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THEORECTICAL ANALYSIS FOR CHEMICAL KINETICS SYSTEM USING LAPLACE TRANSFORM METHOD

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Abstract: In this article, Laplace transform and new perturbation methods are implemented to study the problem of the chemical kinetics problem analytically. This method is used to solve the chemical kinetics problem. This problem is formed by a system of nonlinear ordinary differential equations. In this perturbation method the solution is obtained in the approximate form with simply computed components. The results of the maximal error remained values show that the present method is very effective and reliable.

Keywords: Mathematical modelling; Laplace transform; New perturbation method; Chemical Kinetics.

1. Introduction

There are several parameters and variables linked to each other in any phenomenon in real life under the law imperative on that phenomenon. We typically derive a mathematical model of the problem when the relationships between the parameters and variables are described in mathematical language, which can be an equation, a differential equation, an integral equation, a system of integral equations, 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:

$$A \to B \tag{1}$$

$$B + C \to A + C \tag{2}$$

$$B + B \to C \tag{3}$$

Let u, v and w 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 α. This means that the rate at which u decreases, and at which v increases, because of this reaction, will be equal to αu. 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 β , meaning that the increase of u, and the decrease of w, in this reaction will have a rate equal to $\beta v w$. Finally, the production of C from B will have a rate constant equal to c, meaning that the rate at which this reaction takes place will be γv^2.

2. Mathematical formulation

We find the system of differential equations for the variance of the three concentrations in time to be:

$$\frac{du}{dt} = -\alpha u + \beta v w \tag{4}$$

$$\frac{dv}{dt} = \alpha u - \beta v w - \gamma v^2 \tag{5}$$

$$\frac{dw}{dt} = \gamma v^2 \tag{6}$$

Subject to the initial conditions:

$$u(0) = c_1, \quad v(0) = c_2, \quad w(0) = c_3 \tag{7}$$

If the three reaction rates are moderately small numbers, if they do not vary significantly in magnitude, then this is a simple question.

Many different methods have recently introduced to solvenonlinear problems, such as, variational iteration method(Abassy et al., 2007; Biazar and Ghazvini, 2007; Goha et al.,2010; He, 2000; Sweilam and Khader, 2007; Sweilam andKhader, 2010), Adomian decomposition method (Sen, 1988;Wazwaz, 1998; Yang et al., 2009) and homotopy perturbation method (He, 1999; Liao, 2005; Nayfeh, 1973; Sweilam et al.,2008; Sweilam and Khader,2009).

The method of Adomian decomposition provides solutions as a sequence by using the so-called Adomian polynomials that are connected to nonlinearity derivatives; thus, these nonlin earities must be analytical functions of dependent variables, and this has often been overlooke d in the literature for the existence and uniqueness of solutions to problems of initial value, fo r example, in the literature.(Kelley and Petterson, 2004; Ramos,2008a, b). However, the decomposition method may be formulated in a manner that does not require that the nonlinearitiesbe differentiable with respect to the dependent variables and their derivatives (Ramos, 2009). Other techniques also require that the nonlinearities be analytical functions of the dependent variable and provide either convergent series or asymptotic expansions to the solution including perturbation methods(Nayfeh, 1973), the homotopy perturbation technique and the homotopy analysis procedure (Liao, 2005).

By way of contrast, iterative techniques are used for solving a large class of linear or nonlinear differential equations without the tangible restriction of sensitivity to the degree ofthe nonlinear term and also they reduce the size of calculations besides, their interactions are direct and straight forward. These techniques include the well-known Picard fixed-pointiterative procedure (Agarwal et al., 2001; Khader and Al-Bar, 2011; Kreyszig, 1989).Some highlights of new developments of PIM include work by Ramos, who solved the nonlinear second-order differential equations (Ramos, 2008a), nonlinear ordinary differential equations (Ramos, 2008a), and the nonlinear advection–reaction–diffusion equations (Ramos, 2009).

Hussanan et al. 2014, Studied an influence of Newtonian heating on Casson fluid past an oscillatory vertical plate by Laplace transform. Kumar et al.2013, investigated a new approximate method, namely homotopy perturbation transform method (HPTM) which is a combination of homotopy perturbation method (HPM) and Laplace transform method (LTM) to provide an analytical approximate solution to time-fractional Cauchy-reaction diffusion equation. In this study, analytical approximation to the of the chemical kinetics problem using combination of new perturbation method and Laplace transform is presented.

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

Let us rewrite the Eqs. (4), (5) and (6) as:

$$u' = -\alpha u + \beta v w \tag{8}$$

$$v' = \alpha u - \beta v w - \gamma v^2 \tag{9}$$

$$w' = \gamma v^2 \tag{10}$$

To illustrate new perturbation, we limit ourselves to consider the following system of nonlinear ordinary differential equations (NODEs) in the type of the solving Laplace transform method as follows:

Taking Laplace variables eqns. (8-10) and using new perturbation of initial substitute as follows:

$$L(u') + \alpha L(u) - \beta c_2 c_3 = 0 \tag{11}$$

$$L(v') - \alpha c_1 + \beta c_3 L(v) + \gamma L(v^2) = 0 \tag{12}$$

$$L(w') - \gamma (c_2)^2 = 0 \tag{13}$$

We obtain the solution the eqns. (11) and (13),

$$\bar{u}(s) = \frac{c_1}{s+\alpha} + \frac{\beta c_2 c_3}{s(s+\alpha)} \tag{14}$$

$$\bar{v}(s) = \frac{c_2}{s+\beta c_3} + \frac{\alpha c_1}{s(s+\beta c_3)} - \frac{\gamma c_2^2}{s(s+\beta c_3)} \tag{15}$$

$$\bar{w}(s) = \frac{\gamma c_2^2}{s^2} + \frac{c_3}{s} \tag{16}$$

Finally, we take inverse Laplace transform for solutions (14) and (16) we get

$$u(t) = c_1 \exp(-\alpha t) + \frac{\beta c_2 c_3}{\alpha} (1 - \exp(-\alpha t) \tag{17}$$

$$v(t) = c_2 \exp(-\beta c_3 t) + \frac{\alpha c_1 - \gamma c_2^2}{\beta c_3} (1 - \exp(-\beta c_3 t) \tag{18}$$

$$w(t) = t \gamma c_2^2 + c_3 \tag{19}$$

4. Results and Discussion

In this study, this technique is used to solve the chemical kinetics problem. The governing equation which is a pair first order ordinary differential equations were solved analytically by using the new perturbation method (HPM) and Laplace transform. The behavior of the approximate solutions $u(t)$, $v(t)$ and $w(t)$ using the new perturbation method (HPM) and Laplace transform with those values obtainedby the analytical method are given in Figs. 1–3. In allof these figures, we used the fixed values of the constants α, β and γ, and the following initial conditions(7), c_1, c_2 and c_3. In figures (1-3), it is observed that there will not be any changes in the graph as t increases; hence the value t is restricted. In these figures represented the consideration of $u(t)$, $v(t)$ and $w(t)$ concentrations. . It is noticed that while the values of the parameters are increasing the values of the concentration is decreasing.

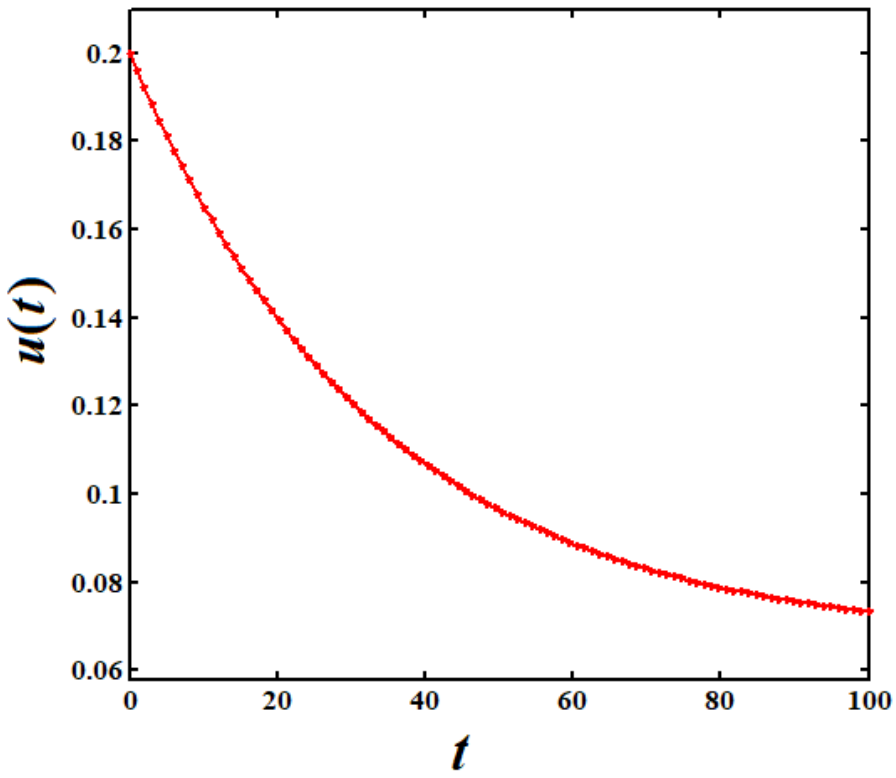

Fig.1. The solution of $u(t)$ using analytical solution for fixed values for $\alpha = 0.03,\ \beta = 0.04$ $c_1 = 0.2,\ c_2 = 0.5, c_3 = 0.1$

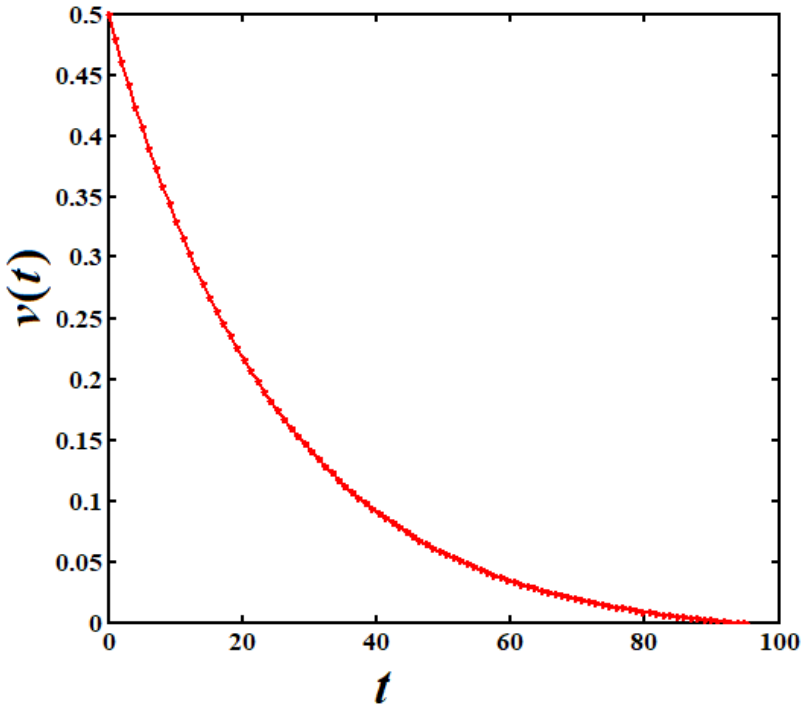

Fig.2. The solution of $v(t)$ using analytical solution for fixed values for $\alpha = 0.03,\ \beta = 0.4$ $\gamma = 0.01,\ c_1 = 0.2,\ c_2 = 0.5, c_3 = 0.1$

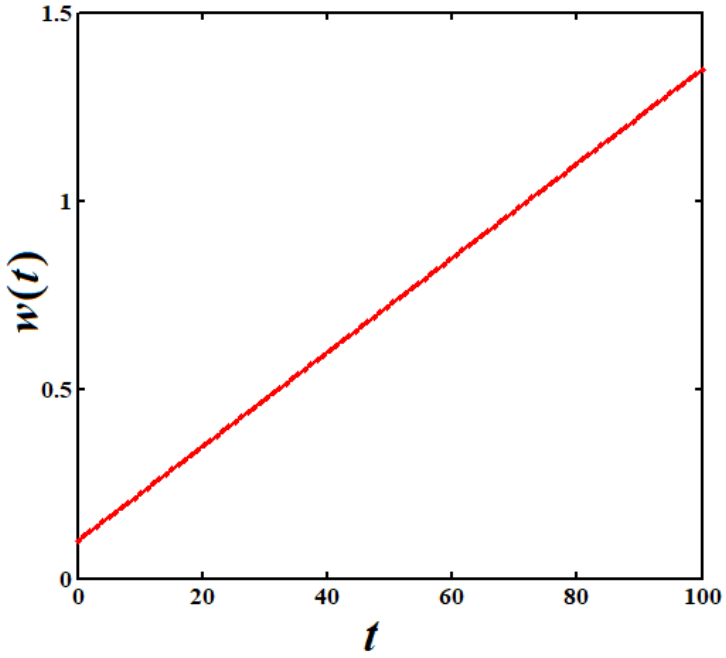

Fig.3. The solution of $w(t)$ using analytical solution for fixed values for $\alpha = 0.03,\ \beta = 0.04$ $\gamma = 0.05,\ c_1 = 0.2,\ c_2 = 0.5, c_3 = 0.1$

5. Conclusion

In current paper, the new perturbation method and Laplace transform has been successfully applied to elucidate a system of ordinary differential equations which symbolise of one of a mathematical models of a chemical kinetics problems. The new perturbation method and Laplace transformaffords the solutions in the form of approximately withsimply computed components. It is efficient in terms of computer power/memory and does not involve monotonous calculations without any regulated assumption and it is seeming that the new perturbation method and Laplace transform appears to be very truthful to employ with consistent results. It has been achieved that from figures and table that the maximal error remainders decreased when the number of iterations are increased.

REFERENCES

1. Abassy, T.A., El-Tawil, Magdy A., El Zoheiry, H., 2007. Solvingnonlinear partial differential equations using the modified variationaliteration Pade´ technique. J. Comput. Appl. Math. 207, 73–91.
2. Agarwal, R.P., Meehan, M., O'Regan, D., 2001. Fixed Point Theoryand Applications. Cambridge University Press, New York.
3. Aminikhah, H., 2011. An analytical approximation to the solution ofchemical kinetics system. J. King Saud Univ.-Sci. 23 (2), 167–170.
4. Baker, G.A.J., 1975. Essentials of Pade´ Approximants. AcademicPress.
5. Biazar, J., Ghazvini, H., 2007. He's variational iteration method forsolving hyperbolic differential equations. Int. J. Nonlinear Sci.Numer. Simul. 8 (3), 311–314.

6. Butcher, J.C., 2003. Numerical Methods for Ordinary Differential Equations. John Wiley and Sons.
7. Goha, S.M., Noorani, M.S.M., Hashim, I., 2010. Introducing variationaliteration method to a biochemical reaction model. NonlinearAnal.: Real World Appl. 11, 2264–2272.
8. He, J.H., 1999. Homotopy perturbation technique. Comput. MethodsAppl. Mech. Eng. 178 (3–4), 257–262.
9. He, J.H., 2000. Variational iteration method for autonomous ordinarydifferential systems. Appl. Math. Comput. 114 (2-3), 115–123.
10. Kelley, W., Petterson, A., 2004. The Theory of Differential Equations:Classical and Qualitative. Pearson Education Inc, Upper SaddleRiver, NJ.
11. Khader, M.M., Al-Bar, R.F., 2011. Application of Picard–Pade´technique for obtaining the exact solution of 1-D hyperbolictelegraph equation and coupled system of Burger's equations.Global J. Pure Appl. Math. 7 (2), 173–190.
12. Kreyszig, E., 1989. Introductory Functional Analysis with Applications.John Wiley & Sons, New York.
13. Liao, S., 2005. Comparison between the homotopy analysis methodand homotopy perturbation method. Appl. Math. Comput. 169,1186–1194.
14. Nayfeh, A.H., 1973. Perturbation Methods. John Wiley and Sons,New York.
15. Ramos, J.I., 2008a. On the Picard–Lindelof method for nonlinearsecond-order differential equations. Appl. Math. Comput. 203,238–242.
16. Ramos, J.I., 2008b. A non-iterative derivative-free method fornonlinear ordinary differential equations. Appl. Math. Comput.203, 672–678.
17. Ramos, J.I., 2009. Picard's iterative method for nonlinear advectionreaction-diffusion equations. Appl. Math. Comput. 215, 1526–1536.
18. Schnell, S., Mendoza, C., 1997. Closed form solution for timedependentenzyme kinetics. J. Theor. Biol. 187, 207–212.
19. Sen, A.K., 1988. An application of the Adomian decompositionmethod to the transient behavior of a model biochemical reaction.J. Math. Anal. Appl. 131, 232–245.
20. Sweilam, N.H., Khader, M.M., 2007. Variational iteration method forone dimensional nonlinear thermoelasticity. Chaos, Solitons Fractals32, 145–149.
21. Sweilam, N.H., Khader, M.M., 2009. Exact solutions of some couplednonlinear partial differential equations using the homotopyperturbation method. Comput. Math. Appl. 58, 2134–2141.
22. Sweilam, N.H., Khader, M.M., 2010. On the convergence of VIM fornonlinear coupled system of partial differential equations. Int. J.Computer Math. 87 (5), 1120–1130.
23. Sweilam, N.H., Khader, M.M., Al-Bar, R.F., 2008. Homotopyperturbation method for multi-dimensional nonlinear coupledsystem of parabolic and hyperbolic equations. Topol. MethodsNonlinear Anal. 31, 295–304.
24. Wazwaz, A.M., 1998. A comparison between Adomian decompositionmethod and Taylor series method in the series solution. Appl.Math. Comput. 97, 37–44.
25. Yang, P., Chen, Y., Zhi-Bin, Li, 2009. ADM-Pade´ technique for thenonlinear lattice equations. Appl. Math. Comput. 210, 362–375.
26. Hussanan A, ZukiSalleh M, Tahar RM, Khan I. Unsteady boundary layer flow and heat transfer of a casson fluid past an oscillating vertical plate with Newtonian heating. PLoS ONE 2014;9:108763.
27. Abid H, Anwar MI, Farhad A, Khan I, Sharidan S. Natural convection flow past an oscillating plate with Newtonian heating. Heat Transf Res 2014;45:119–37.
28. S. Kumar, A new fractional modelling arising in Engineering Sciences and its analytical approximate solution, Alexandria Eng. J. 52 (4) (2013) 813–819, http://dx.doi.org/10.1016/j.aej.2013.09.005.