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ORIGINAL ARTICLE

An analytical approximation to the solution of chemical kinetics system

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Abstract In this paper, homotopy perturbation method is applied to solve chemical kinetics problem. Theoretical considerations are discussed. Numerical results are presented, to illustrating the efficiently and simplicity of the method.

1. Introduction

In every phenomenon in real life, there are many parameters and variables related to each other under the law imperious on that phenomenon. When the relations between the parameters and variables are presented in mathematical language we usually derive a mathematical model of the problem, which may be an equation, a differential equation, an integral equation, a system of integral equations and etc. Consider a model of a chemical process (Butcher, 2003) consisting of three species, which are denoted by A, B and C. The three reactions are

$$A \rightarrow B, \tag{1}$$
$$B + C \rightarrow A + C, \tag{2}$$
$$B + B \rightarrow C. \tag{3}$$

Let, y_1, y_2 and y_3 denote the concentrations of A, B and C, respectively. We assume these are scaled so that the total of the three concentrations is 1, and that each of three constituent reactions will add to the concentration of any of the species exactly at the expense of corresponding amounts of the reactants. The reaction rate of Eq. (1) will be denoted by k_1. This means that the rate at which y_1 decreases, and at which y_2 increases, because of this reaction, will be equal to $k_1 y_1$. In the second reaction Eq. (2), C acts as a catalyst in the production of A from B and the reaction rate will be written as k_2, meaning that the increase of y_1, and the decrease of y_3, in this reaction will have a rate equal to $k_2 y_2 y_3$. Finally, the production of C from B will have a rate constant equal to k_3, meaning that the rate at which this reaction takes place will be $k_3 y_2^2$. Putting all these elements of the process together, we find the system of differential equations for the variation with time of the three concentrations to be

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$$\frac{dy_1}{dx} = -k_1 y_1 + k_2 y_2 y_3,$$
$$\frac{dy_2}{dx} = k_1 y_1 - k_2 y_2 y_3 - k_3 y_2^2,$$
$$\frac{dy_3}{dx} = k_3 y_2^2.$$

If, the three reaction rates are moderately small numbers, are not greatly different in magnitude, then this is a straightforward problem.

Homotopy perturbation method has been used by many mathematicians and engineers to solve various functional equations. This method was further developed and improved by He (1999) and applied to nonlinear oscillators with discontinuities (He, 2004), nonlinear wave equations (He, 2005), boundary value problem (He, 2006), limit cycle and bifurcation of nonlinear problems (He, 2005), and many other subjects (He, 1999, 2000, 2004, 2003). It can be said that He's homotopy perturbation method is a universal one, is able to solve various kinds of nonlinear functional equations. For examples it was applied to nonlinear Schrödinger equations (Biazar and Ghazvini, 2007), to nonlinear equations arising in heat transfer (Ganji, 2006), to the quadratic Riccati differential equation (Abbasbandy, 2006), and to other equations (Odibat and Momani, 2008; Aminikhah and Hemmatnezhad, 2010; Biazar et al., 2009; Aminikhah and Salahi, 2009, 2010; Aminikhah and Biazar, 2010).

The rest of this paper is organized as follows:

In Section 2, the basic idea of homotopy perturbation method is presented. In Section 3, the uses of HPM for solving system of chemical kinetics is presented. And conclusion will be appeared in Section 4.

2. Basic idea of homotopy perturbation method (He, 1999)

To illustrate the basic ideas of the method, we consider the following system of nonlinear differential equations

$$A(U) - f(r) = 0, \quad r \in \Omega, \tag{4}$$

with the boundary conditions

$$B\left(u, \frac{\partial u}{\partial n}\right) = 0, \quad r \in \Gamma. \tag{5}$$

where A is a general differential operator, B is a boundary operator, $f(r)$ a known analytical function and Γ is the boundary of the domain Ω.

The operator A can be divided into two parts, which are L and N, where L is a linear, but N is nonlinear. Eq. (4) can be, therefore, rewritten as follows:

$$L(u) + N(u) - f(r) = 0. \tag{6}$$

By the homotopy technique, we construct a homotopy $U(r,p) : \Omega \times [0,1] \to \mathbb{R}$, which satisfies:

$$H(U,p) = (1-p)[L(U) - L(u_0)] + p[A(U) - f(r)] = 0, \quad p \in [0,1], \quad r \in \Omega, \tag{7}$$

or

$$H(U,p) = L(U) - L(u_0) + pL(u_0) + p[N(U) - f(r)] = 0, \tag{8}$$

where $p \in [0,1]$ is an embedding parameter, u_0 is an initial approximation of Eq. (4), which satisfies the boundary conditions. Obviously, from Eqs. (7) and (8) we will have

$$H(U,0) = L(U) - L(u_0) = 0, \tag{9}$$
$$H(U,1) = A(U) - f(r) = 0, \tag{10}$$

The changing process of p form zero to unity is just that of $U(r,p)$ from $u_0(r)$ to $u(r)$. In topology, this is called homotopy. According to the (HPM), we can first use the embedding parameter p as a small parameter, and assume that the solution of Eqs. (7) and (8) can be written as a power series in p:

$$U = U_0 + pU_1 + p^2 U_2 + \ldots. \tag{11}$$

Setting $p = 1$, results in the approximate solution of Eq. (4)

$$u = \lim_{p \to 1} U = U_0 + U_1 + U_2 + \ldots. \tag{12}$$

The combination of the perturbation method and the homotopy method is called the homotopy perturbation method (HPM), which has eliminated the limitations of the traditional perturbation methods. On the other hand, this technique can have full advantage of the traditional perturbation techniques. The series Eq. (12) is convergent for most cases.

3. HPM for system of chemical kinetics

Consider the following nonlinear system of ordinary differential equations (chemical kinetics model) with initial conditions

$$\begin{aligned}
&\tfrac{dy_1}{dx} = -k_1 y_1 + k_2 y_2 y_3, \quad y_1(0) = \alpha_1,\\
&\tfrac{dy_2}{dx} = k_1 y_1 - k_2 y_2 y_3 - k_3 y_2^2, \quad y_2(0) = \alpha_2,\\
&\tfrac{dy_3}{dx} = k_3 y_2^2, \quad y_3(0) = \alpha_3.
\end{aligned} \tag{13}$$

For solving system Eq. (13), by homotopy perturbation method, we first construct a homotopy as follows

$$\begin{aligned}
&(1-p)\left(\tfrac{dY_1}{dx} - \tfrac{dy_{1,0}}{dx}\right) + p\left(\tfrac{dY_1}{dx} + k_1 Y_1 - k_2 Y_2 Y_3\right) = 0,\\
&(1-p)\left(\tfrac{dY_2}{dx} - \tfrac{dy_{2,0}}{dx}\right) + \left(\tfrac{dY_2}{dx} - k_1 Y_1 + k_2 Y_2 Y_3 + k_3 Y_2^2\right) = 0,\\
&(1-p)\left(\tfrac{dY_3}{dx} - \tfrac{dy_{3,0}}{dx}\right) + \left(\tfrac{dY_3}{dx} - k_3 Y_2^2\right) = 0.
\end{aligned} \tag{14}$$

And consider the solution of Eq. (14) as a series say:

$$Y_i(x) = Y_{i,0}(x) + pY_{i,1}(x) + p^2 Y_{i,2}(x) + \cdots, \quad i = 1,2,3, \tag{15}$$

where $Y_{i,j}(x)$ $i = 1,2,3$, $j = 0,1,2,\ldots$ are functions which will be determined.

Substituting Eqs. (15) into (14) and comparing the coefficients of identical degrees of p, for $i = 1,2,3$, we have

$$p^0 : \begin{cases} \frac{dY_{1,0}}{dx} = \frac{dy_{1,0}}{dx}, \\ \frac{dY_{2,0}}{dx} = \frac{dy_{2,0}}{dx}, \\ \frac{dY_{3,0}}{dx} = \frac{dy_{3,0}}{dx}, \end{cases} \tag{16}$$

$$p^1 : \begin{cases} \frac{dY_{1,1}}{dx} = -\frac{dy_{1,0}}{dx} - k_1 Y_{1,0} + k_2 Y_{2,0} Y_{3,0}, \\ \frac{dY_{2,1}}{dx} = -\frac{dy_{2,0}}{dx} + k_1 Y_{1,0} - k_2 Y_{2,0} Y_{3,0} - k_3 Y_{2,0}^2, \\ \frac{dY_{3,1}}{dx} = -\frac{dy_{3,0}}{dx} + k_3 Y_{2,0}^2. \end{cases}$$

$$p^j : \begin{cases} \frac{dY_{1,1}}{dx} = -k_1 Y_{1,j-1} + k_2 \sum_{k=0}^{j-1} Y_{2,k} Y_{3,j-k-1}, \\ \frac{dY_{2,1}}{dx} = k_1 Y_{1,j-1} - k_2 \sum_{k=0}^{j-1} Y_{2,k} Y_{3,j-k-1} - k_3 \sum_{k=0}^{j-1} Y_{2,k} Y_{2,j-k-1}, \quad j = 1,2,\ldots \\ \frac{dY_{3,1}}{dx} = k_3 \sum_{k=0}^{j-1} Y_{2,k} Y_{2,j-k-1}. \end{cases}$$

The initial approximation $Y_{i,0}(x)$ or $y_{i,0}(x)$ can be chosen freely, here we set

$$Y_{i,0}(x) = y_{i,0}(x) = \alpha_i, \quad i = 1, 2, 3. \tag{17}$$

Therefore, the solution of Eq. (16) can be readily obtained

$$\begin{aligned} Y_{1,j}(x) &= -k_1 \int_0^x Y_{1,j-1}(t)dt + k_2 \int_0^x \sum_{k=0}^{j-1} Y_{2,k}(t) Y_{3,j-k-1}(t)dt, \\ Y_{2,j}(x) &= k_1 \int_0^x Y_{1,j-1(t)dt} - k_2 \int_0^x \sum_{k=0}^{j-1} Y_{2,k}(t) Y_{3,j-k-1}(t)dt - k_3 \int_0^x \sum_{k=0}^{j-1} Y_{2,k}(t) Y_{2,j-k-1}(t)dt, \quad j = 1, 2, \ldots \\ Y_{3,j}(x) &= k_3 \int_0^x \sum_{k=0}^{j-1} Y_{2,k}(t) Y_{2,j-k-1}(t)dt. \end{aligned} \tag{18}$$

Therefore, we will have

$$y_i(x) = \lim_{p \to 1} Y_i(x) = \sum_{j=0}^{\infty} Y_{i,j}(x), \quad i = 1, 2, 3. \tag{19}$$

If we set, $k_1 = 0.04$, $k_2 = 0.003$, $k_3 = 0.05$, $y_1(0) = 10$, $y_2(0) = 5$, $y_3(0) = 20$, therefore, approximations to the solutions with seven terms are as follows

$$\begin{aligned} y_1^*(x) &\approx \sum_{j=0}^{6} Y_{1,j}(x) = 0.00001011918609x^6 + 0.00001255479161x^5 - 0.0003823567710x^4 \\ &\quad + 0.003645833333x^3 - 0.02312500000x^2 - 0.1000000000x + 10, \\ y_2^*(x) &\approx sum_{j=0}^{6} Y_{2,j}(x) = 0.001143169397x^6 - 0.004658487082x^5 + 0.01899511718x^4 \\ &\quad - 0.07745833333x^3 + 0.3106250000x^2 - 1.1500000000x + 5, \\ y_3^*(x) &\approx \sum_{j=0}^{6} Y_{3,j}(x) = -0.001153288583x^6 + 0.004645932290x^5 - 0.01861276041x^4 \\ &\quad + 0.07381250000x^3 - 0.2875000000x^2 + 1.250000000x + 20. \end{aligned}$$

Some numerical results are presented in Table 1 and Fig. 1.

If we set, $k_1 = 0.1$, $k_2 = 0.02$, $k_3 = 0.009$, $y_1(0) = 10$, $y_2(0) = 5$, $y_3(0) = 20$, therefore, approximations to the solutions with seven terms are as follows

$$\begin{aligned} y_1^*(x) &\approx \sum_{j=0}^{6} Y_{1,j}(x) = -0.00003988741217x^6 + 0.0006702295838x^5 - 0.006752067708x^4 \\ &\quad + 0.05096666667x^3 - 0.2837500000x^2 + x + 10, \\ y_2^*(x) &\approx \sum_{j=0}^{6} Y_{2,j}(x) = 0.0001639414130x^6 - 0.001348128474x^5 + 0.01009689896x^4 \\ &\quad - 0.06563479167x^3 + 0.3388750000x^2 - 1.225000000x + 5, \\ y_3^*(x) &\approx \sum_{j=0}^{6} Y_{3,j}(x) = -0.0001240540009x^6 + 0.0006778988906x^5 - 0.003344831250x^4 \\ &\quad + 0.01466812500x^3 - 0.05512500000x^2 + 0.2250000000x + 20. \end{aligned}$$

Some numerical results are presented in Table 2 and Fig. 2.

Table 1 Numerical values of solutions of chemical kinetic model by HPM for $k_1 = 0.04$, $k_2 = 0.003$, $k_3 = 0.05$.

x	$y_1(x)$	$y_2(x)$	$y_3(x)$
0	10	5	20
0.5	9.944651132	4.494033438	20.56131543
1	9.880161150	4.098646466	21.02119238
1.5	9.808548358	3.786293183	21.40515846
2	9.731598340	3.550846463	21.71755520
2.5	9.651195643	3.422280269	21.92652409
3	9.569769303	3.494212621	21.93601808
3.5	9.490852205	3.964309224	21.54483857
4	9.419754293	5.187547743	20.39269796
4.5	9.364349610	7.742342740	7.742342740
5	9.335977191	12.50953127	13.15449154

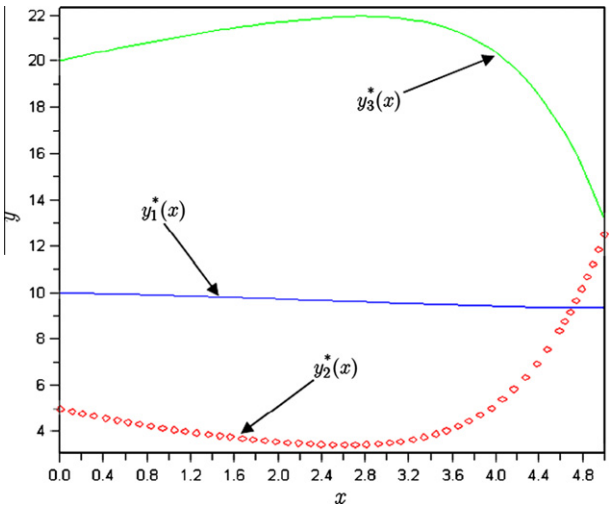

Figure 1 The plots of approximations of chemical kinetics model for $k_1 = 0.04$, $k_2 = 0.003$, $k_3 = 0.05$.

Table 2 Numerical values of solutions of chemical kinetic model by HPM for $k_1 = 0.1$, $k_2 = 0.02$, $k_3 = 0.009$.

x	$y_1(x)$	$y_2(x)$	$y_3(x)$
0	10	5	20
0.5	10.43503165	4.464605890	20.10036245
1	10.76109494	4.057152920	21.18175214
1.5	11.00402787	3.746196924	20.24977521
2	11.18359480	3.509324189	20.30708101
2.5	11.31487799	3.332706833	20.35241517
3	11.40922038	3.212502512	20.37827711
3.5	11.47471966	3.158098469	20.36718187
4	11.51627359	3.197199938	20.28652648
4.5	11.53517660	3.382762863	20.08206054
5	11.52826765	3.801770988	19.66996136

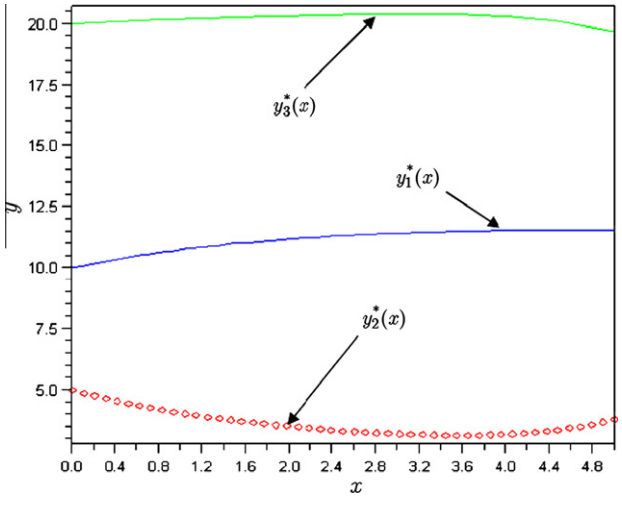

Figure 2 The plots of approximations of chemical kinetics model for $k_1 = 0.1$, $k_2 = 0.02$, $k_3 = 0.009$.

4. Conclusions

Homotopy perturbation method has been known as a powerful device for solving many functional equations such as ordinary, partial differential equations, integral equations and so many other equations. In this article, we have applied homotopy perturbation method for solving the nonlinear system of chemical kinetics. Numerical methods such as Runge–Kutta and Euler methods commonly used for solving these equations, either need a lot of computations and have less convergence speed and accuracy or solve only certain types of problems. In many cases one or two terms approximations have enough accuracy, i.e. fast convergence which can be mentioned as an advantage of the homotopy perturbation method. The main advantage of the HPM over ADM. is that this method provides the solution without a need for calculating Adomian's polynomials (Aminikhah and Salahi, 2010). It can be concluded that He's homotopy perturbation method is very powerful and efficient technique in finding exact solutions for wide classes of problems.

The computations associated with the examples in this paper were performed using Maple 10.

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