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Research Article

Third-Order Approximate Solution of Chemical Reaction-Diffusion Brusselator System Using Optimal Homotopy Asymptotic Method

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The objective of this paper is to investigate the effectiveness and performance of optimal homotopy asymptotic method in solving a system of nonlinear partial differential equations. Since mathematical modeling of certain chemical reaction-diffusion experiments leads to Brusselator equations, it is worth demanding a new technique to solve such a system. We construct a new efficient recurrent relation to solve nonlinear Brusselator system of equations. It is observed that the method is easy to implement and quite valuable for handling nonlinear system of partial differential equations and yielding excellent results at minimum computational cost. Analytical solutions of Brusselator system are presented to demonstrate the viability and practical usefulness of the method. The results reveal that the method is explicit, effective, and easy to use.

1. Introduction

The Brusselator model, the nonlinear system of partial differential equations, arises in the modeling of certain chemical reaction-diffusion processes. This 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 in numerous coupling among models [1]. A pair of variables are involved in dealing with these chemical reactions; intermediates with input and output chemicals, whose concentrations are likely to be controlled during the reaction process, are substantial under quite genuine conditions and are discussed by Nicolis and Prigogine in [2, 3]. This model has been revealed as the trimolecular model [4].

The two-dimensional nonlinear reaction-diffusion Brusselator system is

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

subject to the initial condition:

$$\begin{aligned}u(x,y,0) &= h(x,y),\\ v(x,y,0) &= g(x,y),\end{aligned} \tag{2}$$

where $u(x,y,t)$, $v(x,y,t)$ are unknown functions representing the dimensionless concentrations of two reactants, x, y, and t denote spatial and temporal independent variables, respectively, A and B are constant concentrations of the two reactants, μ represent the diffusion coefficient, and h and k are known functions. It is evident that, for small values of diffusion coefficient μ, 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 keen interest in the existence of solution of the Brusselator reaction model when $1-A+B^2 \not> 0$ [5–7]. In this paper, we have made a successful attempt to find the solution of such types of Brusselator system.

Numerical methods need large size of computational works and generally the consequence of round-off error causes loss of precision in the results for system of nonlinear partial differential equations. Analytical methods mostly used for solving these equations are very restricted and can

be used in very special cases. Therefore, an optimal technique is required to resolve such circumstances.

The OHAM was recently introduced by Marinca and Herişanu [8–11]. In series of papers, authors [12–16] have applied this method effectively to validate the solutions of currently important problems. Iqbal et al. [12–15] used OHAM for linear and nonlinear differential equations and time dependent partial differential equations. Similarly, Idrees et al. [16] validated OHAM for nonlinear phenomena of fluid mechanics.

In this presentation, we have extended OHAM formulation for system of partial differential equations. Particularly, the extended formulation is demonstrated by illustrative example of nonlinear Brusselator system partial differential equations.

2. OHAM Formulation for Brusselator System

The optimal homotopy asymptotic method (OHAM) is given in [8–16]; we formulate this method for fractional order partial differential equations in the following steps.

(a) Write the governing partial differential equation system as

$$\frac{\partial}{\partial t}u(x,y,t) = u^2v - (A+1)u + \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + B,$$
$$\frac{\partial}{\partial t}v(x,y,t) = -u^2v + Au + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right), \tag{3}$$

subject to the initial condition:

$$u(x,y,0) = h(x,y),$$
$$v(x,y,0) = g(x,y), \tag{4}$$

where $u(x,y,t)$, $v(x,y,t)$ are unknown functions; x, y, and t denote spatial and temporal independent variables, respectively.

(b) Construct an optimal homotopy for system of partial differential equations, $\phi_1(x,y,t;p) : \Omega \times [0,1] \to R, \phi_2(x,y,t;p) : \psi \times [0,1] \to R$, which satisfies

$$H(\phi_1(x,y,t;p),p) = (1-p)\frac{\partial}{\partial t}\phi_1(x,y,t) - H_1(x,y,t;p)\left(\frac{\partial \phi_1}{\partial t} - \phi_1^2\phi_2 + (A+1)\phi_1 - \mu\left(\frac{\partial^2\phi_1}{\partial x^2} + \frac{\partial^2\phi_1}{\partial y^2}\right) - B\right) = 0$$
$$H(\phi_2(x,y,t;p),p) = (1-p)\frac{\partial}{\partial t}\phi_2(x,y,t) - H_2(x,y,t;p)\left(\frac{\partial \phi_2}{\partial t} - \phi_1^2\phi_2 - A\phi_1 - \mu\left(\frac{\partial^2\phi_1}{\partial x^2} + \frac{\partial^2\phi_1}{\partial y^2}\right)\right) = 0, \tag{5, 6}$$

where $p \in [0,1]$ is an embedding parameter, $H_1(x,y,t;p)$ and $H_2(x,y,t;p)$ are nonzero auxiliary functions for $p \neq 0$ and $H_1(x,y,t;\ 0) = 0, H_2(x,y,t;\ 0) = 0$, and, clearly, we have

$$H_1(x,y,t;p) = H_2(x,y,t;p) = pK_1(x,y,t;c_1) + p^2K_2(x,y,t;c_2) + \cdots + p^mK_m(x,y,t;c_m), \tag{7}$$

where $c_1, c_2, c_3, \ldots, c_m$ are convergence control parameters. The selection of functions $K_m(x,y,t;c_i)$ might be different type of polynomial and so on. It is very important to choose the functions, since the convergence of the solution very much depends on these functions. The auxiliary function $H(x,y,t;c)$ provides us with a simple way to adjust and control the convergence. It also increases the accuracy of the results and effectiveness of the method [17, 18]. The convergence control parameters adjust and control the convergence, which provides optimal accuracy and effectiveness of the method. The presence of c_i, $i = 1,2,\ldots,m$ ensures the fast convergence.

(c) Expand $\phi_1(x,y,t;p,c)$ and $\phi_2(x,y,t;p,c)$ in Taylor's series about p, to get approximate solutions as

$$\phi_1(x,y,t;p,c_i) = u_0(r,t) + \sum_{k=1}^{m} u_k(r,t;c_i)\,p^k \quad i = 1,2,3,\ldots,m, \tag{8}$$

$$\phi_2(x,y,t;p,c_i) = v_0(r,t) + \sum_{k=1}^{m} v_k(r,t;c_i)\,p^k \quad i = 1,2,3,\ldots,m. \tag{9}$$

(i) It has been observed that the convergence of the series (8) and (9) depends upon the convergence control parameters.

(ii) If it converges at $p = 1$, one has

$$\widetilde{u}(r,t;c_i) = u_0(r,t) + \sum_{k=1}^{m} u_k(r,t;c_i) \quad i = 1,2,3,\ldots,m, \tag{10}$$

$$\widetilde{v}(r,t;c_i) = v_0(r,t) + \sum_{k=1}^{m} v_k(r,t;c_i) \quad i = 1,2,3,\ldots,m. \tag{11}$$

(d) Equate the coefficients of like powers of p after substituting (8) and (9) in (5) and (6), respectively; one can get zeroth-order system given by (12), first-order and second-order system given by (13)-(14), respectively, and the higher order system if needed:

$$p^0: \quad \frac{\partial}{\partial t}u_0(x,y,t) = 0, \qquad \frac{\partial}{\partial t}v_0(x,y,t) = 0 \tag{12}$$

$$p^1: \quad Bc_1 - c_1u_0 - Ac_1u_0 + c_1u_0^2v_0 + \mu c_1\frac{\partial^2 u_0}{\partial y^2} + \mu c_1\frac{\partial^2 u_0}{\partial x^2} - (1+c_1)\frac{\partial u_0}{\partial t} + \frac{\partial u_1}{\partial t} = 0,$$
$$Ac_1u_0 - c_1u_0^2v_0 + \mu c_1\frac{\partial^2 v_0}{\partial y^2} + \mu c_1\frac{\partial^2 v_0}{\partial x^2} - (1+c_1)\frac{\partial v_0}{\partial t} + \frac{\partial v_1}{\partial t} = 0 \tag{13}$$

$$p^2: \quad Bc_2 - c_2u_0 - Ac_2u_0 - c_1u_1 - Ac_1u_1 + c_2u_0^2v_0 + 2c_1u_0u_1v_0 + c_1u_0^2v_1 + \mu c_2\frac{\partial^2 u_0}{\partial y^2} + \mu c_1\frac{\partial^2 u_1}{\partial y^2} + \mu c_2\frac{\partial^2 u_0}{\partial x^2} + \mu c_1\frac{\partial^2 u_1}{\partial x^2} - c_2\frac{\partial u_0}{\partial t} - (1+c_1)\frac{\partial u_1}{\partial t} + \frac{\partial u_2}{\partial t} = 0,$$
$$Ac_2u_0 + Ac_1u_1 - c_2u_0^2v_0 - 2c_1u_0u_1v_0 - c_1u_0^2v_1 + \frac{1}{4}c_2\frac{\partial^2 v_0}{\partial y^2} + \mu c_1\frac{\partial^2 v_1}{\partial y^2} + \mu c_2\frac{\partial^2 v_0}{\partial x^2} + \mu c_1\frac{\partial^2 v_1}{\partial x^2} - c_2\frac{\partial v_0}{\partial t} - (1+c_1)\frac{\partial v_1}{\partial t} + \frac{\partial v_2}{\partial t} = 0 \tag{14}$$

and so on.

(e) The above system of nonlinear equations, that is, zeroth-order, first-order, and higher order systems (if needed), can be easily solved. Put these solutions of different order problems in (10) and (11); one can obtain the approximate solutions $\widetilde{u}(r,t;c_i)$ and $\widetilde{v}(r,t;c_i)$, respectively.

(f) Determine the convergence control parameters, $c_1, c_2, c_3, \ldots$, by using one of the methods given in [8–11]. Using auxiliary constants in (10) and (11), one can get the approximate solutions $u(x,y,t)$ and $v(x,y,t)$, respectively.

3. Application

Example 1. Let us consider with $A = 1$, $\mu = 1/4$, $B = 0$, $h(x,y) = e^{(-x-y)}$, and $g(x,y) = e^{(x+y)}$ two-dimensional Brusselator system (1) can be written in the following form:

$$\frac{\partial u(x,y,t)}{\partial t} = u^2v - 2u + \frac{1}{4}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right),$$
$$\frac{\partial v(x,y,t)}{\partial t} = u - u^2v + \frac{1}{4}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right), \tag{15}$$

subject to the initial conditions:

$$u(x,y,0) = e^{(-x-y)}, \qquad v(x,y,0) = e^{(x+y)}, \qquad (x,y,t) \in \mathbb{R}^2 \times [0,2]. \tag{16}$$

The exact solutions of (15) is found to be [19]

$$u(x,y,t) = e^{(-x-y-t/2)}, \qquad v(x,y,t) = e^{(x+y+t/2)}. \tag{17}$$

OHAM formulation presented in Section 2 generates the series of problems, which can be written as

$$\frac{\partial}{\partial t}u_0(x,y,t) = 0, \qquad \frac{\partial}{\partial t}v_0(x,y,t) = 0,$$
$$-2c_1u_0 + c_1u_0^2v_0 + \frac{1}{4}c_1\frac{\partial^2 u_0}{\partial y^2} + \frac{1}{4}c_1\frac{\partial^2 u_0}{\partial x^2} - (1+c_1)\frac{\partial u_0}{\partial t} + \frac{\partial u_1}{\partial t} = 0,$$
$$-c_1u_0 - c_1u_0^2v_0 + \frac{1}{4}c_1\frac{\partial^2 v_0}{\partial y^2} + \frac{1}{4}c_1\frac{\partial^2 v_0}{\partial x^2} - (1+c_1)\frac{\partial v_0}{\partial t} + \frac{\partial v_1}{\partial t} = 0,$$
$$-2c_2u_0 - 2c_1u_1 + c_2u_0^2v_0 + 2c_1u_0u_1v_0 + c_1u_0^2v_1 + \frac{1}{4}c_2\frac{\partial^2 u_0}{\partial y^2} + \frac{1}{4}c_1\frac{\partial^2 u_1}{\partial x^2} - c_2\frac{\partial u_0}{\partial t} - (1+c_1)\frac{\partial u_1}{\partial t} + \frac{\partial u_2}{\partial t} = 0,$$
$$-c_2u_0 + c_1u_1 - c_2u_0^2v_0 - 2c_1u_0u_1v_0 - c_1u_0^2v_1 + \frac{1}{4}c_2\frac{\partial^2 v_0}{\partial y^2} + \frac{1}{4}c_1\frac{\partial^2 v_1}{\partial y^2} + \frac{1}{4}c_2\frac{\partial^2 v_0}{\partial x^2} + \frac{1}{4}c_1\frac{\partial^2 v_1}{\partial x^2} - c_2\frac{\partial v_0}{\partial t} - (1+c_1)\frac{\partial v_1}{\partial t} + \frac{\partial v_2}{\partial t} = 0,$$

$$
\begin{aligned}
&-2c_3u_0-2c_2u_1-2c_1u_2+c_3u_0^2v_0+2c_2u_0u_1v_0+c_1u_1^2v_0\\
&\quad+2c_1u_0u_2v_0+c_2u_0^2v_1+2c_1u_0u_1v_1+c_1u_0^2v_2\\
&\quad+\frac{1}{4}c_3\frac{\partial^2u_0}{\partial y^2}+\frac{1}{4}c_2\frac{\partial^2u_1}{\partial y^2}+\frac{1}{4}c_1\frac{\partial^2u_2}{\partial y^2}+\frac{1}{4}c_3\frac{\partial^2u_0}{\partial x^2}\\
&\quad+\frac{1}{4}c_2\frac{\partial^2u_1}{\partial x^2}+\frac{1}{4}c_1\frac{\partial^2u_2}{\partial x^2}+c_3\frac{\partial u_0}{\partial t}-c_2\frac{\partial u_1}{\partial t}\\
&\quad-\left(1+c_1\right)\frac{\partial u_2}{\partial t}+\frac{\partial u_3}{\partial t}=0,\\
&c_3u_0+c_2u_1+c_1u_2-c_3u_0^2v_0-2c_2u_0u_1v_0-c_1u_1^2v_0\\
&\quad-2c_1u_0u_2v_0-c_2u_0^2v_1-2c_1u_0u_1v_1-c_1u_0^2v_2\\
&\quad+\frac{1}{4}c_3\frac{\partial^2v_0}{\partial y^2}+\frac{1}{4}c_2\frac{\partial^2v_1}{\partial y^2}+\frac{1}{4}c_1\frac{\partial^2v_2}{\partial y^2}+\frac{1}{4}c_3\frac{\partial^2v_0}{\partial x^2}\\
&\quad+\frac{1}{4}c_2\frac{\partial^2v_1}{\partial x^2}+\frac{1}{4}c_1\frac{\partial^2v_2}{\partial x^2}-c_3\frac{\partial v_0}{\partial t}-c_2\frac{\partial v_1}{\partial t}\\
&\quad-\left(1+c_1\right)\frac{\partial v_2}{\partial t}+\frac{\partial v_3}{\partial t}=0.
\end{aligned}
\tag{18}
$$

The above zeroth-order, first-order, second-order, and third-order problems are given in (18) which can easily be solved. We get

$$
\begin{aligned}
u_0(x,y,t)&=e^{(-x-y)},\\
v_0(x,y,t)&=e^{(x+y)},\\
u_1(x,y,t)&=\frac{t}{2}e^{(-x-y)}c_1,\\
v_1(x,y,t)&=\frac{-t}{2}e^{(x+y)}c_1,\\
u_2(x,y,t)&=\frac{t}{8}e^{(-x-y)}\left(4c_1+4c_1^2+tc_1^2+4c_2\right),\\
v_2(x,y,t)&=\frac{t}{8}e^{(x+y)}\left(-4c_1-4c_1^2+tc_1^2-4c_2\right),\\
u_3(x,y,t)&=\frac{t}{48}e^{(-x-y)}\left(24c_1+48c_1^2+12tc_1^2+24c_1^3\right.\\
&\quad\left.+12tc_1^3+t^2c_1^3+24c_2+48c_1c_2+12tc_1c_2+24c_3\right),\\
v_3(x,y,t)&=\frac{-t}{48}e^{(x+y)}\left(24c_1+48c_1^2-12tc_1^2+24c_1^3\right.\\
&\quad\left.-12tc_1^3+t^2c_1^3+24c_2+48c_1c_2-12tc_1c_2+24c_3\right).
\end{aligned}
\tag{19}
$$

Substituting (19) in (10) and (11), respectively, we obtain

$$
\begin{aligned}
u(x,y,t)&=\frac{e^{-x-y}}{48}\left(18t\left(4+t\right)c_1^2\right.\\
&\quad\left.+tc_1^3\left(24+12t+t^2\right)+12tc_1\left(6+\left(4+t\right)c_2\right)\right.\\
&\quad\left.+24\left(2+2tc_2+tc_3\right)\right),\\
v(x,y,t)&=\frac{-e^{xy}}{48}\left(-18t\left(-4+t\right)c_1^2\right.\\
&\quad\left.+tc_1^3\left(24-12t+t^2\right)-12tc_1\left(-6+\left(-4+t\right)c_2\right)\right.\\
&\quad\left.+24\left(-2+2tc_2+tc_3\right)\right).
\end{aligned}
\tag{20}
$$

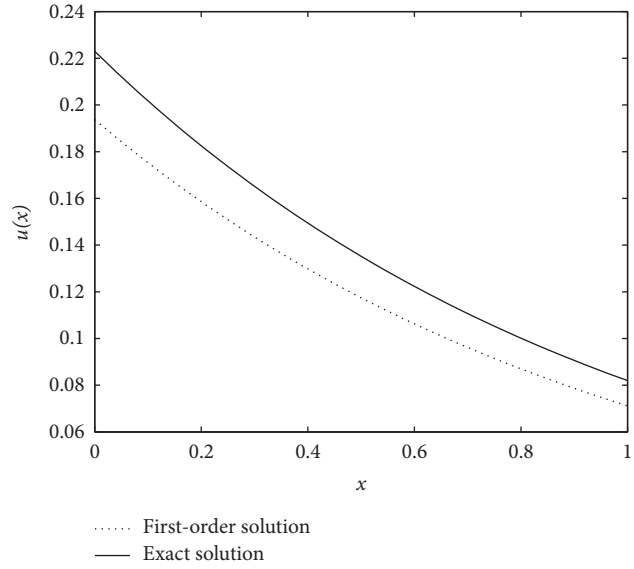

Figure 1: Convergence of first-order solution of $u(x, y, t)$ at $t = y = 1$.

Auxiliary constants shown in (20) can be found by using step (f) in Section 2.

4. Results and Discussions

The formulation of OHAM for two-dimensional nonlinear Brusselator system with $A = 1$, $B = 0$, and $\mu = 0.25$ is presented in Section 2 and the demonstration of the formulation is presented in Example 1.

The third-order approximate solutions of $u(x, y, t)$, $v(x, y, t)$ are given in (19). These solutions depend upon the optimal convergence control parameters which are given in Table 1. The simplicity and accuracy of the presented method are illustrated by computing $|u_{\text{Exact}} - u_{\text{OHAM}}|$, $|v_{\text{Exact}} - v_{\text{OHAM}}|$. Tables 2 and 3 at different gird points show the comparisons of absolute error of $u(x, y, t)$ and $v(x, y, t)$ between OHAM and the exact solutions, respectively. In this study, only up to third-order solutions are considered. From Tables 2 and 3, it is clear that OHAM achieves accurate solutions at only third-order term of approximation without any spatial discretization. Thus the third-order approximate solutions of Brusselator reaction-diffusion system converge.

Figures 1, 2, and 3 show the convergence of first-order, second-order, and third-order approximate solutions of $u(x, y, t)$ obtained by OHAM, respectively. Figures 4, 5,

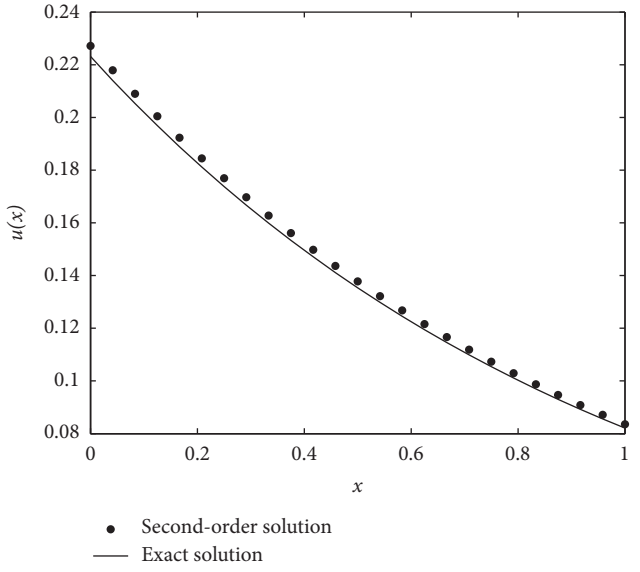

Figure 2: Convergence of second-order solution of $u(x, y, t)$ at $t = y = 1$.

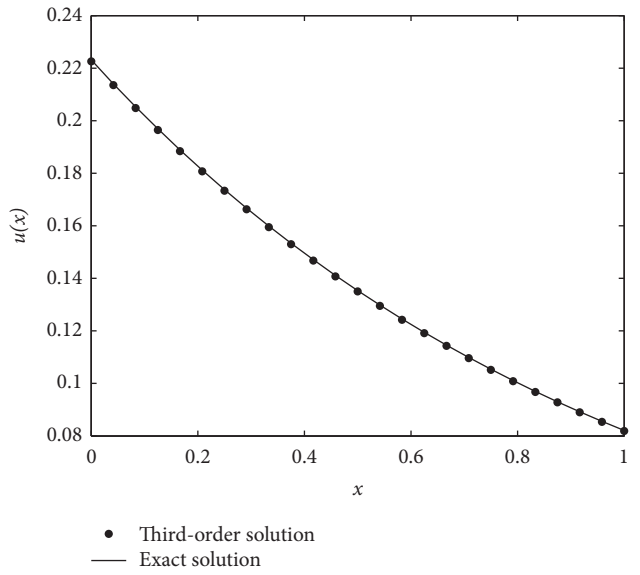

Figure 3: Convergence of third-order solution of $u(x, y, t)$ at $t = y = 1$.

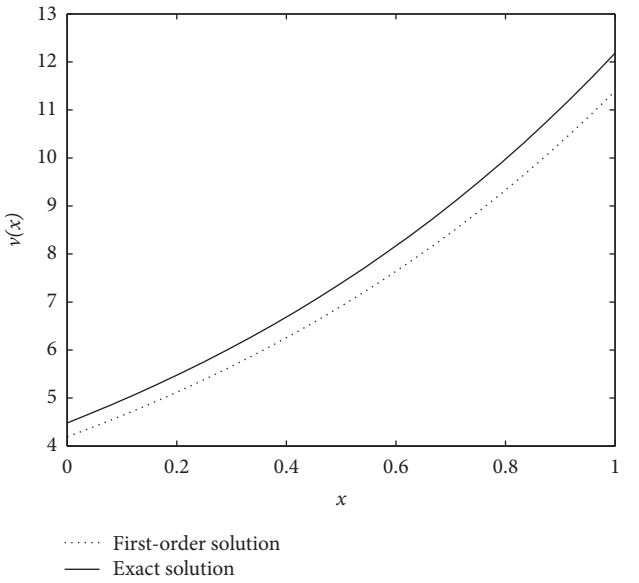

Figure 4: Convergence of first-order solution of $v(x, y, t)$ at $t = y = 1$.

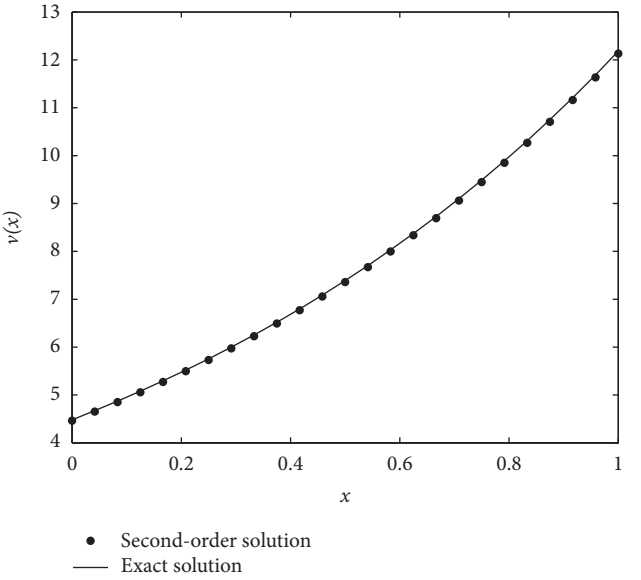

Figure 5: Convergence of second-order solution of $v(x, y, t)$ at $t = y = 1$.

Table 1: Convergence control parameters of example for $u(x, y, t)$ and $v(x, y, t)$.

	c_1	c_2	c_3
$u(x, y, t)$	−0.945983141	0.0083062488	0.0004400396
$v(x, y, t)$	−1.0838346562	0.0032355216	−0.0012528760

and 6 show the convergence of first-order, second-order, and third-order approximate solutions of $v(x, y, t)$ obtained by OHAM, respectively. Figure 7 shows the error convergence with the order of approximation of $u(x, y, t)$ and $v(x, y, t)$. It is clear from the figures that the behaviour of approximate solutions is highly same as exact solution. It can also be clear from Figures 3 and 6 that third-order approximate solution converges and there is no need to compute extra terms when OHAM is used. It is observed that as we move along the domain we get consistent accuracy. It can also be observed that approximate solutions by formulation are in excellent agreement with the exact solutions. Thus the series

Table 2: Comparison of absolute errors of $u(x, y, t)$ at different orders of approximation.

t	x	y	OHAM	Exact	Absolute error $= \lvert u_{\text{exact}} - u_{\text{OHAM}} \rvert$		
					1st-order error	2nd-order error	3rd-order error
0.25	0.25	0.25	0.535285	0.535261	0.000451741	0.000544293	2.31736×10^{-5}
		0.5	0.41688	0.416862	0.000351816	0.000423896	1.80476×10^{-5}
		0.75	0.324667	0.324652	0.000273995	0.000330131	1.40555×10^{-5}
0.5	0.5	0.25	0.367815	0.367879	0.00722559	0.000930733	6.44165×10^{-5}
		0.5	0.286455	0.286505	0.00562729	0.000724856	5.01676×10^{-5}
		0.75	0.223091	0.22313	0.00438254	0.000564518	3.90706×10^{-5}
0.75	0.75	0.25	0.367815	0.367879	0.00722559	0.000930733	6.44165×10^{-5}
		0.5	0.286455	0.286505	0.00562729	0.000724856	5.01676×10^{-5}
		0.75	0.223091	0.22313	0.00438254	0.000564518	3.90706×10^{-5}

Table 3: Comparison of absolute errors of $v(x, y, t)$ at different orders of approximation.

t	x	y	OHAM	Exact	Absolute error $= \lvert v_{\text{exact}} - v_{\text{OHAM}} \rvert$		
					1st-order error	2nd-order error	3rd-order error
0.01	0.2	0.25	1.57619	1.57617	0.000637758	0.0000770919	1.81338×10^{-5}
		0.5	2.02387	2.02385	0.000818897	0.000098988	2.32843×10^{-5}
		0.75	2.5987	2.59867	0.00105149	0.000127103	2.98976×10^{-5}
0.02	0.4	0.25	1.93484	1.93479	0.00150979	0.000180195	4.29601×10^{-5}
		0.5	2.48438	2.48432	0.00193861	0.000231375	5.51618×10^{-5}
		0.75	3.19	3.18993	0.00248922	0.000297091	7.08292×10^{-5}
0.03	0.8	0.25	2.90093	2.90084	0.00327045	0.000385405	9.32357×10^{-5}
		0.5	3.72487	3.72475	0.00419935	0.00049487	1.19717×10^{-4}
		0.75	4.78283	4.78267	0.00539207	0.000635425	1.5372×10^{-4}

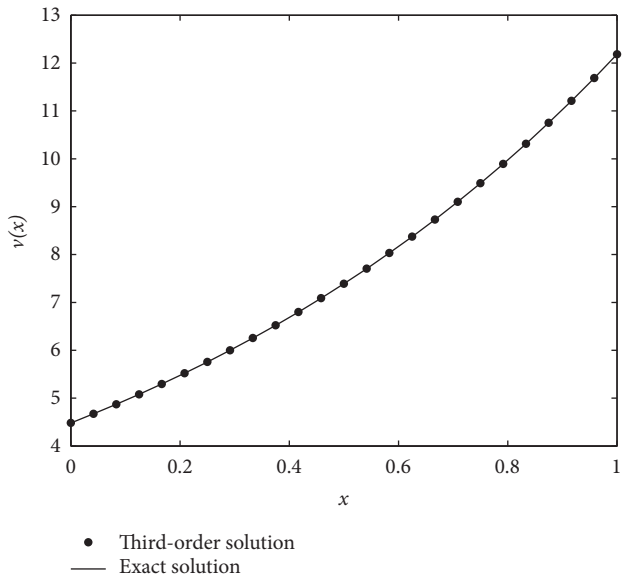

Figure 6: Convergence of third-order solution of $v(x, y, t)$ at $t = y = 1$.

solutions for fractional equations converge. Results indicate the performance of the method nonlinear system of partial differential equations in precisely approximating the solution at less computational cost.

5. Conclusion

In this work, we employed a new powerful semianalytic technique, optimal homotopy asymptotic method to solve Brusselator reaction-diffusion system. The objective of this work is to illustrate the usefulness of the technique. This technique is simple in applicability, as it does not need discretization like numerical methods. Furthermore, this technique delivers an appropriate way to control the convergence by optimally shaping the convergence control parameters. Additionally, this method converges rapidly at lower order of approximations. Therefore, OHAM exhibits its concealed supremacy and is latent for the solution of nonlinear problems in real life applications. One substantial objective of this effort is the investigation of convergence and practicality of the method. By using this method, we acquire a new effective recurrent relation to solve nonlinear Brusselator system. The results demonstrate that the method is a prevailing mathematical tool for solving systems of nonlinear partial differential equations having extensive applications in science and engineering.

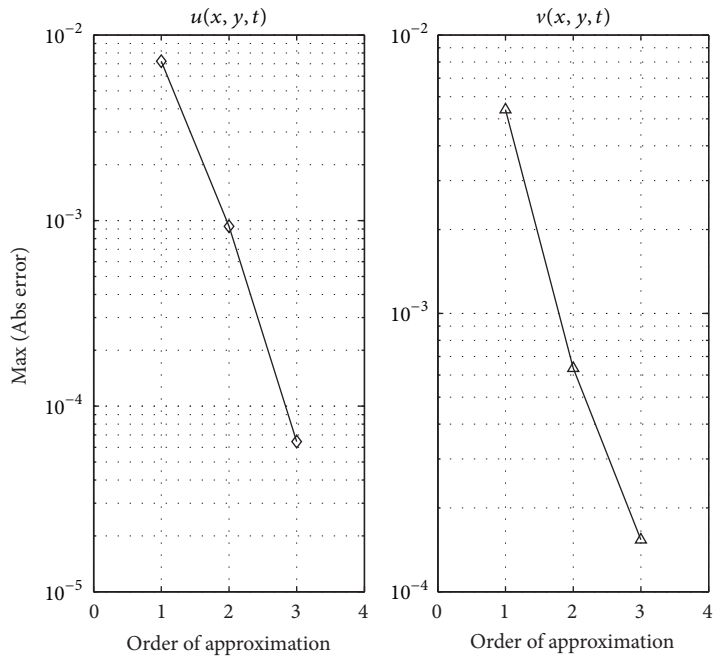

Figure 7: Error convergence with the order of approximation of $u(x, y, t)$ and $v(x, y, t)$.

Competing Interests

The author declares that there is no conflict of interests regarding the publication of this paper.

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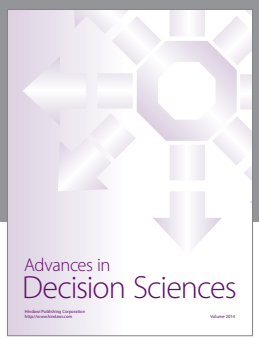

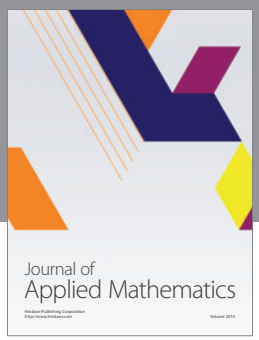

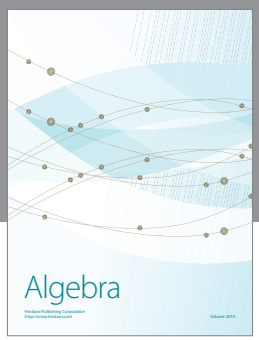

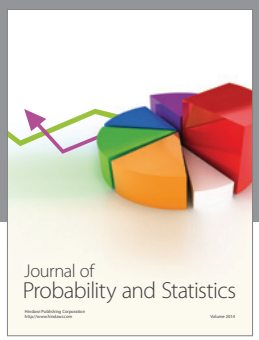

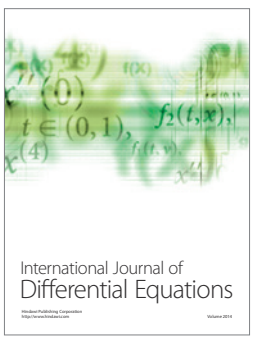

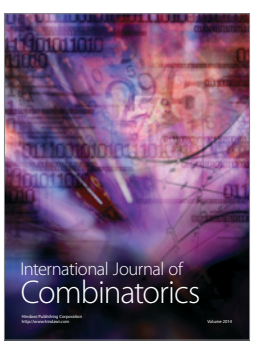
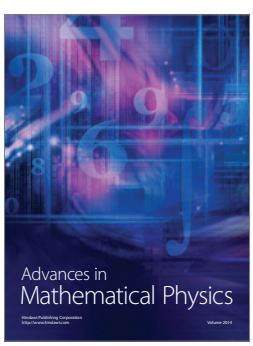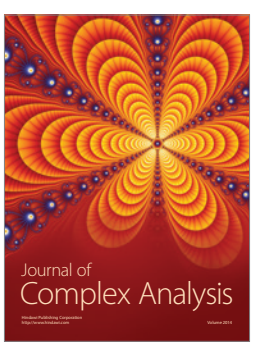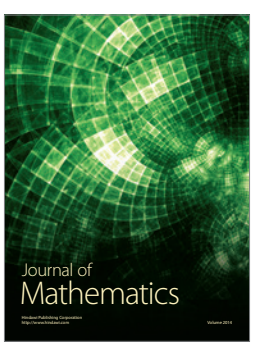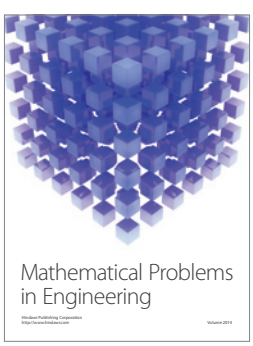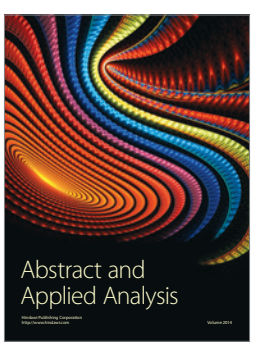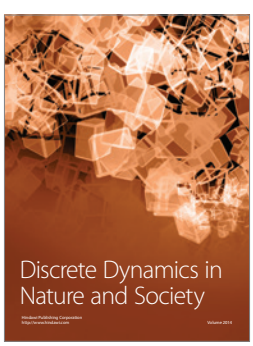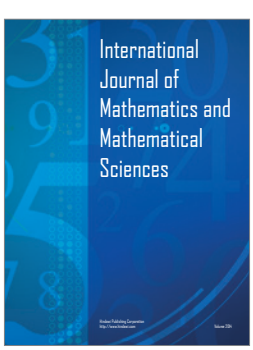
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