Advances and Applications in Mathematical Sciences
Volume 21, Issue 4, February 2022, Pages 1957-1963

THEORETICAL ANALYSIS OF CHEMICAL REACTIONS SYSTEM USING HOMOTOPY PERTURBATION METHOD

I. ATHAL and M. K. SIVASANKARI

Assistant Professor
Department of Mathematics
PSNA College of Engineering and Technology
Dindigul, Tamilnadu, India
E-mail: athalbabloo@psnacet.edu.in

Assistant Professor
Department of Mathematics
Pasumpon Muthuramalinga Thevar College
Usilampatti, Tamilnadu, India
E-mail: sujipriya18@rediffmail.com

Abstract

This study uses mathematical approaches to describe a chemical furnace and the reaction suction system. Energy absorption equipment and chemical kinetics are used in chemical processing plants worldwide. For simulation, optimization, and scale-up in the process/chemical engineering field, precise modelling of chemical reactors and reactive absorption systems is essential. Chemical furnaces and reactive absorption systems must be accurately modelled for simulation, optimization, and scale-up in the process/chemical engineering discipline. The Concentration specification is obtained using an efficient, simple, and precise homotopy perturbation method (HPM) to solve differential equations. The approximation analytical results are generally preferred using a set of unknown parameters found by applying the initial conditions.

1. Introduction

Chemical reactants and absorbers are essential components of chemical

2020 Mathematics Subject Classification: 34Bxx; 76-10; 80A30.
Keywords: Mathematical modelling, Homotopy perturbation method, Chemical reaction system, Initial condition.
Received November 2, 2021; Accepted December 27, 2021

reactions. At different scales, the reactors could be ideally (continuous stirred-tank reactors and plug flow reactors) or non-ideal. Only a few variables determine reaction kinetics and reactors efficiencies, such as temperature, pressure, and concentration [1]. Kinetics deriving from the law of mass action, such as Michaelis-Menten kinetics or Hill kinetics, are crucial in chemistry and biology [2-7]. Mathematical models based on mass-action kinetics are widely used in chemistry and biology [8-11]. The analytical formulation of the current generated by the electrochemical reaction in a porous rotating disc electrode was developed by Visuvasam et al. [12]. Ravi Kanth and Aruna created the DTM to solve linear and non-linear Klein-Gordon equations, demonstrating that the method is computationally efficient and accurate [13]. The functional model's sensitivity analysis finds the most (or least) factors to the modelling result [14]. The researchers are developing a numerical method for determining the model's parametric identifiability, including model estimation criteria and approaches for the difference attributed to and lower the kinetic model's size [15]. A kinetic model's sensitivity analysis entails identifying how much the function depends on the variation of a given parameter and which parameters are critical to the model and which have a minor impact on the solution when changed [16-18].

The Variational Iteration Method (VIM) [19], the Adomian Decomposition Method (ADM) [20], the Homotopy Analysis Method (HAM) [21], the Harmonic Balance Method (HBM) [22], the Homotopy-Perturbation Method (HPM) [23], the Haar wavelet quasi linearization method [24], and the Haar wavelet operational matrix method [25] are some well-known methods for finding numerical and analytical series solutions for nonlinear problems. Although nonlinear analytical techniques are constantly improving, they are still insufficient for mathematicians and engineers.

To the best of our knowledge, HPM has not yet been used to solve challenges in chemical reaction engineering. This study aims to look into the capabilities and performance of nonlinear problems in chemical reaction process engineering [26]. This study uses HPM to determine the solutions to the governing equations for these instances. The performance of techniques is then evaluated in terms of dependability and accuracy by comparing approximate results to readily available analytical answers. This

communication aims to use the Homotopy perturbation method to develop approximate analytical formulations for the concentration profile of a chemical reaction.

2. Mathematical Formulation

Consider the following reaction as a series-elementary first-order single molecule reaction [27].

$$A \xrightarrow{k_1} R \xrightarrow{k_1} S \tag{1}$$

The reaction begins with component A, which has a starting concentration of C_{A0}, using the kinetic reaction. For the component R, the mass balance equation is as follows: [27]

$$\frac{dC_R}{dt} + k_2 C_R - k_1 C_{A0} \exp(-k_1 t) = 0 \tag{2}$$

Initial condition are

$$t = 0,\ C_R = 0 \tag{3}$$

The following is the exact results (solution) of the preceding first-order linear differential equation (Equation 2):

$$C_R = \frac{k_1 C_{A0}}{k_2 - k_1} [\exp(-k_1 t) - \exp(-k_2 t)] \tag{4}$$

Many authors have shown that the homotopy perturbation approach is an effective mathematical tool for solving various nonlinear problems [28, 29]. In terms of applicability, precision, and efficiency, the HPM is unique. The following concentration profile expressions can be obtained by solving eqns. (2) and (3) using the homotopy perturbation method.

$$C_R(t) = C_{A0} - C_{A0} \exp(-k_1 t) - k_2 C_{A0} t + \frac{k_2 C_{A0}}{k_1} - \frac{k_2 C_{A0} \exp(-k_1 t)}{k_1} + \frac{k_2^2 C_{A0} t^2}{2}$$

$$- \frac{k_2^2 C_{A0} t}{k_1} + \left(\frac{k_2}{k_1}\right)^2 C_{A0} - \left(\frac{k_2}{k_1}\right)^2 C_{A0} \exp(-k_1 t) \tag{5}$$

3. Results and Discussion

This approach is used to solve the chemical kinetics problem in this study. The homotopy perturbation method is used to obtain approximate analytical results (solution) for the first-order differential equation. The behavior of the approximate solutions of the concentration $C_R(t)$ using the homotopy perturbation method (HPM) with those values obtained by the analytical method is given in Figures 1 and 2.

The Approximate analytical results and exact results of concentration of $C_R(t)$ for fixed values for $k_1 = 2$ and $k_1 = 0.1$ in figures 1 and 2, it can be seen that as t increases, the graph does not change; thus, the value of t is limited. The consideration of concentration $C_R(t)$ was depicted in these diagrams. It's worth noting that as the parameter values increase, the concentration level decreases.

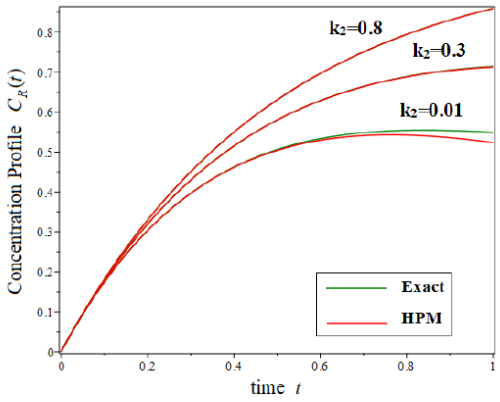

Figure 1. The Approximate analytical results and Exactresults of Concentration of $C_R(t)$ for fixed values for $k_1 = 2$.

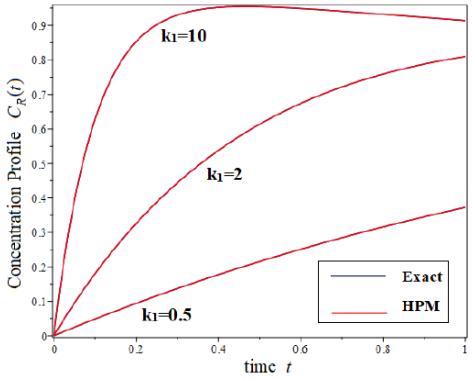

Figure 2. The Approximate analytical results and Exactresults of Concentration of $C_R(t)$ for fixed values for $k_2 = 0.1$.

4. Conclusion

The homotopy perturbation approach has been used to solve a system of ordinary differential equations representing one of the mathematical models of chemical reaction systems in this study. When compared to exact solutions, the approximate analytical solution is highly accurate. It is efficient in computer power/memory usage and does not require tedious calculations. It appears that the homotopy perturbation method is very accurate to use and produces reliable results. The maximal error remainders decreased as the number of iterations was increased, as shown in the figures.

References

[1] M. E. Davis and R. J. Davis, Fundamentals of chemical reaction engineering, Reactors for Measuring Reaction Rates 1st ed. Mc Graw-Hill 3 (2003), 64-99.

[2] B. L. Clarke, Advances in chemical physics, (Eds.: I. Prigogine, S. A. Rice), John Wiley, Hoboken NJ 43 (1980), 1-216.

[3] P. Érdi and J. Tóth, Mathematical models of chemical reactions, Manchester University Press, Manchester, 1989.

[4] J. Gunawardena, Chemical Reaction Network Theory for in-silico biologists, avail. at 2003, http://vcp.med.harvard.edu/papers.html.

[5] H. de Jong, Modeling and simulation of genetic regulatory systems: a literature review, J. Comput. Biol. 9 (2002), 67-103.

[6] E. D. Sontag, Structure and stability of certain chemical networks and applications to

the kinetic proofreading model of *T*-cell receptor signal transduction, IEEE Trans. Autom. Control 46 (2001), 1028-1047.

[7] E. O. Voit, H. A. Martens and S. W. Omholt, 150 Years of the Mass Action Law, PLoS Comput. Biol. 11 (2015), e1004012,

[8] B. L. Clarke, Stability of complex reaction networks, In Advances in Chemical Physics, (Eds.: I. Prigogine, S. A. Rice), John Wiley, Hoboken NJ 43 (1980), 1-216.

[9] B. P. Ingalls, Mathematical modelling in systems biology: An Introduction, The MIT Press, Cambridge, (2013).

[10] M. D. Johnston, D. Siegel and G. Szederkényi, J. Math. Chem. 50 (2012), 274-288.

[11] J. Visuvasam, A. Molina, E. Laborda and L. Rajendran, Mathematical models of the infinite porous rotating disk electrode, Int. J. Electrochem. Soc. 13 (2018), 9999-10022.

[12] A. S. V. Ravi Kanth and K. Aruna, Differential transform method for solving the linear and nonlinear klein-gordon equation, Computer Physics Communications 180(5) (2009), 708-711.

[13] A. Saltelli, M. Ratto, S. Tarantola and F. Campolongo, Sensitivity analysis for chemical models, Chemical Reviews 105(7) (2005), 2811-2828.

[14] L. F. Nurislamova and I. M. Gubaydullin, Journal of Mathematical Chemistry 55 (2017), 1779.

[15] Andrea Saltelli, Marco Ratto, Stefano Tarantola and Francesca Campolongo, Sensitivity analysis of complex kinetic systems. Tools and applications Sensitivity Analysis for Chemical Models, Chem. Rev. 105(7) (2005), 2811-2828.

[16] Y. Shi, H-W Ge, J. L. Brakora and R. D. Reitz, Automatic Chemistry mechanism reduction of hydrocarbon fuels for HCCI engines based on DRGEP and PCA methods with error control, Energy Fuels 24 (2010), 1646-1654.

[17] He JH. Variational iteration method-a kind of non-linear analytical technique: some examples, Int. J. Non Linear Mech. 34 (1999), 699-708.

[18] K. Abbaoui and Y. Cherruault, Convergence of Adomian's method applied to differential equations, Comput. Math. Appl. 28 (1994), 103-109.

[19] S. Liao, On the homotopy analysis method for nonlinear problems, Appl. Math. Comput. 147 (2004), 499-513.

[20] MSH. Chowdhury, MA. Hosen and K. Ahmad et al. High-order approximate solutions of strongly nonlinear cubic-quintic Duffing oscillator based on the harmonic balance method, Results Phys. 7 (2017), 3962-3967.

[21] JH. He, Homotopy perturbation method: a new nonlinear analytical technique, Appl. Math. Comput. 135 (2003), 73-79.

[22] S. Mt Aznam, NA. Ghani and M.S.H. Chowdhury, A numerical solution for nonlinear heat transfer of fin problems using the Haar wavelet quasilinearization method, Results Phys. 14 (2019), 102393.

[23] S. Mt Aznam and M. S. H. Chowdhury, Generalized Haar wavelet operational matrix

method for solving hyperbolic heat conduction in thin surface layers, Results Phys 11 (2018), 243-252.

[24] J. H. He, Homotopy perturbation technique, Computational Methods in Applied Mechanics and Engineering 178 (1999), 257-262.

[25] A. G. Xi, D. V. Michelangeli and P. A. Makar, Atmospheric Chemistry and Physics 9 (2009), 4341.

[26] R. N. Barik, G. C. Dash and P. K. Rath, Homotopy Perturbation Method (HPM) Solution for Flow of a Conducting Visco-elastic Fluid Through a Porous Medium, Proc. Natl. Acad. Sci. India Sect. Phys. Sci. 84 (2014), 55-61.

[27] M. K. Sivasankari and I. Athal, Mathematical models of solving partial differential equations in Variational Iteration method, Advances and Applications in Mathematical Sciences 18(10) (2019), 1087-1092.

[28] M. K. Sivasankari and M. Karthivel, Analytical solution of steady state substrate concentration of an immobilized enzyme kinetics by Adomian decomposition method, Advances and Applications in Mathematical Sciences 18(10) (2019), 1063-1070.

[29] M. Karthivel and M. K. Sivasankari, Mathematical modeling for 2-D fluorescence spectra based using Laplace transform method, European Journal of Molecular and Clinical Medicine 7(11) (2020), 1739-1743.

[30] M. Karthivel and M. K. Sivasankari, Approximate solutions of chemical reaction-diffusion brusselator system and coupled schrodinger-kdv equation using New iterative method, International Journal of Modern Agriculture 10(1) (2021), 168-175.

[31] Murali Kirthiga, Solayappan Balamurugan, James Visuvasam, Lakshmanan Rajendran and Abukhaled Marwan, Theoretical analysis of single-stage and multi-stage monod model of landfill degradation through mathematical modelling, Current Biochemical Engineering 7(1) (2021), 48-62.