Analytic solution of nonlinear batch reaction kinetics equations

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Abstract

The classical nonlinear reaction kinetics equations are solved using an analytic technique for solving nonlinear problems known as the homotopy analysis method. An explicit analytic solution for the concentration of reactants and products that is uniformly valid for all times is presented. Numerical simulations based on Runge–Kutta initial value problem solvers verify our analytic solutions with good agreement.

Contents

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1 Introduction

Batch reactors provide flexible means of producing high value-added products in specialty chemical, bio-technical, and pharmaceutical industries. To realize the production objectives, these batch reactors have to be operated optimally in a precise fashion. Batch reactor design has been studied from various perspective in order to develop systematic optimization tools to improve performance [1]. Friedrich and Perne [2] presented that the design of batch reactors means not only the design of equipment, but also the design of operation.

In the last four decades or so, many chemical producers moved from the relatively stable world of large continuous plant production to the much more turbulent environment of multi-product batch production in order to better adjust to changing market conditions. Kawarasaki et al. [3] intensively investigated and optimized several reaction conditions of cell-free protein synthesis such as temperature, buffers, tRNAS, and creatine phosphate.

Fulcher et al. [4] investigated and then provided insight into, the physical behaviour of the reaction mixture, and to evaluate the effectiveness of intrusive nutrient addition. The study showed that results for unstirred, batch zeolite A reaction systems the non-solid gel-fraction changed during the course of the reaction. Bonvin [5] presented a personal, thus necessarily subjective, view of the operation of batch and semi-batch reactors. The emphasis in this review was on the analysis of industrial challenges and the definition of academic opportunities.

Van Woezik and Westerterp [6] focused on the thermal dynamics of a semi-batch reactor, in which multiple exorthermic, liquid-liquid reactions are carried out. Muske et al. [7] presented a comparison of results obtained from deterministic and stochastic model-based optimization approaches for the determination of the optimal open-loop operating policy for a semi-batch reaction system. Hua et al. [8] proposed a cascade closed-loop optimization and control strategy for batch reactors.

Zhang and Smith [9] addressed a systematic methodology for batch and semi-batch reactor design and optimization for ideal and non-ideal mixing. The method starts from a general representation in the form of a temporal superstructure based on the similarity of between plug flow reactors and ideal batch reactors. Goncalves et al. [10] compared the performance of batch and semi-batch reactors, under optimal operational conditions of amoxicillin enzymic synthesis at 25° and pH ≈ 6.5. Most recently, Jana and Adari [11] dealt with the advanced adaptive control of a batch reactive distillation column for the production of ethyle.

Few, if any, attempted to solve batch problems analytically. To that end, this paper aims to obtain an analytic solution of these nonlinear batch reaction kinetics equations by using the homotopy analysis method (HAM). This is a fairly new technique that has been successfully applied in the analysis of systems of nonlinear equations in other areas of science and engineering particularly in fluid dynamics. Liao [12] gave a systematic description of homotopy analysis method (HAM), by means of an operator to denote non-linear differential equations in general. They also generally discussed the convergence of the related approximate solution sequences and showed that, as long as the approximate solution sequence given by the HAM is convergent, it must converge to one solution of the non-linear problem under consideration. Liao [13] further improved the homotopy analysis method and systematically described it through a typical non-linear problem.

Liao [14] applied the HAM to give a convergent series solution of non-similarity boundary-layer flows. Mehmood and Ali [16] investigated the incompressible generalized viscous flow with heat transfer analysis in the presence of viscous dissipation. Complete analytic solutions for velocity and temperature were obtained by homotopy analysis method. Ali and Mehmood [17] dealt with the unsteady boundary layer flow of viscous fluid in porous medium started due to the impulsively stretching of the plane wall using the homotopy analysis method. Mehmood et al. [18] presented a complete analytic solution to the unsteady heat transfer flow of an incompressible viscous fluid over a permeable plane wall. The homotopy analysis method was also used by Hayat et al. [19] to investigate the flow of a fourth grade fluid past a porous plate. Sajid and Hayat [20] proved that the perturbation and homotopy perturbation solutions for two problems, (i) unsteady convective-radiative equation and (ii) non-linear convective-radiative conduction equation, are only valid for weak non-linearity.

Cheng et al. [21] presented a similar solution for the nano boundary layer with a Navier boundary condition. The work considered three types of flow: (i) flow past a wedge; (ii) flow in a convergent channel; (iii) flow driven by an exponentially varying outer flow. The resulting differential equations are solved by the homotopy analysis method. Alizadeh-Pahlavan and Sadegy [22] studied unsteady MHD flow of a Maxwellian fluid above an impulsively stretched sheet, under the assumption that boundary layer approximation is applicable. Bararnia et al. [23] employed the homotopy analysis method to investigate the momentum, heat and mass transfer characteristics of MHD natural convection flow and heat generation fluid driven by a continuously moving permeable surface immersed in fluid saturated porous medium. Khan et al. [24] applied the homotopy analysis to develop an analytic approach for nonlinear differential equations with time delay. Allan [25] used the HAM to solve a non-linear, chaotic system of ordinary differential equations (Lorenz system). Xu et al. [26] investigated the time fractional partial differential equations by means of the homotopy analysis method.

Liao [15] details the HAM technique in solving nonlinear differential equations.

2 Mathematical formulation

We consider a batch reactor operated isothermally with negligible volume change due to reaction and with two elementary reactions

$$A + B \longrightarrow C \quad \text{and} \quad C + B \longrightarrow D. \tag{1}$$

Examples of chemical processes that are governed by mechanism (1) include

$$\text{potassium permanganate (A)} + \text{ethanol (B)} \rightarrow \text{acetic acid (C)}, \tag{2}$$

and then

$$\text{acetic acid (C)} + \text{ethanol (B)} \rightarrow \text{ethyl acetate (D)}, \tag{3}$$

and also the nitric acid oxidation of 2 octanol to 2 octanone and further oxidation of 2 octanone to carboxylic acids. Application of the material balance for the constant volume reactor gives the following differential equations

$$\frac{d[A]}{dt} = -k_1[A][B], \tag{4}$$

$$\frac{d[B]}{dt} = -k_1[A][B] - k_2[C][B], \tag{5}$$

$$\frac{d[C]}{dt} = k_1[A][B] - k_2[C][B], \tag{6}$$

$$\frac{d[D]}{dt} = k_2[C][B], \tag{7}$$

where k_1 and k_2 are reaction rate constants, and where $[\cdot]$ denotes concentration. The initial concentrations are

$$[A](0) = A_0\,, \quad [B](0) = B_0\,, \quad [C](0) = 0\,, \quad [D](0) = 0\,. \tag{8}$$

For brevity, we introduce the following notation to denote the concentrations of the reactants and products

$$y_1(t) = [A](t), \quad y_2(t) = [B](t), \quad y_3(t) = [C](t), \quad y_4(t) = [D](t). \tag{9}$$

Equation (7) is uncoupled from system (4)–(6), thus the solution for $[D](t)$ can obtained by integration of (7) when the solutions for $[B](t)$ and $[C](t)$ are known. Using the notation (9), equations (4)–(6) transform to

$$\frac{dy_1(t)}{dt} = -k_1y_1(t)y_2(t), \qquad (10)$$

$$\frac{dy_2(t)}{dt} = -k_1y_1(t)y_2(t) - k_2y_3(t)y_2(t), \qquad (11)$$

$$\frac{dy_3(t)}{dt} = k_1y_1(t)y_2(t) - k_2y_3(t)y_2(t). \qquad (12)$$

The initial conditions become

$$y_1(0) = A_0\,, \quad y_2(0) = B_0\,, \quad y_3(0) = 0\,. \qquad (13)$$

In the next section equations (10)–(13) are solved using the homotopy analysis method (HAM).

3 Homotopy analysis method solution

The concentrations for the reacting species A, B and C all tend to zero as $t \to \infty$. We therefore assume that

$$y_1(t) = \sum_{j=1}^{+\infty} a_j e^{-j\beta t}, \quad y_2(t) = \sum_{j=1}^{+\infty} b_j e^{-j\beta t}, \quad y_3(t) = \sum_{j=1}^{+\infty} c_j e^{-j\beta t}, \qquad (14)$$

where a_j, b_j and c_j are coefficients. The parameter β is a convergence controlling auxiliary parameter that is characteristic of the HAM approach and is carefully selected in such a way that the resulting HAM solution conforms to the rule of solution expression. These expressions provide us with the so-called rule of solution expressions for solving the governing equations (10)–(13). The β value is experimentally selected through trial and error for a fixed value of the HAM auxiliary parameter $\hbar$. However, a fixed value of $\hbar$

in most cases will work for a reasonable non-zero values of β and still gives similar agreement between the numerical solution and the HAM solution.

To obtain solutions in the form of (14), we use the HAM auxiliary linear operators

$$\mathcal{L}_i\left[\Phi_i(t;q)\right] = \frac{\partial \Phi_i(t;q)}{\partial t} + \beta\Phi_i(t;q), \tag{15}$$

which have the properties

$$\mathcal{L}_i\left[C_i e^{-\beta t}\right] = 0\,, \tag{16}$$

where C_i $(i = 1,2,3)$ are integral coefficients, $q \in [0,1]$ is the HAM embedding parameter, $\Phi_i(t;q)$ are unknown functions. The governing equations (10)–(12) suggest that we define the following HAM nonlinear operators:

$$\mathcal{N}_1\left[\Phi_i(t;q)\right] = \frac{\partial \Phi_1(t;q)}{\partial t} + k_1\Phi_1(t;q)\Phi_2(t;q), \tag{17}$$

$$\mathcal{N}_2\left[\Phi_i(t;q)\right] = \frac{\partial \Phi_2(t;q)}{\partial t} + k_1\Phi_1(t;q)\Phi_2(t;q) + k_2\Phi_2(t;q)\Phi_3(t;q), \tag{18}$$

$$\mathcal{N}_3\left[\Phi_i(t;q)\right] = \frac{\partial \Phi_3(t;q)}{\partial t} - k_1\Phi_1(t;q)\Phi_2(t;q) + k_2\Phi_2(t;q)\Phi_3(t;q). \tag{19}$$

Let $\hbar$ be an auxiliary parameter and $H(t)$ be an auxiliary function. Using the embedding parameter q we construct the so called zeroth order deformation equations as

$$(1-q)\mathcal{L}_i\left[\Phi_i(t;q) - y_{i,0}(t)\right] = \hbar\, q\, H(t)\mathcal{N}_i\left[\Phi_i(t;q)\right] \tag{20}$$

subject to the conditions $\Phi_i(t,0) = y_{i,0}(t)$, where $y_{i,0}(t)$ are the initial guesses of $y_i(t)$. Considering the initial conditions (13) and the expressions (14) we choose the initial guesses

$$y_{1,0}(t) = A_0 e^{-\beta t}, \quad y_{2,0}(t) = B_0 e^{-\beta t}, \quad y_{3,0}(t) = 0\,. \tag{21}$$

When $q = 0$ and $q = 1$ we have

$$\Phi_i(t;0) = y_{i,0}(t), \quad \Phi_i(t;1) = y_i(t). \tag{22}$$

Thus, as q varies from 0 to 1, the solutions $\Phi_i(t;q)$ vary from the initial guesses $y_{i,0}(t)$ to the exact solutions $y_i(t)$. Expanding $\Phi_i(t;q)$ using Taylor series with respect to q, we obtain,

$$\Phi_i(t;q) = \Phi_i(t;0) + \sum_{m=1}^{+\infty} y_{i,m}(t)q^m, \tag{23}$$

where

$$y_{i,m}(t) = \frac{1}{m!}\frac{\partial^m \Phi_i}{\partial q^m}\bigg|_{q=0}. \tag{24}$$

Importantly, the HAM approach gives us freedom to choose the auxiliary parameter $\hbar$ and function $H(t)$. Assuming that $\hbar$ and $H(t)$ are carefully selected so that series (23) converges at $q = 1$, we have

$$y_i(t) = y_{i,0}(t) + \sum_{m=1}^{+\infty} y_{i,m}(t). \tag{25}$$

The auxiliary function $H(t)$ must be chosen in such a way that the resulting solutions conform to the rule of solution expression (14).

To obtain the so called higher order deformation equations, we define the vectors

$$\vec{y}_{i,n} = \big(y_{i,0}(t), y_{i,1}(t), y_{i,2}(t), \ldots, y_{i,n}(t)\big). \tag{26}$$

Differentiating (20) m times with respect to q, then setting $q = 0$, and finally dividing the resulting equations by $m!$, we obtain the mth order deformation equations

$$\mathcal{L}_i\left[y_{i,m}(t) - \chi_m y_{i,m-1}(t)\right] = \hbar\, H(t)\, R_{i,m}(\vec{y}_{i,m-1}(t)), \tag{27}$$

subject to the initial conditions

$$y_{i,m}(0) = 0 \tag{28}$$

where

$$R_{1,m} = y'_{1,m-1} + k_1 \sum_{j=0}^{m-1} y_{1,j} y_{2,m-1-j}, \tag{29}$$

$$R_{2,m} = y'_{2,m-1} + k_1 \sum_{j=0}^{m-1} y_{1,j} y_{2,m-1-j} + k_2 \sum_{j=0}^{m-1} y_{2,j} y_{3,m-1-j}, \tag{30}$$

$$R_{3,m} = y'_{3,m-1} - k_1 \sum_{j=0}^{m-1} y_{1,j} y_{2,m-1-j} + k_2 \sum_{j=0}^{m-1} y_{2,j} y_{3,m-1-j}. \tag{31}$$

and

$$\chi_m = \begin{cases} 0, & m \leqslant 1, \\ 1, & m > 1. \end{cases} \tag{32}$$

Equations (27)–(32) , form a system of uncoupled first order differential equations. Since the HAM approach allows us to choose the convergence-control auxiliary function $H(t)$ and parameter $\hbar$, we set $H(t) = e^{-\beta t}$. This choice of $H(t)$ ensures that the resulting approximate solutions for $y_i(t)$ do not violate the rule of solution (14). Setting $m = 1$, substituting the initial guesses $y_{i,0}(t)$ in (27)–(32) gives

$$y'_{1,1} + \beta y_{1,1} = -\hbar A_0 \left[\beta e^{-2\beta t} + B_0 k_1 e^{-3\beta t}\right], \tag{33}$$

$$y'_{2,1} + \beta y_{2,1} = -\hbar B_0 \left[\beta e^{-2\beta t} + A_0 k_1 e^{-3\beta t}\right], \tag{34}$$

$$y'_{3,1} + \beta y_{3,1} = -\hbar A_0 B_0 k_1 e^{-3\beta t}. \tag{35}$$

Solving the above equations subject to the initial conditions $y_{i,m}(0) = 0$ gives

$$y_{1,1}(t) = \frac{A_0 \hbar}{2\beta} \left[B_0 k_1 e^{-3\beta t} + 2\beta e^{-2\beta t} - (2\beta + B_0 k_1) e^{-\beta t}\right], \tag{36}$$

$$y_{2,1}(t) = \frac{B_0 \hbar}{2\beta} \left[A_0 k_1 e^{-3\beta t} + 2\beta e^{-2\beta t} - (2\beta + A_0 k_1) e^{-\beta t}\right], \tag{37}$$

$$y_{3,1}(t) = \frac{A_0 B_0 k_1 \hbar}{2\beta} \left[e^{-3\beta t} - e^{-\beta t}\right]. \tag{38}$$

The solutions for $y_{i,m}(t)$ $(m \geqslant 2)$ can easily be found in a similar manner, especially using symbolic computation software such as Maple, Mathematica, MATLAB and others.

3.1 Explicit series solution of the batch reaction kinetics equations

By considering the first few solutions for $y_{i,m}(t)$ we obtain

$$y_{1,m} = \sum_{j=1}^{2m+1} a_{m,j} e^{-\beta j t}, \quad y_{2,m} = \sum_{j=1}^{2m+1} b_{m,j} e^{-\beta j t}, \quad y_{3,m} = \sum_{j=1}^{2m+1} c_{m,j} e^{-\beta j t}, \tag{39}$$

where $a_{m,j}$, $b_{m,j}$ and $c_{m,j}$ are coefficients. Substituting the series (39) into equations (27)–(32) we obtain the following recurrence formulas, for $2 \leqslant j \leqslant 2m+1$,

$$a_{m,j} = \chi_m \chi_{2m-j+1} a_{m-1,j} + \hbar \chi_{2m-j+4} a_{m-1,j-1} - \frac{\hbar k_1 \chi_{j-1} \lambda_{m,j-1}}{\beta(j-1)}, \tag{40}$$

$$b_{m,j} = \chi_m \chi_{2m-j+1} b_{m-1,j} + \hbar \chi_{2m-j+4} b_{m-1,j-1} - \frac{\hbar \chi_{j-1}(k_1 \lambda_{m,j-1} + k_2 \gamma_{m,j-1})}{\beta(j-1)}, \tag{41}$$

$$c_{m,j} = \chi_m \chi_{2m-j+1} c_{m-1,j} + \hbar \chi_{2m-j+4} c_{m-1,j-1} - \frac{\hbar \chi_{j-1}(k_2 \gamma_{m,j-1} - k_1 \lambda_{m,j-1})}{\beta(j-1)}, \tag{42}$$

where

$$\lambda_{m,j} = \sum_{j=0}^{m-1} \sum_{r=\max\{1,i+2j-2n+1\}}^{\min\{i-1,2j+1\}} a_{j,r} b_{m-1-j,i-r} \tag{43}$$

and

$$\gamma_{m,j} = \sum_{j=0}^{m-1} \sum_{r=\max\{1,i+2j-2n+1\}}^{\min\{i-1,2j+1\}} b_{j,r} c_{m-1-j,i-r} \,. \tag{44}$$

From the initial conditions $y_{i,m}(0) = 0$, we obtain

$$a_{0,1} = A_0\,, \quad b_{0,1} = B_0\,, \quad \text{and} \quad c_{0,1} = 0\,. \tag{45}$$

Also,

$$a_{m,1} = -\sum_{j=2}^{2m+1} a_{m,j}, \quad b_{m,1} = -\sum_{j=2}^{2m+1} b_{m,j}, \quad c_{m,1} = -\sum_{j=2}^{2m+1} c_{m,j}. \tag{46}$$

Using the above recurrence relations, we obtain, in succession, all the coefficients starting from the coefficients of the initial guesses (45) and the solutions (36)–(38). This process results in the explicit series solution

$$\begin{aligned} y_1(t) &= \sum_{m=1}^{+\infty} \sum_{j=1}^{2m+1} a_{m,j} e^{-j\beta t}, \\ y_2(t) &= \sum_{m=1}^{+\infty} \sum_{j=1}^{2m+1} b_{m,j} e^{-j\beta t}, \\ y_3(t) &= \sum_{m=1}^{+\infty} \sum_{j=1}^{2m+1} c_{m,j} e^{-j\beta t}. \end{aligned} \tag{47}$$

The mth order approximation is

$$\begin{aligned} y_1(t) &\approx \sum_{m=1}^{M} \sum_{j=1}^{2m+1} a_{m,j} e^{-j\beta t}, \\ y_2(t) &\approx \sum_{m=1}^{M} \sum_{j=1}^{2m+1} b_{m,j} e^{-j\beta t}, \\ y_3(t) &\approx \sum_{m=1}^{M} \sum_{j=1}^{2m+1} c_{m,j} e^{-j\beta t}. \end{aligned} \tag{48}$$

4 Results and discussion

We present the HAM approach results and compare them to numerical methods of solution. We used Maple to obtain successive solutions of $A(t)$, $B(t)$, $C(t)$ and $D(t)$ for $m \geqslant 1$. When applying the HAM technique, the auxiliary parameter $\hbar$ is critical in determining the convergence of the series. The convergence rate and region of the HAM solution series depends on the careful selection of the auxiliary parameter $\hbar$. As pointed out by Liao [15], the admissible values of $\hbar$ are chosen from the so called $\hbar$-curve in which some derivative property of the governing function, say $y_1'(0)$ in the case of the current problem, is considered to be an independent variable and plotted against $\hbar$. The valid region of $\hbar$ where the series converges is the horizontal segment of each $\hbar$-curve. This study found that $\hbar = -1/4$ was appropriate to be used. Using this choice of the auxiliary parameter the HAM approximation at order $m = 15$ was found to converge to the numerical solution. Figures 1–4 show comparisons of the HAM analytical solutions with numerical results obtained using MATLAB initial value solvers. As can be clearly observed in the figures, there is an excellent agreement between the two approaches for all values of time t. As expected, in Figure 1 we observe that as the reaction rate k_1 increases, concentration $A(t)$ which is a reactant is greatly reduced. It quickly diminishes for bigger values of the reaction rate. In Figure 2 we observe that the concentration profiles of reactant $B(t)$ are reduced as values of k_1 increase. The reduction of $B(t)$ is not as great as that of $A(t)$ since reactant $B(t)$ is also added to react with reactant $C(t)$ at the next phase of the batch reaction process. As expected, we observe in Figure 3 that concentration $C(t)$ increases as the reaction rate k_1 increases and reaches a peak before steadily decreases as it then reacts with $B(t)$ to produce concentrate $D(t)$. The optimal time at which the concentration of the product $C(t)$ is maximum can be deduced from Figure 3 and then the reactor quenched at this time. In Figure 4 we observe that as the reaction rate k_1 increases, the product concentration $D(t)$ increases as expected.

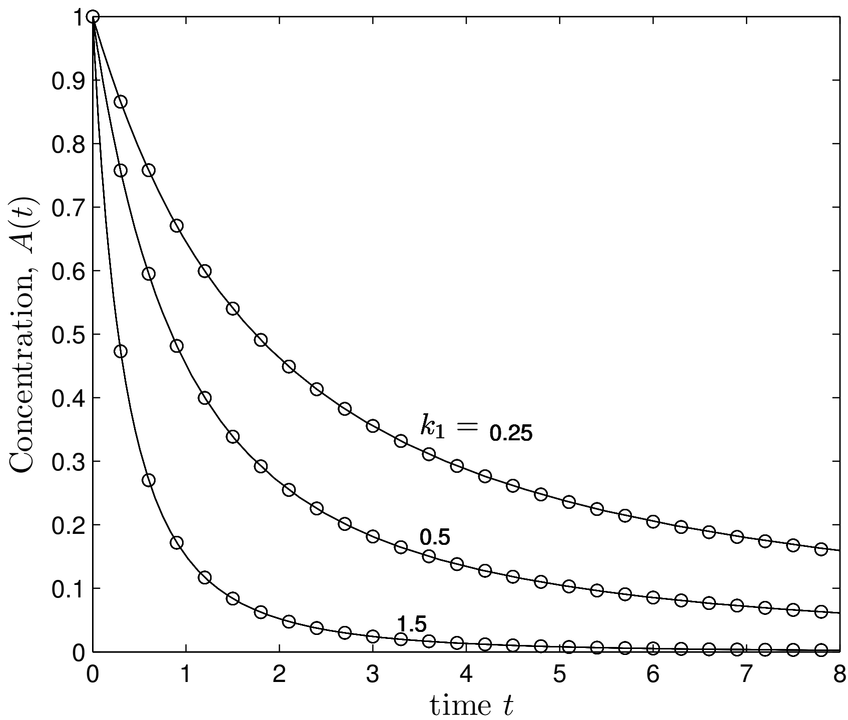

FIGURE 1: Comparison of the numerical solution of $A(t)$ with the 15th order HAM approximate solution when $\hbar = -0.25$, $k_2 = 0.5$, $\beta = 0.15$. The solid line denotes the numerical solution and the circles denote the HAM solutions

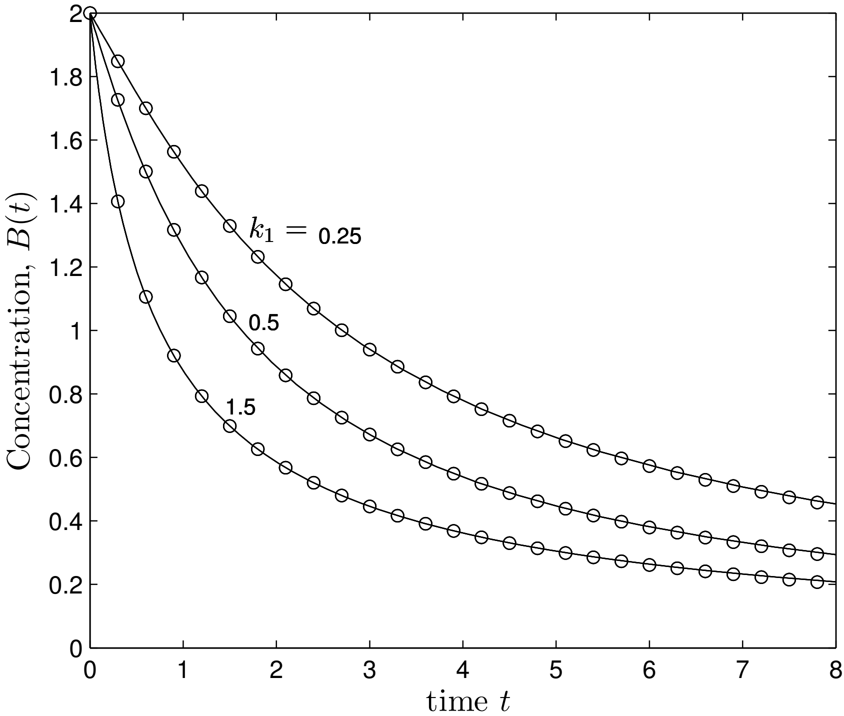

Figure 2: Comparison of the numerical solution of $B(t)$ with the 15th order HAM approximate solution when $\hbar = -0.25$, $k_2 = 0.5$, $\beta = 0.15$. The solid line denotes the numerical solution and the circles denote the HAM solutions

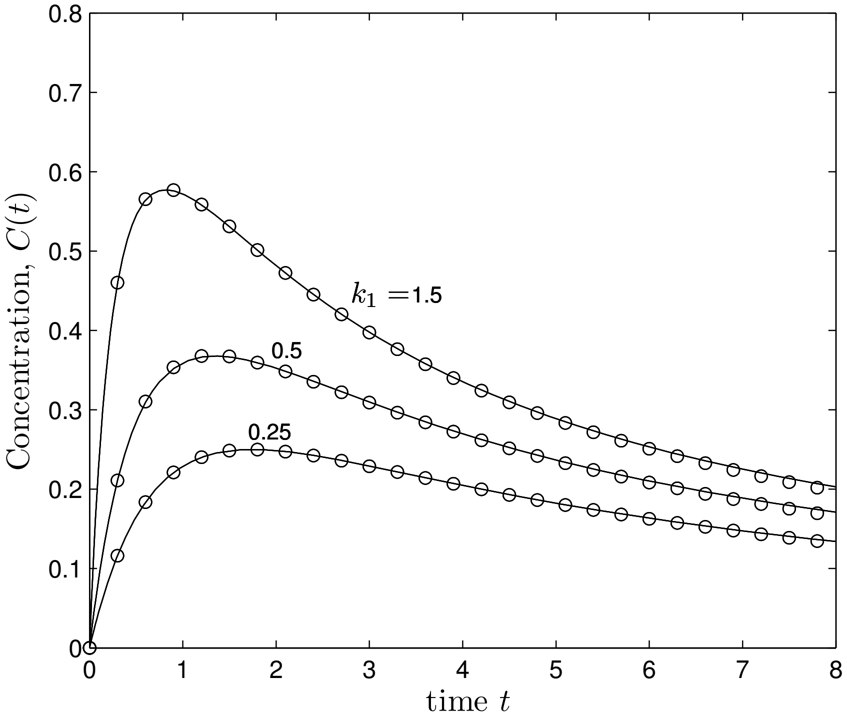

FIGURE 3: Comparison of the numerical solution of $C(t)$ with the 15th order HAM approximate solution when $\hbar = -0.25$, $k_2 = 0.5$, $\beta = 0.15$. The solid line denotes the numerical solution and the circles denote the HAM solutions

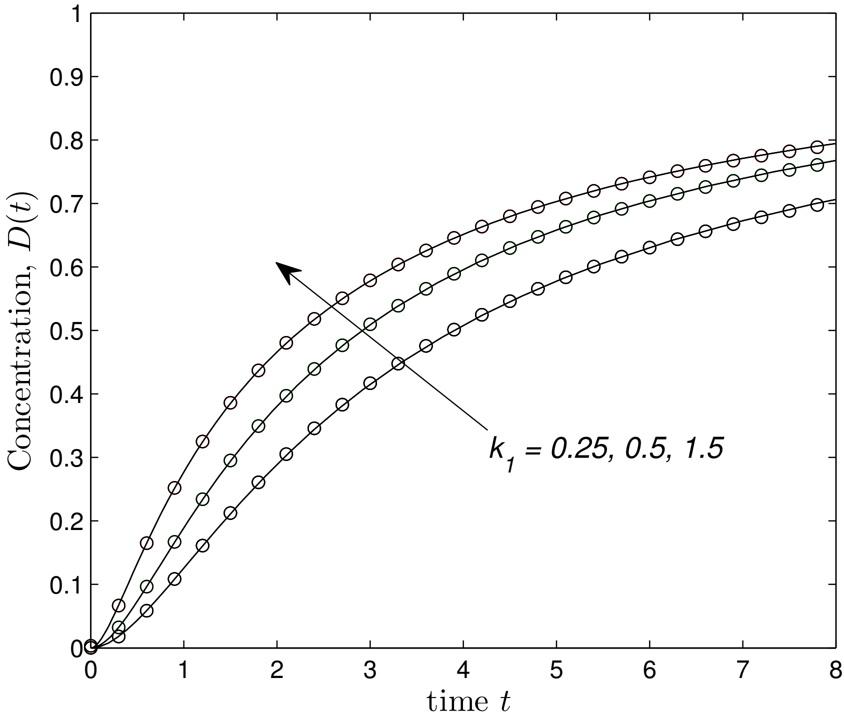

Figure 4: Comparison of the numerical solution of $D(t)$ with the 15th order HAM approximate solution when $\hbar = -0.25$, $k_2 = 0.5$, $\beta = 0.15$. The solid line denotes the numerical solution and the circles denote the HAM solutions

5 Conclusion

The homotopy analysis method is used to solve the nonlinear batch reaction kinetic equations. Explicit series solutions describing the time evolution of the underlying reaction kinetics equations are obtained. Our HAM results are found to be in excellent agreement with numerical results. This confirms the power and significance of the HAM approach as an effective technique for solving nonlinear systems of equations. The value of 0.15 for β was arrived at when the appropriate value of $\hbar = -1/4$ was used. We hope that the HAM approach presented here will spawn further interest in the analysis of reaction kinetic models that fully characterize the reactions without making assumptions of small or large concentration, initial or long term effects, quasi-steady or steady state effects.

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