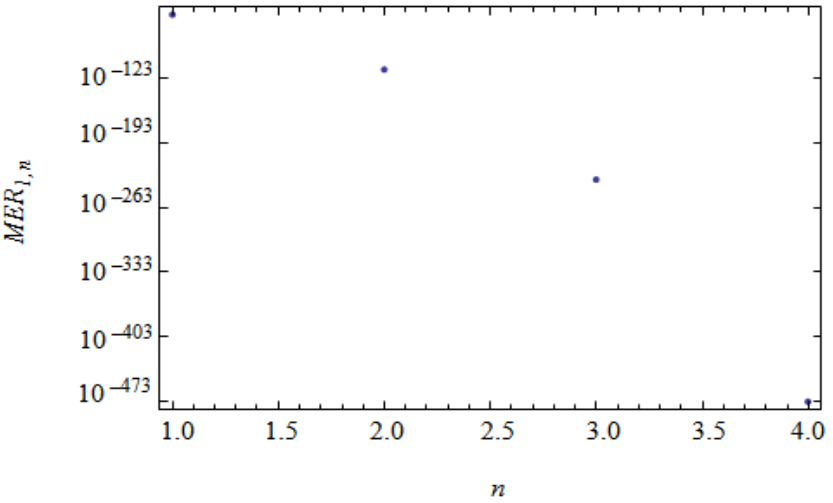

Fig.3: Logarithmic plots of $MER_{1,n}$ versus *n* is 1 through 4 and *m*=30

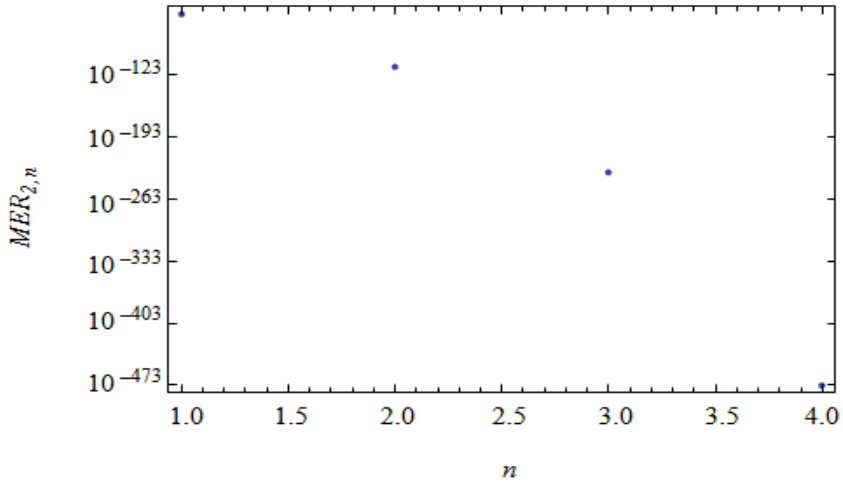

Fig.4: Logarithmic plots of $MER_{2,n}$ versus *n* is 1 through 4 and *m*=30

Tables 3 and 4 show the maximal error remainders are decreases when the power of x is increases for both $u_n(x)$ and $v_n(x)$:

Table.3: the maximal error remainder: $MER_{1,n}$ by the VIM Where n=1,…,4 and the power of x is m

n \ m	1	2	3	4
1	0.00799	0.00319	0.00128	0.00051
5	0.07998×10^{-5}	2.84315×10^{-16}	6.16298×10^{-33}	6.16298×10^{-33}
10	0.35998×10^{-15}	1.36406×10^{-35}	4.77101×10^{-75}	1.44069×10^{-154}
15	0.83998×10^{-25}	3.24398×10^{-55}	1.18909×10^{-114}	3.96065×10^{-234}
20	1.51998×10^{-35}	5.92394×10^{-75}	2.22109×10^{-154}	7.75660×10^{-314}
25	2.39998×10^{-45}	9.40392×10^{-95}	3.57308×10^{-194}	1.28311×10^{-393}
30	3.47998×10^{-55}	1.36839×10^{-114}	5.24508×10^{-234}	1.91847×10^{-473}
35	4.75998×10^{-65}	1.87639×10^{-134}	7.23708×10^{-274}	2.68179×10^{-553}
40	6.23998×10^{-75}	2.46439×10^{-154}	9.54908×10^{-314}	3.57308×10^{-633}
45	7.91998×10^{-85}	3.13239×10^{-174}	1.21810×10^{-353}	4.59234×10^{-713}
50	9.79998×10^{-95}	3.88039×10^{-194}	1.51330×10^{-393}	5.73960×10^{-793}

Table.4: the maximal error remainder: $MER_{2,n}$ by the VIM Where n=1,…,4 and the power of x is m

n \ m	1	2	3	4
1	0.00399	0.00159	0.00064	0.00025
5	0.07999×10^{-5}	2.84359×10^{-16}	4.93038×10^{-32}	4.93038×10^{-32}
10	0.35999×10^{-15}	1.36411×10^{-35}	4.77118×10^{-75}	1.44074×10^{-154}
15	0.83999×10^{-25}	3.24403×10^{-55}	1.18911×10^{-114}	3.96071×10^{-234}
20	1.51999×10^{-35}	5.92399×10^{-75}	2.22111×10^{-154}	7.75670×10^{-314}
25	2.39999×10^{-45}	9.40397×10^{-95}	0.35731×10^{-193}	1.28312×10^{-393}
30	3.47999×10^{-55}	0.13684×10^{-113}	0.52451×10^{-233}	1.91848×10^{-473}
35	4.75999×10^{-65}	1.87639×10^{-134}	7.23710×10^{-274}	2.68179×10^{-553}
40	6.23999×10^{-75}	2.46439×10^{-154}	9.54909×10^{-314}	3.57308×10^{-633}
45	7.91999×10^{-85}	3.13239×10^{-174}	1.21810×10^{-353}	4.59235×10^{-713}
50	9.79999×10^{-95}	3.88039×10^{-194}	1.51330×10^{-393}	5.73960×10^{-793}

VI. Conclusion

In this paper, He's variational iteration method has been successfully applied to calculate the concentrations of carbon dioxide absorbed into phenyl glycidyl ether. The VIM provides the solutions in the form of convergent series with easily computed components. Unlike the ADM where computational algorithms required to calculate the Adomian polynomials to handle the nonlinear terms. Comparison with Adomian's decomposition method reveals that the numerical solutions obtained by the VIM converge faster than those of Adomian's method. It has been achieved that from figures and tables that the maximal error remainders decreased when the number of iterations are increased. Moreover, as the power of x (initial approximation) is increased the maximal error remainders decreased.

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