

Approximate Solutions Of Chemical Reaction - Diffusion Brusselator System And Coupled Schrodinger - Kdv Equation Using New Iterative Method

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Abstract

This article, presents the approximate solutions of Chemical Reaction-Diffusion Brusselator system and Coupled Schrodinger – Korteweg - de Vries equation by a reliable algorithm of New Iterative Method. Results obtained by proposed method are compared with exact solutions as well as with the results obtain by Optimal Homotopy Asymptotic Method, Homotopy Perturbation Method and Variational Iterational Method. New Iterative Method is an improvement with regard to its accuracy and rapid convergence. Since mathematical analysis leads to Brusselator equations for some chemical reaction-diffusion experiments, it is worth demanding a new technique to solve such a method. We are creating a modern and successful recurring method. Numerical results indicate that the approach suggested is accurate and efficient. The method's precision increases with the number of iterations increasing.

Keywords: *New Iterative Method, Chemical Reaction-Diffusion Brusselator system, Coupled Schrodinger-KdV equations.*

1. Introduction

The Brusselator model arises in the modelling of certain chemical reaction - diffusion processes. The Brusselator reaction-diffusion model plays a substantial role in the study of cooperative processes of chemical kinetics. This system occurs in a large number of physical problems. It arises in the creation of ozone by atomic oxygen through a triple collision, in enzymatic reactions, and in plasma and laser physics [1]. A pair of variables is involved in dealing with these chemical reactions with input and output chemicals, whose concentrations are likely to be controlled during the reaction process and are substantial under quite genuine conditions. The coupled Schrodinger-KdV equations are extensively used to model nonlinear dynamics of one-dimensional Langmuir and ion acoustic waves in the system of coordinates moving at the speed of ion acoustic. The two dimensional chemical-diffusion reaction brusselator system takes the following form

$$\begin{aligned} \frac{\partial u(x, y, t)}{\partial t} &= u^2 v - (A+1)u + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + B, \\ \frac{\partial v(x, y, t)}{\partial t} &= -u^2 v + Au + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right), \end{aligned} \tag{a}$$

subject to the initial conditions

$$\begin{aligned} u(x, y, 0) &= h(x, y), \\ v(x, y, 0) &= g(x, y), \end{aligned}$$

where $u(x, y, t)$ and $v(x, y, t)$ are unknown functions representing the dimensionless concentrations of two reactants, x, y , and t denote the spatial and temporal independent variables, respectively. A and B are constant concentrations of the two reactants, μ represents the diffusion coefficient, and h and k are known functions. It is evident that for small values of diffusion coefficient μ , the steady state solution of Brusselator system converges to the equilibrium point $(B, A/B)$ if $1-A+B^2 > 0$. During the last few years, the researchers have shown keen interest in the existence of solution of the Brusselator reaction model when $1 - A + B^2 \geq 0$ [5–7]. The Coupled Schrodinger Korteweg-de Vries (KdV) equation is given by

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} &= \frac{\partial^2 v(x,t)}{\partial x^2} + v(x,t)w(x,t), \\ \frac{\partial v(x,t)}{\partial t} &= -\frac{\partial^2 u(x,t)}{\partial x^2} - u(x,t)w(x,t), \\ \frac{\partial w(x,t)}{\partial t} &= -6w \frac{\partial w(x,t)}{\partial x} - \frac{\partial^3 w(x,t)}{\partial x^3} + 2u(x,t) \frac{\partial w(x,t)}{\partial x} + 2v(x,t) \frac{\partial v(x,t)}{\partial x}. \end{aligned} \tag{b}$$

These problems remained the center of research and study for many years and have been investigated by many researchers. Many authors have investigated the approximate solution of these equations by various techniques [2-9].

In this research article, we have extended New Iterative Method (NIM) for finding the approximate solution of above mentioned problems. The method was proposed by Daftardar- Gejji and Jafari and is one of the most reliable and effective techniques to solve linear and nonlinear functional equations [10-13]. This method produces a series of analytical solution to such nonlinear equations which converges to the exact solution.

2. Analysis of NIM for Coupled System of PDE's

Consider the system of partial differential equations in the form of

$$u_{i,0} = f_i + \zeta_i(u_1, u_2, \dots, u_n) \quad i = 1, 2, 3, \dots, n, \tag{1}$$

where f_i are known function and ζ_i are nonlinear operators. Let $\tilde{u} = (u_1, u_2, \dots, u_n)$ be the solution of system (1) where u_i having the series form,

$$u_i = \sum_{j=0}^{\infty} u_{i,j} \quad i = 1, 2, 3, \dots, n. \tag{2}$$

We decompose the nonlinear operator N_i as

$$\zeta_i(\tilde{u}) = \zeta_i \left(\sum_{j=0}^{\infty} u_{1,j}, \dots, \sum_{j=0}^{\infty} u_{n,j} \right) \tag{3}$$

$$= \zeta_i(u_{1,0}, u_{2,0}, \dots, u_{n,0}) + \sum_{k=0}^{\infty} \left\{ \left(\zeta_i \sum_{j=0}^{\infty} u_{1,j}, \dots, \sum_{j=0}^{\infty} u_{n,j} - \zeta_i \sum_{j=0}^{k-1} u_{1,j}, \dots, \sum_{j=0}^{k-1} u_{n,j} \right) \right\}. \tag{4}$$

By virtue of above equations, Equation (1) takes the following form

$$\sum_{j=0}^{\infty} u_{i,j} = f_i + \zeta_i(u_{1,0}, u_{2,0}, \dots, u_{n,0}) + \sum_{k=1}^{\infty} \left\{ \left(\zeta_i \sum_{j=0}^k u_{1,j}, \dots, \sum_{j=0}^k u_{2,j} - \zeta_i \sum_{j=0}^{k-1} u_{1,j}, \dots, \sum_{j=0}^{k-1} u_{n,j} \right) \right\}. \tag{5}$$

For $i = 1, 2, 3, \dots, n$, we define recurrence relation as

$$u_{i,m+1} = \left(\zeta_i \sum_{j=0}^m u_{1,j}, \dots, \sum_{j=0}^m u_{2,j} - \zeta_i \sum_{j=0}^{m-1} u_{1,j}, \dots, \sum_{j=0}^{m-1} u_{n,j} \right), \quad m = 1, 2, 3, \dots, \tag{6}$$

then

$$u_i = \sum_{j=0}^{\infty} u_{i,j}. \tag{7}$$

The k-th order approximate to u_i is given by

$$u_i = \sum_{j=0}^{k-1} u_{i,j}. \tag{8}$$

The k-th iteration ($k=2,3,4, \dots$) is given by the following relations

$$u_{1,k} = \zeta_1 \left(\sum_{i=0}^{k-1} u_{1,i}, \dots, \sum_{i=0}^{k-1} u_{n,i} \right) - \zeta_1 \left(\sum_{i=0}^{k-2} u_{1,i}, \dots, \sum_{i=0}^{k-2} u_{n,i} \right), \tag{9}$$

$$u_{j,k} = \zeta_j \left(\sum_{i=0}^k u_{1,i}, \dots, \sum_{i=0}^k u_{i-1,i}, \sum_{i=0}^{k-1} u_{i,i}, \dots, \sum_{i=0}^{k-1} u_{i-1,i} \right) - \zeta_j \left(\sum_{i=0}^{k-1} u_{1,i}, \dots, \sum_{i=0}^{k-1} u_{j-1,i}, \sum_{i=0}^{k-2} u_{j,i}, \dots, \sum_{i=0}^{k-2} u_{n,i} \right), \tag{10}$$

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$$u_{n,k} = \zeta_n \left(\sum_{i=0}^k u_{1,i}, \dots, \sum_{i=0}^k u_{n-1,i}, \sum_{i=0}^{k-1} u_{n,i} \right) - \zeta_n \left(\sum_{i=0}^{k-1} u_{1,i}, \dots, \sum_{i=0}^{k-1} u_{n-1,i}, \sum_{i=0}^{k-2} u_{n,i} \right). \tag{11}$$

Thus

$$\zeta_i(\tilde{u}) = \zeta_i \left(\sum_{j=0}^{\infty} u_{1,j}, \dots, \sum_{j=0}^{\infty} u_{n,j} \right) = \sum_{j=1}^{\infty} u_{i,j}. \quad (12)$$

Hence we have

$$\tilde{u} = \sum_{j=0}^{\infty} u_{i,j} \quad (13)$$

3. Numerical Examples

3.1: Chemical Reaction-Diffusion Brusselator System

Consider Eq. (a) with $(A = 1, \mu = \frac{1}{4}, B = 0, h(x, y) = e^{(-x-y)}, \text{ and } g(x, y) = e^{(x+y)})$,

we have

$$\begin{aligned} \frac{\partial u(x, y, t)}{\partial t} &= u^2 v - 2u + \frac{1}{4} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \\ \frac{\partial v(x, y, t)}{\partial t} &= u - u^2 v + \frac{1}{4} \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right), \\ u(x, y, 0) &= e^{(-x-y)}, \quad v(x, y, 0) = e^{(x+y)}. \end{aligned} \quad (14) \text{ with initial conditions}$$

The exact solutions are

$$u(x, y, t) = e^{(-x-y-\frac{t}{2})}, \quad v(x, y, t) = e^{(x+y+\frac{t}{2})}.$$

The equivalent integral forms of the Eq. (14) can be written as

$$\begin{aligned} u &= \int_0^t (u^2 v) dt - 2 \int_0^t u dt + \frac{1}{4} \int_0^t \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) dt, \\ v &= \int_0^t u dt - \int_0^t (u^2 v) dt + \frac{1}{4} \int_0^t \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) dt. \end{aligned} \quad (15)$$

Using NIM formulation discussed in section 2, we have the following approximations:

$$\begin{aligned} u_0(x, y, t) &= e^{(-x-y)}, \\ v_0(x, y, t) &= e^{(x+y)}, \\ u_1(x, y, t) &= -\frac{1}{2} e^{(-x-y)} t, \\ v_1(x, y, t) &= \frac{1}{2} e^{(x+y)} t, \\ u_2(x, y, t) &= \frac{1}{2} e^{(-x-y)} t + \frac{3}{4} e^{(-x-y)} \left(-2t + \frac{t^2}{2} \right) + \frac{1}{8} e^{(-x-y)} \left(8t - 2t^2 - \frac{2t^3}{2} + \frac{t^4}{4} \right), \\ v_2(x, y, t) &= -\frac{1}{2} e^{(x+y)} t - \frac{1}{2} e^{(-x-y)} \left(-2t + \frac{t^2}{2} \right) + \frac{1}{4} e^{(x+y)} \left(2t + \frac{t^2}{2} \right) - \frac{1}{8} e^{(-x-y)} \\ &\quad \left(8t - 2t^2 - \frac{2t^3}{2} + \frac{t^4}{4} \right), \end{aligned} \quad (16)$$

$$u_3(x, y, t) = \frac{1}{2} e^{(-x-y)} \left(-2t + \frac{t^2}{2} \right) - \frac{1}{4} e^{(-x-y)} \left(8t - 2t^2 - \frac{-2t^3}{3} + \frac{t^4}{4} \right) + \frac{1}{96} e^{(-x-y)} \left(96 - 24t^2 + 4t^3 - 2t^4 + \frac{3t^5}{5} \right) + \frac{1}{192} e^{-3(x+y)} \left(2t^4 - \frac{3t^5}{5} + 4e^{2(x+y)} t(24 + 6t + t^2) - \frac{1}{884736} e^{-3(x+y)} \left(18432t^4 + \frac{101376t^5}{5} + 10752t^6 - \frac{35328t^7}{7} + 2496t^8 - \frac{2768t^9}{3} + \frac{1264t^{10}}{5} - 72t^{11} + 18t^{12} - \frac{2713t^{13}}{13} + e^{2(x+y)} \left(88736t - 221184t^2 + 36864t^3 - 36864t^4 + 13824t^5 - 1152t^6 + \right) \right) \right) \quad (17)$$

$$v_3(x, y, t) = \frac{1}{2} e^{(-x-y)} \left(-2t + \frac{t^2}{2} \right) - \frac{1}{4} e^{(-x-y)} \left(8t - 2t^2 - \frac{-2t^3}{3} + \frac{t^4}{4} \right) + \frac{1}{96} e^{(-x-y)} \left(96 - 24t^2 + 4t^3 - 2t^4 + \frac{3t^5}{5} \right) + \frac{1}{192} e^{-3(x+y)} \left(2t^4 - \frac{3t^5}{5} + 4e^{2(x+y)} t(24 + 6t + t^2) - \frac{1}{884736} e^{-3(x+y)} \left(18432t^4 + \frac{101376t^5}{5} + 10752t^6 - \frac{35328t^7}{7} + 2496t^8 - \frac{2768t^9}{3} + \frac{1264t^{10}}{5} - 72t^{11} + 18t^{12} - \frac{2713t^{13}}{13} + e^{2(x+y)} \left(88736t - 221184t^2 + 36864t^3 - 36864t^4 + 13824t^5 - 1152t^6 + \frac{7872t^7}{7} - 480t^8 + \frac{64t^9}{3} - \frac{72t^{10}}{5} + \frac{108t^{11}}{11} \right) \right) \right) \quad (18)$$

Similarly we can find the remaining terms with the help of Mathematica 7.0. Finally we have

$$\begin{cases} \tilde{u}(x, y, t) = u_0(x, y, t) + u_1(x, y, t) + u_2(x, y, t) + u_3(x, y, t), \\ \tilde{v}(x, y, t) = v_0(x, y, t) + v_1(x, y, t) + v_2(x, y, t) + v_3(x, y, t). \end{cases} \quad (19)$$

3.2: Coupled Schrodinger-KdV equation

Consider Schrodinger-KdV equation of the following form

$$\begin{aligned} \frac{\partial u(x, t)}{\partial t} &= \frac{\partial^2 v(x, t)}{\partial x^2} + v(x, t)w(x, t), \\ \frac{\partial v(x, t)}{\partial t} &= -\frac{\partial^2 u(x, t)}{\partial x^2} - u(x, t)w(x, t), \\ \frac{\partial w(x, t)}{\partial t} &= -6w \frac{\partial w(x, t)}{\partial x} - \frac{\partial^3 w(x, t)}{\partial x^3} + 2u(x, t) \frac{\partial w(x, t)}{\partial x} + 2v(x, t) \frac{\partial v(x, t)}{\partial x}, \end{aligned} \quad (20)$$

with initial conditions

$$\begin{aligned} u(x, 0) &= \text{Cos}(x), \\ v(x, 0) &= \text{Sin}(x), \\ w(x, 0) &= \frac{3}{4}. \end{aligned} \quad (21)$$

The exact solutions of Eq. (20) is given by

$$\begin{aligned}
 u(x,t) &= \text{Cos}\left(x + \frac{t}{4}\right), \\
 v(x,t) &= \text{Sin}\left(x + \frac{t}{4}\right), \\
 w(x,t) &= \frac{3}{4}.
 \end{aligned}
 \tag{22}$$

The equivalent integral forms of the Eq. (14) can be written as

$$\begin{aligned}
 u(x,t) &= \int_0^t \frac{\partial^2 v(x,t)}{\partial x^2} dt + \int_0^t \frac{\partial^2 v(x,t)}{\partial x^2} + \int_0^t v(x,t)w(x,t)dt, \\
 v(x,t) &= -\int_0^t \frac{\partial^2 u(x,t)}{\partial x^2} dt - \int_0^t u(x,t)w(x,t)dt, \\
 w(x,t) &= -6\int_0^t w \frac{\partial w(x,t)}{\partial x} dt - \int_0^t \frac{\partial^3 w(x,t)}{\partial x^3} dt + 2\int_0^t u(x,t) \frac{\partial w(x,t)}{\partial x} dt + \int_0^t 2v(x,t) \frac{\partial v(x,t)}{\partial x} dt.
 \end{aligned}
 \tag{23}$$

Using NIM formulation discussed in section 2, we get the following approximations:

$$\begin{aligned}
 u_0(x,t) &= \text{cos}(x), & v_0(x,t) &= \text{Sin}(x), & w_0(x,t) &= \frac{3}{4}, \\
 u_1(x,t) &= -\frac{1}{4}t \text{Sin}(x), & v_1(x,t) &= \frac{1}{4}t \text{Cos}(x), & w_1(x,t) &= 2t \text{Cos}(x) \text{Sin}(x), \\
 u_2(x,t) &= -\frac{1}{32}t^2 \text{Cos}(x) + \frac{1}{2}t^2 \text{Sin}(x) \text{Sin}(2x) + \frac{1}{12}t^3 \text{Cos}(x) \text{Sin}(2x), \\
 v_2(x,t) &= -\frac{1}{32}t^2 \text{Sin}(x) - \frac{1}{2}t^2 \text{Cos}(x) \text{Sin}(x) + \frac{1}{12}t^3 \text{Sin}(x) \text{Sin}(2x).
 \end{aligned}
 \tag{24}$$

Similarly we can find the remaining terms with the help of Mathematica 7.0.

Finally we can get the following expression as

$$\begin{cases}
 \tilde{u}(x,t) = u_0(x,t) + u_1(x,t) + u_2(x,t), \\
 \tilde{v}(x,t) = v_0(x,t) + v_1(x,t) + v_2(x,t), \\
 \tilde{w}(x,t) = w_0(x,t) + w_1(x,t) + w_2(x,t),
 \end{cases}
 \tag{25}$$

4. Results and Discussion

We implemented NIM for finding the approximate solutions of Chemical Reaction-Diffusion Brusselator system and Coupled Schrodinger-KdV equations. The results obtained by NIM for Chemical Reaction-Diffusion Brusselator system. Table 1 and 2 shows the comparison of absolute errors of NIM and OHAM for $u(x, y, t)$ and $v(x, y, t)$ part of Chemical Reaction-Diffusion Brusselator system. From the numerical values and graphs it is clear that NIM is very powerful tool for solution of coupled system of partial differential equations. The accuracy of the NIM can further be increased by taking higher order approximations.

Table 1

3rd order approximate solution $u(x, y, t)$ obtained by NIM in comparison with exact Solution and third order OHAM solution [14] at $t = 0.25$

x/t	y	NIM	Exact	Absolute Error OHAM [14]	Absolute Error NIM
0.5	0.25	0.535261	0.535248	2.317×10^{-5}	1.338×10^{-5}
0.5	0.5	0.416862	0.416847	1.804×10^{-5}	1.464×10^{-5}
0.5	0.75	0.324652	0.324639	1.405×10^{-5}	1.339×10^{-5}

Table 2

3rd order approximate solution $v(x, y, t)$ obtained by NIM in comparison with exact

Solution and third order OHAM solution [14] at $x = 0.2, t = 0.01$

x/t	y	NIM	Exact	Absolute Error OHAM [14]	Absolute Error NIM
0.2 / 0.01	0.25	1.57617	1.57617	1.813×10^{-5}	1.041×10^{-10}
0.2 / 0.01	0.5	2.02385	2.02385	2.328×10^{-5}	7.683×10^{-11}
0.2 / 0.01	0.75	2.59867	2.59867	2.989×10^{-5}	4.105×10^{-11}

Table 3

Absolute errors of NIM corresponding to exact solution at different time level for $u(x, t)$ of Eq. (20)

x	$t = 0.5$	$t = 0.2$	$t = 0.1$	$t = 0.01$	$t = 0.001$
-3	320577×10^{-4}	969838×10^{-4}	219824×10^{-4}	1.99424×10^{-6}	1.97382×10^{-8}
-2	126114×10^{-4}	139541×10^{-2}	346466×10^{-3}	344318×10^{-5}	3.44103×10^{-7}
-1	184298×10^{-4}	149928×10^{-2}	378698×10^{-3}	382186×10^{-5}	3.82535×10^{-7}
0	325267×10^{-4}	2.60395×10^{-7}	1.62757×10^{-8}	1.62759×10^{-12}	2.22045×10^{-16}
1	167187×10^{-4}	156128×10^{-2}	386448×10^{-3}	382961×10^{-5}	3.82612×10^{-7}
2	144604×10^{-4}	13572×10^{-2}	341691×10^{-3}	343841×10^{-5}	3.44055×10^{-7}
3	323446×10^{-4}	606891×10^{-4}	174455×10^{-4}	1.94887×10^{-6}	1.96929×10^{-8}

Table 4

Absolute errors of NIM corresponding to exact solution at different time level for $v(x, t)$ of Eq. (20)

x	$t = 0.5$	$t = 0.2$	$t = 0.1$	$t = 0.01$	$t = 0.001$
-3	338461×10^{-2}	548551×10^{-3}	137723×10^{-3}	138251×10^{-5}	1.38304×10^{-7}
-2	320732×10^{-2}	583162×10^{-3}	151629×10^{-3}	156886×10^{-5}	1.57412×10^{-7}
-1	695665×10^{-2}	103475×10^{-2}	252166×10^{-3}	246299×10^{-5}	2.45713×10^{-7}
0	325267×10^{-4}	208307×10^{-5}	2.60409×10^{-6}	2.60417×10^{-9}	2.60417×10^{-12}
1	532745×10^{-2}	930478×10^{-3}	239132×10^{-3}	244996×10^{-5}	2.45583×10^{-7}
2	466805×10^{-2}	67665×10^{-3}	163315×10^{-3}	158055×10^{-5}	1.57529×10^{-7}
3	353116×10^{-2}	557933×10^{-3}	138896×10^{-3}	138368×10^{-5}	1.38315×10^{-7}

Table 5

Comparison of NIM solution with exact solution for $w(x, t)$ Eq. (20)

x	NIM	Exact
-3	3 / 4	3 / 4
-2	3 / 4	3 / 4
-1	3 / 4	3 / 4
0	3/4	3 / 4

1	3/4	3 /4
2	3/4	3 /4
3	3/4	3 /4

5. Conclusion

New Iterative Method converges rapidly to the exact solution at lower order of approximations for Chemical Reaction-Diffusion Brusselator system and Coupled Schrodinger-Korteweg-de Vries equation. The results obtained by proposed method are very encouraging in comparison with OHAM, HPM and VIM. As a result it will be more appealing for researchers to apply this method for solving systems of nonlinear partial differential equations in different fields of science especially in fluid dynamics and physics.

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