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APPROXIMATE ANALYTICAL SOLUTIONS FOR CHEMICAL KINETICS SYSTEM IN BROMINE USING LAPLACE TRANSFORM METHOD

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Abstract

This communication describes the Homotopy Perturbation Method with Laplace Transform (LT-HPM), which is used to solve the chemical kinetics problem analytically investigated. This technique is used to solve the chemical kinetics problem in bromine. Coupled nonlinear ordinary differential equations form this problem. In this perturbation method, the solution is obtained in the approximate form with easily computed components. The Laplace transform used to accelerate the convergence of the power series, and the results are shown in the graphs, which have good agreement with the other existing method in the literature. The results show that LTHPM is very effective and easy to implement.

Keywords : Mathematical modelling; Laplace transform; Homotopy Perturbation Method, Chemical Kinetics, First Order Reactions.

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1. INTRODUCTION

The most general form for a coupled set of first-order reactions is the one in which every component is reacting to form every other piece. The equations for several simple systems have been integrated with exact results. There do not appear to be many coupled systems that are strictly first order. Radioactive decay series come to mind, but these rarely involve feedback. If feedback is not applied, the equations can be integrated by traditional means. The reactions in the early stages of an Initiating self- chain are all first-order as follows [1].

$$Br_2 \overset{k_2}{\leftrightarrow} 2\,Br \qquad (1)$$

A coupled multi reaction system is relatively stable to small changes in rate constants. Therefore, it is proposed to replace a second-order reaction with a first-order reaction with a variable rate constant. This constant will contain a concentration term and will be evaluated
by successive approximation. The formulation will be tested on a simple system for which an exact integration is possible. Since the $\boldsymbol{H_2 - Br_2}$ reaction is to be discussed in some detail in the next

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section, it will be of interest to take the $\boldsymbol{Br_2}$dissociate. The following mechanism has been shown to account for the rate of reaction of hydrogen and bromine.

2. Mathematical Formulation

we find the system of coupled first order differential equations for the variation with time of the two concentrations to be:

$$\frac{dBr_2}{dt} = -k_1\ Br_2 + k_6\ Br \tag{2}$$

$$\frac{dBr}{dt} = 2\ k_1\ Br_2 - 2\ k_5\ Br \tag{3}$$

Subject to the initial conditions:

$$Br_2(0) = Br_2^*, \quad Br(0) = Br^* \tag{4}$$

we propose LT-HPM, a new hybrid of Laplace transform and new homotopy perturbation methods(NHPM) for solving chemical kinetics problem. This method is simple and finds exact solution of the equations analytically using the initial condition only.

In order to obtain an analytical solution of non-linear differential equations, several analytical methods such as the Variational Iteration method [2], Adomain decomposition method [3], Taylor series method [4], Homotopy analysis method [5-7] and Homotopy perturbation method [8-10] are considered. Compared to these methods, the new approach to Homotopy perturbation method [11-13] gives a better simple approximate solution in the zeroth iteration itself. The technique employs a Homotopy transform to generate a convergent series solution of differential equations. The advantage of this method is that it does not need a small parameter in the system and hence has a wide application in solving non-linear differential equations.

Kumar [14] investigated a new approximate method, namely the homotopy perturbation transform method (HPTM), which is a combination of homotopy perturbation method (HPM) and Laplace transform approach (LTM) to provide an approximate analytical solution to the time-fractional Cauchy-reaction diffusion equation. The MHD free convection

of water at 4°C through a fluid flow bounded by a moving boundary layer was portrayed mathematically [15]. An analytical approximation to the solution of the problem of forced convection over a horizontal flat plate using a combination of the Homotopy perturbation method and Laplace transform is presented [16]. In this study, the analytical approximation of the chemical kinetics problem using a combination of the new perturbation method and Laplace transform is presented.

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3. Solving the system of chemical kinetics new homotopy perturbation method and Laplace transform

Let us rewrite the Eqs. (2) and (3) as:

$$\frac{dBr_2}{dt} + k_1\ Br_2 - k_6\ Br = 0 \tag{5}$$

$$\frac{dBr}{dt} - 2\ k_1\ Br_2 + 2\ k_5\ Br = 0 \tag{6}$$

To illustrate homotopy perturbation method, we limit ourselves to consider the following system of nonlinear ordinary differential equations (NODEs) as follows:

Consider the function

$$A(u) - f(r) = 0 \tag{7}$$

with the boundary condition of

$$B\left(u, \frac{\partial u}{\partial n}\right) = 0 \tag{8}$$

where $A(u)$ is defined as

$$A(u) = L(u) - N(u) \tag{9}$$

Homotopy Perturbation procedure is shown as:

$$H(v,p) = L(v) - L(u_0) + pL(u_0) + p[N(v) - f(r)] = 0 \tag{10}$$

or

$$H(v,p) = (1-p)[L(v) - L(u_0)] + p[A(v) - f(r)] = 0 \tag{11}$$

According to the homotopy perturbation method form of the Eq. (5) and (6) is constructed as follows

$$(1-P)\left[\frac{dBr_2}{dt} + k_1\ Br_2\right] + P\left[\frac{dBr_2}{dt} + k_1\ Br_2 - k_6\ Br\right] = 0 \tag{12}$$

$$(1-P)\left[\frac{dBr}{dt} + 2\ k_5\ Br\right] + P\ \left[\frac{dBr}{dt} - 2\ k_1\ Br_2 + 2\ k_5\ Br\right] = 0 \tag{13}$$

A solution of Eq. (12) and (13) can then be obtained in the form

$$Br_2(t) = Br_{20}(t) + p\,Br_{21}(t) + p^2\ Br_{22}(t) + \ldots \tag{14}$$

$$Br(t) = Br_0(t) + p\,Br_1(t) + +p^2\ Br_2(t) + +\ldots \tag{15}$$

Substituting Eq. (17) and (18) into (19) and (20), yields Comparing the coefficients of p, p^2 and solving u_0, u_1, θ_0 and θ_1.

$$p^0 : \frac{dBr_{2_0}}{dt} + k_1\ Br_{2_0} = 0 \tag{16}$$

$$p^0 : \frac{dBr_0}{dt} + 2\ k_5\ Br_0 = 0 \tag{17}$$

$$p^1 : \frac{dBr_{2_1}}{dt} + k_1\ Br_{2_1} - k_6\ Br_0 = 0 \tag{18}$$

$$p^0 : \frac{dBr_1}{dt} + 2\ k_5\ Br_1 - 2k_1\,Br_{2_0} = 0 \tag{19}$$

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with boundary conditions are as follows

$$t = 0, \quad Br_{2_0} = Br_2^*, \quad Br_0 = Br^* \tag{20}$$

$$t = 0, \quad Br_{2_1} = 0, \quad Br_1 = 0 \tag{21}$$

Taking Laplace variables eqns. (16-10) and Laplace transform using initial substitute as follows:

$$\overline{Br}_{2_0}(s) = \frac{Br_2^*}{s + k_1} \tag{22}$$

$$\overline{Br}_0(s) = \frac{Br^*}{s + 2k_5} \tag{23}$$

$$\overline{Br}_{2_1}(s) = \frac{k_6 \; Br^*}{(s + 2k_5)\;(s + k_1)} \tag{24}$$

$$\overline{Br}_1(s) = \frac{2k_1 \, Br_2^*}{(s + k_1)\;(s + 2k_5)} \tag{25}$$

we obtain the solution the eqns. (22) and (25),

$$\overline{Br}_2(s) = \frac{Br_2^*}{s + k_1} + \frac{k_6 \; Br^*}{(s + 2k_5)\;(s + k_1)} \tag{26}$$

$$\overline{Br}(s) = \frac{Br^*}{s + 2k_5} + \frac{2k_1 \, Br_2^*}{(s + k_1)\;(s + 2k_5)} \tag{27}$$

Finally, we take inverse Laplace transform for solutions (26) and (27) we get

$$Br_2(t) = Br_2^* \; \exp(-k_1 t) + \frac{k_6 \, Br^*}{2k_5 - k_1}\left[\exp(-k_1 t) - \exp(-2k_5 t)\right] \tag{28}$$

$$Br(t) = Br^* \exp(-2k_5 t) + \frac{2k_1 \, Br_2^*}{2k_5 - k_1}\left[\exp(-k_1 t) - \exp(-2k_5 t)\right] \tag{29}$$

4. Results and Discussion

The non-linear differential equations govern the time-dependent behaviour of the first-order reaction system in a batch reactor. In this work, a new homotopy perturbation method (HPM) and Laplace transform derive the analytical solution for a simple first-order monomolecular reaction system. This technique is used to solve the chemical kinetics problem. The behavior of the approximate solutions of the concentrations of $Br_2(t)$ and $Br(t)$ using the new perturbation method (HPM) and Laplace transform with those values obtained by the analytical method are given in Figs. 1–3.

In figures (1), it is the concentrations of $Br_2(t)$ and $Br(t)$ observed that there will not be any changes in the graph as t decreases with concentrations increases. Figures 1(a) and 2(a) represented

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an $Br_2(t)$ and $Br(t)$ Concentrations increases and leads to a decrease in time t. It is very significant from a practical point of view. Figures 1(b) and 1(b), illustrates that the time t decreases with an increase in the concentrations.

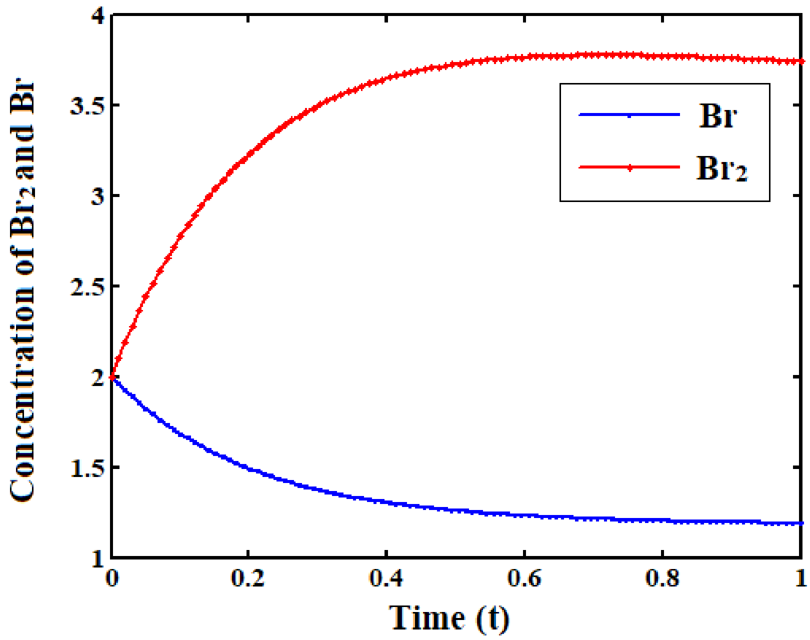

Fig.1. The concentrations of $Br_2(t)$ and $Br(t)$ using analytical solution for fixed values for

$Br_2^* = 1,\ Br^* = 1,\ k_1 = 5,\ k_5 = 0.05$ and $k_6 = 1$

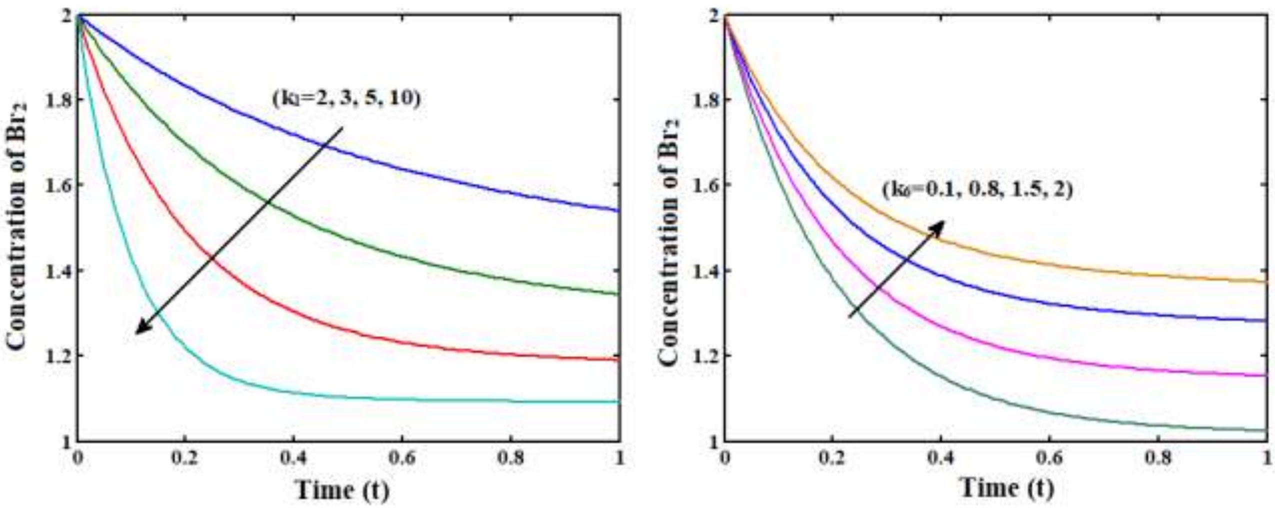

Fig.2. The concentrations of $Br_2(t)$ using analytical solution for fixed values for

$Br_2^* = 1,\ Br^* = 1,\ k_1 = 5,\ k_5 = 0.05$ and $k_6 = 1$

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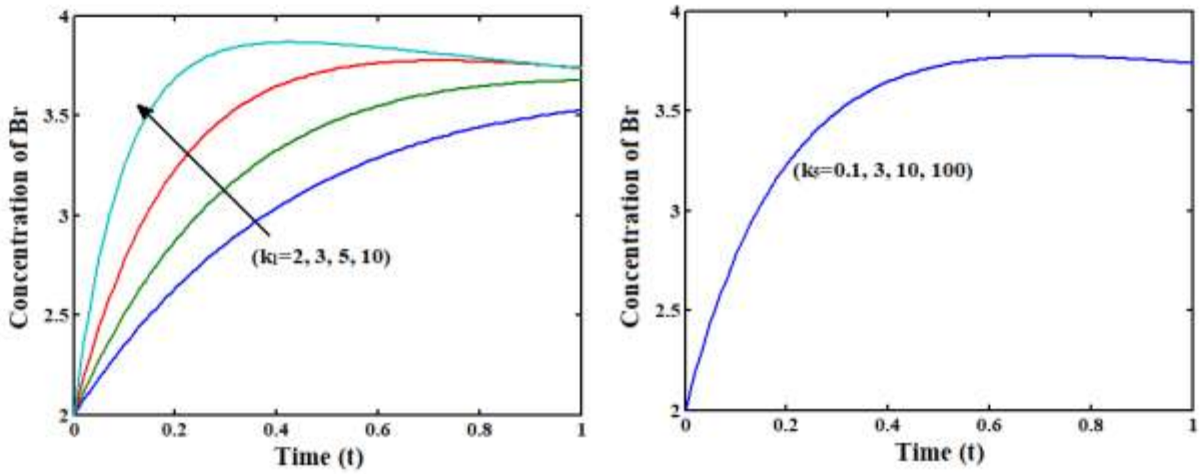

Fig.3. The concentrations of $Br(t)$ using analytical solution for fixed values for

$$Br_2^* = 1,\ Br^* = 1,\ k_1 = 5,\ k_5 = 0.05 \text{ and } k_6 = 1$$

5. Conclusion

In this paper, the analytical solutions for the first order reversible reaction systems are derived using the homotopy perturbation method and Laplace transform (LT-HPM), representing one of the mathematical models of chemical kinetics problems. The homotopy perturbation method and Laplace transform method to provide the solutions in approximately easily computed components. The derived analytical solutions for the two species reacting system are consistent with the solution obtained through Laplace transforms. The obtained results show that the new method developed in the current paper can solve the problem effectively.

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