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Chemical Reactions System: A Theorical Analysis Using Homotopy Perturbation Method

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Abstract: This work describes a chemical furnace and the reaction suction system using mathematical techniques. Chemical processing facilities all around the world employ chemical kinetics and energy absorption technology. In chemical and process engineering, accurate modeling of reactive absorption systems and chemical reactors is crucial for modeling, optimization, and scale-up. Precise modeling of chemical furnaces and reactive absorption systems is necessary for process/chemical engineering simulation, optimization, and scale-up. An effective, straightforward, and accurate homotopy perturbation technique (HPM) for solving differential equations yields the Concentration specification. Generally speaking, the approximation analytical findings with a set of unknown parameters discovered by applying the beginning circumstances are preferable.

Keywords: *The initial condition, chemical reaction system, mathematical modeling, and the homotopy perturbation method.*

1. Introduction

Chemical reactions require both chemical reactants and absorbers as necessary components. The reactors might be non-ideal or ideal at different sizes (continuous stirred-tank reactors and plug flow reactors). Temperature, pressure, and concentration are only a few of the factors that affect reaction kinetics and reactor efficiency [1]. In chemistry and biology, kinetics derived from the law of mass action—such as Michaelis-Menten kinetics or Hill kinetics—are essential [2–7]. In the fields of biology and chemistry, mass-action kinetics-based mathematical models are often employed [8–11]. Visuvasam and colleagues [12] discovered the analytical formulation of the current produced by the electrochemical reaction in a porous rotating disc electrode.

The DTM was developed by Aruna and Ravi Kanth to solve both linear and non-linear Klein-Gordon equations, proving the method's accuracy and computing efficiency [13]. The sensitivity analysis of the functional model determines which factors contribute most (or least) to the modeling outcome [14]. A numerical technique, comprising model estimate criteria and methodologies for the difference attributed to and lower the kinetic model's size, is being developed by the researchers to ascertain the model's parametric identifiability [15]. Sensitivity analysis for a kinetic model include determining which parameters are important to the model and which changes have little effect on the solution [16–18]. It also involves determining how much the function depends on a specific parameter's fluctuation.

Some well-known techniques for determining numerical and analytical series solutions for nonlinear problems are 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]. Despite continuous improvement, nonlinear analytical techniques remain inadequate for engineers and mathematicians.

To the best of our knowledge, chemical reaction engineering problems have not yet been resolved using HPM. The purpose of this research is to investigate the performance and capacities of nonlinear issues in chemical reaction process engineering [26]. The solutions to the governing equations for these cases are found in this study using HPM. The reliability and correctness of the approaches' performance are then assessed by contrasting their approximations with easily accessible analytical solutions. The goal of this communication is to create approximate analytical formulations for a chemical reaction's concentration profile using the Homotopy perturbation approach.

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2. Mathematical formulation

Assume that the reaction that follows is a first-order, series-elementary, single-molecule process [27].

$$A \xrightarrow{k_1} R \xrightarrow{k_1} S \qquad (1)$$

Using the kinetic process, the reaction starts with component A, which has a starting concentration of. The mass balance equation for component R is as follows: [27]:

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

Initial condition are

$$t = 0, \quad C_R = 0 \qquad (3)$$

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

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

Numerous writers have demonstrated the efficacy of the homotopy perturbation method as a mathematical tool for resolving a wide range of nonlinear issues [28, 29]. The HPM is exceptional in terms of its efficiency, accuracy, and application. By utilizing the homotopy perturbation approach to solve equations (2) and (3), the concentration profile expressions that follow may be obtained:

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

4. Results and Discussion

In this work, the chemical kinetics problem is resolved using this method. The first-order differential equation can be approximated analytically and solved using the homotopy perturbation method. Figures 1 and 2 show the behavior of the homotopy perturbation method (HPM) approximate solutions of the concentration with those values acquired by the analytical technique.

Figures 1 and 2 show the approximate analytical findings and exact results of concentration for fixed values. It is evident that the graph does not vary as t grows, indicating that the value of t is restricted. These illustrations illustrated the concept of focus. It is important to note that the concentration level falls as the parameter values rise.

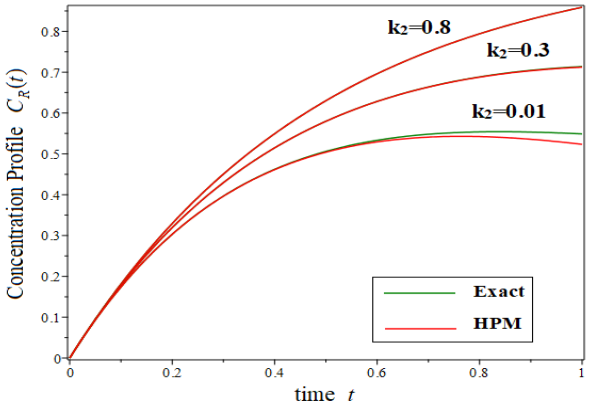

Fig.1. The Approximate analytical results and Exactresults of Concentration of $C_R(t)$ for fixed values for $k_1 = 2$.

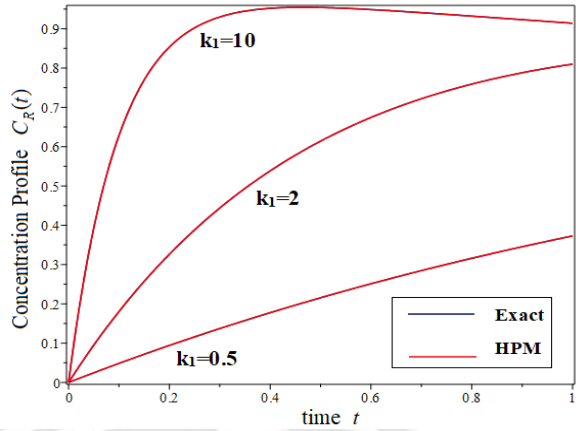

Fig.2. The Approximate analytical results and Exactresults of Concentration of $C_R(t)$ for fixed values for $k_2 = 0.1$.

5. Conclusion

One of the mathematical models of chemical reaction systems in this work is represented by a system of ordinary differential equations that has been solved using the homotopy perturbation technique. The approximate analytical answer is quite accurate when compared to exact solutions. It uses computer power and memory efficiently and doesn't need laborious computations. The homotopy perturbation method seems to be a fairly accurate tool with consistent output. The figures demonstrate how the maximal error remainders dropped as the number of repetitions grew.

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