Analytical solutions of non-linear boundary value problem for chemical reactions of enzyme substrate

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Abstract

A mathematical representation for the non-linear accelerator mechanics response technique is discussed. We have a tendency to ponder dynamic models of reversible hastening agent responses and look at two systems for expository rough arrangements of the model. Logical inexact arrangements of non-linear response conditions for reversible kinetic responses are computed using the homotopy analysis Method and this article mainly focused on the accelerator mechanics answer bind and uses the homotopy analytical procedure to find out an investigative articulation for accelerator reaction technique. Our results are meet numerical simulation results and are found subsequent in the sensible accedence. And we build a regression model.

Keywords

Non-Linear accelerator Equations, Enzyme substrate, mechanics response, Homotopy analytical method, Time dependent analytical Solution. Regression.

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1. Introduction

The enzyme kinetics is the investigation of the substance responses that are catalyzed by chemicals. In catalyst energy, the response rate is estimated and the impacts of shifting the states of the response researched. Concentrate a protein's energy thusly can uncover the reactant instrument of this chemical, its part in digestion, how its movement is controlled, and how a medication or an agonist may repress the compound.

Chemicals are normally protein particles that control different atoms the catalysts substrates. These objective particles tie to a protein's dynamic site and are changed into items through a progression of steps known as the enzymatic systems. These instruments can be partitioned into single-substrate and various substrate components. Motor examinations on compounds that lone tie one substrate, such as triosephosphate isomerism (CH3OCH3 and CH3CH2OH); expect to gauge the liking with which the chemical ties this substrate and the turnover rate.

Compounds are imperative in controlling natural procedures, for instance, as activators or inhibitors in a response. To comprehend their part we need to think about compound energy which is basically the investigation of rates of responses, the fleeting conduct of the different reactants and the conditions which impact them. Presentations with a statistical twisted are given by Rubinow [1], Murray [2], Segel [3] and Roberts [4].

In this paper we discuss about some model response components, which reflect a substantial number of genuine responses, and some broad kinds of response wonders and their relating numerical acknowledge; information of these is fundamental while building models to reflect particular known biochemical properties of an instrument. Be that as it may, to the best of my insight, till date no diagnostic outcomes for catalyst energy response dissemination condition utilizing homotopy analysis technique have been derived.

2. Mathematical Formulation of the Problem

The enzyme kinetics in biochemical frameworks have generally been displayed by common differential conditions which are construct exclusively in light of responses without spatial reliance of the different focuses. The model for a catalyst activity, first clarified by Michaelis and Menten proposed the official of free protein to the reactant shaping a compound reactant. Generally, the reactant atom that ties to the compound is named the substrate S, and the system is regularly composed as [5];

$$E + S \xrightarrow[k_{-1}]{k_1} ES \xrightarrow{k_2} E + P \tag{2.1}$$
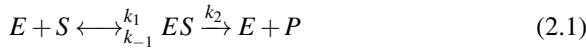
This system outlines the authoritative of substrate S and arrival of item P. E is the free compound and ES is the chemical substrate complex. k_1, k_{-1} and k_2 signify the rates of response of these three procedures. Note that substrate restricting is reversible however item discharge isn't. The convergence of the reactants in the Eq. (2.1) is signified by bring down case letters

$$s = [S], e = [E], c = [SE], p = [P] \tag{2.2}$$

The law of mass activity prompts the arrangement of following non-linear response equations [5]

$$\frac{ds}{dt} = -k_1 es + k_{-1} c \tag{2.3a}$$

$$\frac{de}{dt} = -k_1 es + (k_{-1} + k_2) c \tag{2.3b}$$

$$\frac{dc}{dt} = k_1 es - (k_{-1} + k_2) c \tag{2.3c}$$

$$\frac{dp}{dt} = k_2 c \tag{2.3d}$$

The boundary conditions are

$$s(0) = s_0, e(0) = e_0, c(0), p(0) = 0. \tag{2.4}$$

Adding equations (2.3b) and (2.3c), we get,

$$\frac{de}{dt} + \frac{dc}{dt} = 0 \tag{2.5}$$

Using the initial conditions (2.4), we obtain the following result

$$e(t) + c(t) = e_0 \tag{2.6}$$

With this, the system of ordinary differential equations reduce to only two, for s and c, namely

$$\frac{ds}{dt} = -k_1 e_0 s + (k_1 s + k_{-1}) c \tag{2.7}$$

$$\frac{dc}{dt} = k_1 e_0 s - (k_1 s + k_{-1} + k_2) c \tag{2.8}$$

with initial conditions $s(0) = s_0$, $c(0) = 0$. By introducing the following parameters

$$\tau = \frac{k_1 e_0 t}{\varepsilon}, \ u(\tau) = \frac{s(t)}{s_0}, \ v(\tau) = \frac{c(t)}{e_0}, \ w(\tau) = \frac{p(t)}{e_0}$$

$$\lambda = \frac{k_2}{k_1 s_0}, \ k = \frac{k_{-1} + k_2}{k_1 s_0}, \ \varepsilon = \frac{e_0}{s_0}, \ E(\tau) = \frac{e(t)}{e_0} \tag{2.9}$$

the system of Eqs. (2.7) and (2.8) and the initial conditions [Eqs. (2.4)] can be represented in dimensionless form as follows:

$$\frac{du}{d\tau} = -u\varepsilon + \varepsilon(u + k - \lambda) v \tag{2.10a}$$

$$\frac{dv}{d\tau} = u - (u + k) v \tag{2.10b}$$

$$\frac{dw}{d\tau} = \lambda v \tag{2.10c}$$

$$u(0) = 1, \quad v(0) = 0, \quad w(0) = 0. \tag{2.11}$$

From the Eq. (2.6), we can also obtain the dimensionless concentration of enzyme

$$E(\tau) = 1 - v(\tau) \tag{2.12}$$

Equation (2.3d) is uncoupled with the initial three conditions. The dimensionless concentration of the item is given by

$$w(\tau) = \lambda \int_0^t v(t') dt' \tag{2.13}$$

Eqs. (2.12) and (2.13) represent the new analytical expressions of the concentrations of enzyme $E(\tau)$ and product $w(\tau)$ for the values of parameters k, λ and ε.

3. Solution of Enzyme Kinetics Reaction Diffusion Equations

The homotopy analysis method (HAM) is a powerful analytical method to solve nonlinear problems [6–12] and this method provides a convenient way to guarantee the convergence of approximation series. Furthermore, the obtained result is of high accuracy. Solving Eqs. (2.10a)–(2.10c) and (2.12) using homotopy analysis method and simultaneous equation method, the steady state and transient contributions to the model are given by: The homotopy analysis method (HAM) is a great systematic technique to tackle non-linear issues [6–12] and this technique gives a helpful method to ensure the merging of estimation arrangement. Besides, the got result is of high exactness. Solving Eqs. (2.10a)–(2.10c)

and (2.12) utilizing homotopy analysis method and synchronous condition technique, the enduring state and transient commitments to the model are given by:

$$u(\tau) = e^{-\varepsilon\tau}\left(1 + \frac{h}{k}\right)$$
$$+ \frac{h\varepsilon}{(k-\varepsilon)}\left[\frac{-ke^{-2\varepsilon\tau} + \varepsilon e^{-(k+\varepsilon)\tau}}{k\varepsilon}\right.$$
$$\left. + \frac{(k-\lambda)}{(k-\varepsilon)}\left(\tau(k-\varepsilon)e^{-\varepsilon\tau} + (e^{-k\tau} - e^{-\varepsilon\tau})\right)\right] \quad (3.1)$$

$$v(\tau) = \left(1 + \frac{h}{k}\right)\left(\frac{e^{-\varepsilon\tau} - e^{-k\tau}}{(k-\varepsilon)}\right)$$
$$+ \frac{h(k+\varepsilon)}{k\varepsilon(k-\varepsilon)}\left(e^{-k\tau} - e^{-(k+\varepsilon)\tau}\right)$$
$$+ \frac{h}{(k-\varepsilon)}\left[\left(\frac{\varepsilon+1}{k-2\varepsilon}\right)\left(e^{-k\tau} - e^{-2\varepsilon\tau}\right)\right.$$
$$+ \frac{\varepsilon(k-\lambda)}{(k-\varepsilon)^2}\left(\tau(k-\varepsilon)(e^{-k\tau} + e^{-\varepsilon\tau})\right.$$
$$\left.\left. + 2(e^{-k\tau} - e^{-\varepsilon\tau})\right)\right] \quad (3.2)$$

$$w(\tau) = \frac{h}{(k-\varepsilon)}\left(1 + \frac{h}{k}\right)\left(\frac{(e^{-k\tau}-1)}{k} - \frac{(e^{-\varepsilon\tau}-1)}{\varepsilon}\right)$$
$$+ \frac{h}{(k-\varepsilon)}\left[\left(\frac{\varepsilon+1}{k-2\varepsilon}\right)\left(\frac{e^{-2\varepsilon\tau}-1}{2\varepsilon} - \frac{e^{-k\tau}-1}{k}\right)\right.$$
$$\left. + \left(\frac{k+\varepsilon}{k\varepsilon}\right)\left(\frac{e^{-(\varepsilon+k)\tau}-1}{\varepsilon+k} - \frac{e^{-k\tau}-1}{k}\right)\right]$$
$$+ \frac{h\varepsilon(k-\lambda)}{(k-\varepsilon)^2}\left[\left(\frac{1}{\varepsilon^2} + \frac{1}{k^2}\right)\right.$$
$$+ \frac{2}{(k-\varepsilon)}\left(\frac{e^{-\varepsilon\tau}-1}{\varepsilon} - \frac{e^{-k\tau}-1}{k}\right)$$
$$\left. - \frac{e^{-\varepsilon\tau}}{\varepsilon^2}(\tau\varepsilon+1) - \frac{e^{-k\tau}}{k^2}(\tau k+1)\right] \quad (3.3)$$

$$E(\tau) = 1 - \left(1 + \frac{h}{k}\right)\left(\frac{e^{-\varepsilon\tau} - e^{-k\tau}}{(k-\varepsilon)}\right)$$
$$+ \left(\frac{k+\varepsilon}{k\varepsilon}\right)\left(e^{-k\tau} - e^{-(k+\varepsilon)\tau}\right)$$
$$- \frac{h}{(k-\varepsilon)}\left[\left(\frac{\varepsilon+1}{k-2\varepsilon}\right)\left(e^{-k\tau} - e^{-2\varepsilon\tau}\right)\right.$$
$$+ \frac{\varepsilon(k-\lambda)}{(k-\varepsilon)^2}\left(\tau(k-\varepsilon)(e^{-k\tau} + e^{-\varepsilon\tau})\right.$$

$$+ 2(e^{-k\tau} - e^{-\varepsilon\tau}))\right] \quad (3.4)$$

Eqs. (3.1)–(3.4) fulfill the limit conditions Eq. (2.11). This equation speaks to the new analytical expression of the concentration $u(\tau)$, $v(\tau)$, $w(\tau)$ and $E(\tau)$ for every possible estimation of the parameters.

4. Numerical Simulation

The non-linear equations (Eqs. (2.10a)–(2.10c) and (2.12)) for the boundary conditions (Eq. (2.11)) are explained by numerical strategies. The capacity ode45 in Scilab programming is utilized to take care of the boundary value problems (BVPs) for ordinary differential equations. The numerical outcomes are likewise contrasted and the acquired expository articulations (Eqs. (3.1)–(3.4)).
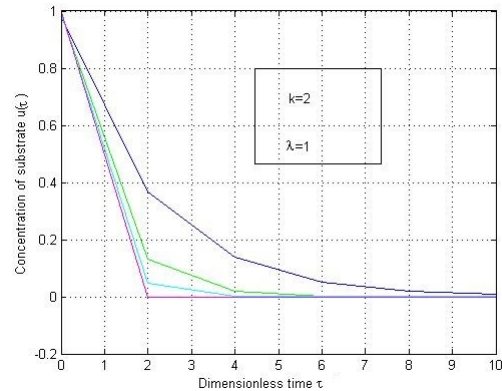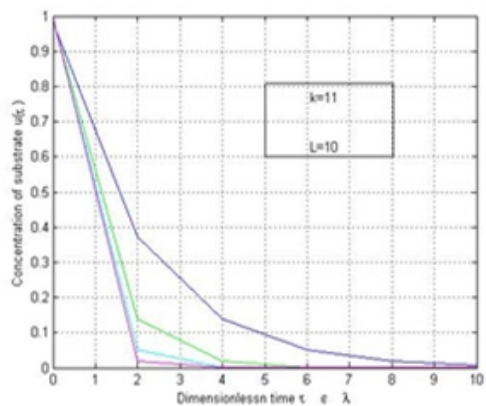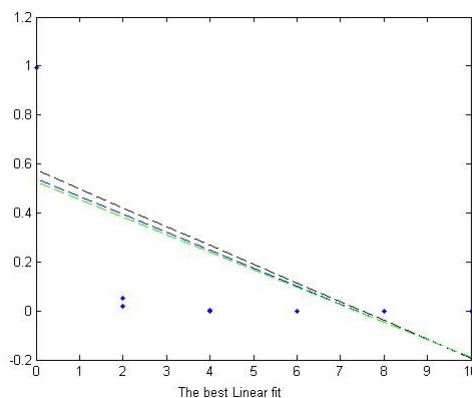

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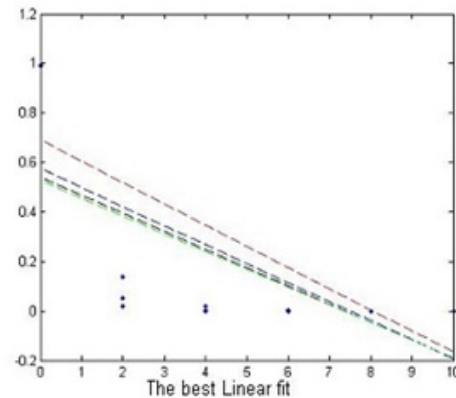
(b)

Figure 4.1. The focus of the substrate $u(\tau)$ are plotted using Eq. (3.1) for the values $k = 2$, $\lambda = 1$, $h = -0.01$, (Blue) $\varepsilon = 0.5$, (Green) $\varepsilon = 1$, $\varepsilon = 1.5$ and $\varepsilon = 2$.
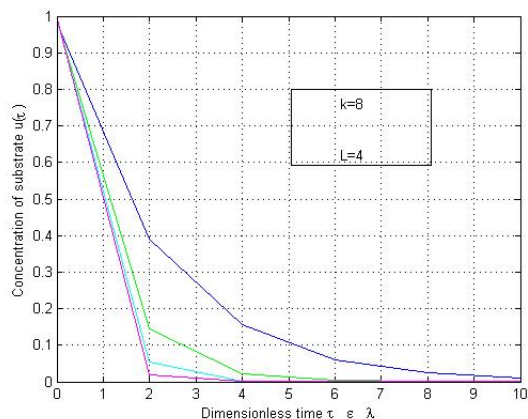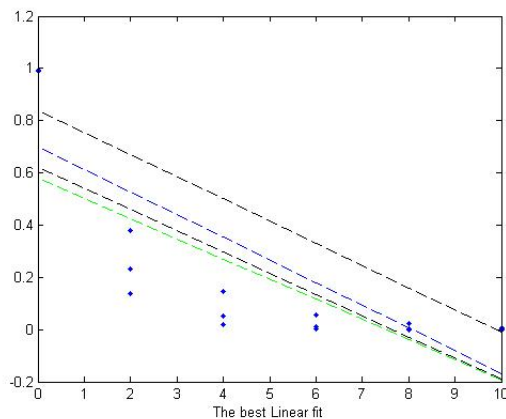
(a)   **(b)**

Figure 4.2. The focus of the substrate $u(\tau)$ are plotted using Eq. (3.1) for the values $k = 11$, $\lambda = 10$, $h = -0.01$, (a) $\varepsilon = 0.5$, (b) $\varepsilon = 1$, (c) $\varepsilon = 1.5$ and (d) $\varepsilon = 2$.
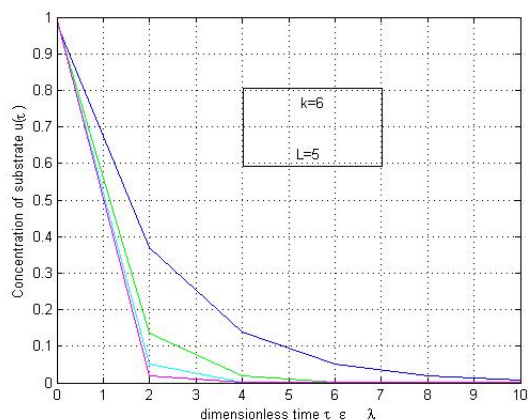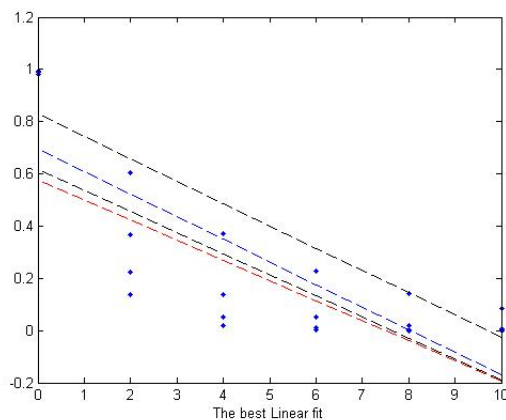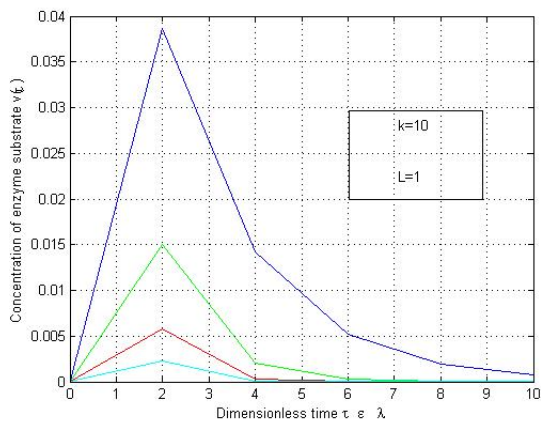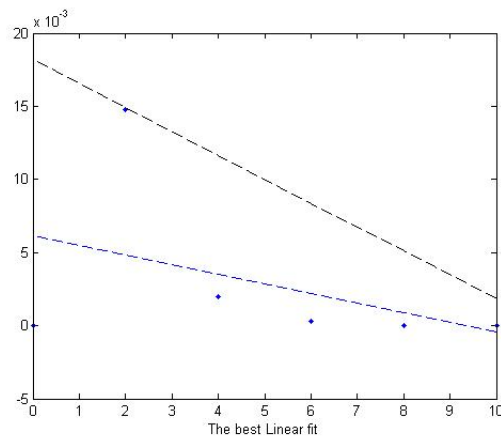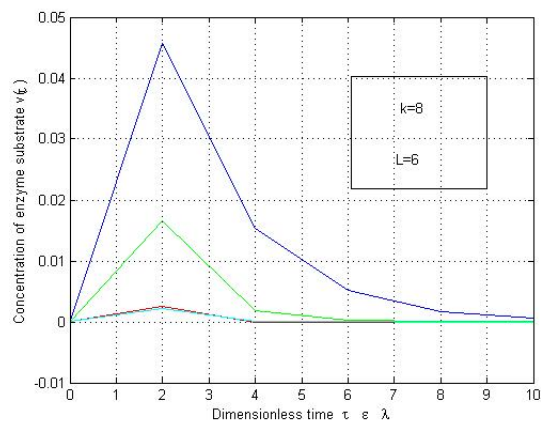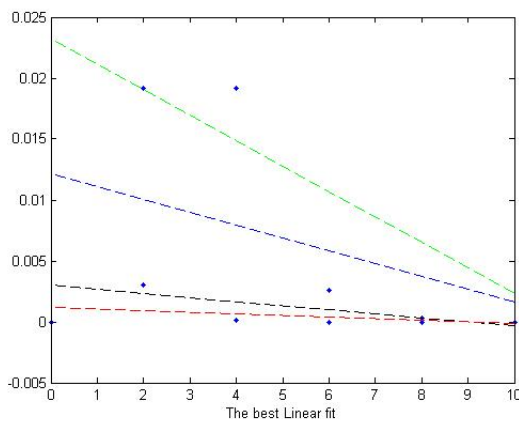

(a)   **(b)**

Figure 4.3. The focus of the substrate $u(\tau)$ are plotted using Eq. (3.1) for the values $k = 8$, $\lambda = 4$, $h = -0.01$, (a) $\varepsilon = 0.5$, (b) $\varepsilon = 1$, (c) $\varepsilon = 1.5$ and (d) $\varepsilon = 2$.


(a)   **(b)**

Figure 4.4. The focus of the substrate $u(\tau)$ are plotted using Eq. (3.1) for the values $k = 6$, $\lambda = 5$, h =-0.01, (a) $\varepsilon = 0.5$,(b) $\varepsilon = 1$, (c) $\varepsilon = 1.5$ and (d) $\varepsilon = 2$.
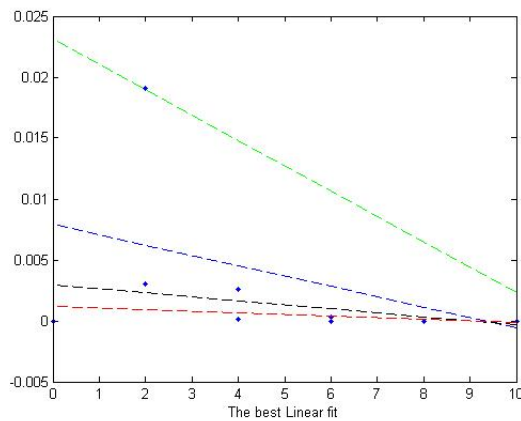
(a)

(b)

Figure 4.5. The concentration of enzyme-substrate $v(\tau)$ are plotted using Eq. (3.2) for the values $k = 10$, $\lambda = 1$, $h = -0.001$, (a) $\varepsilon = 0.5$, (b) $\varepsilon = 1$, (c) $\varepsilon = 1.5$ and (d) $\varepsilon = 2$.
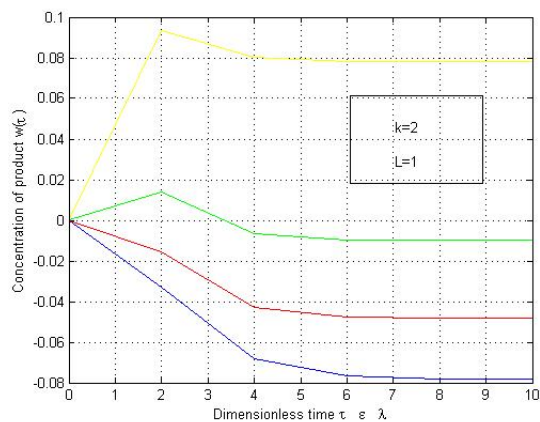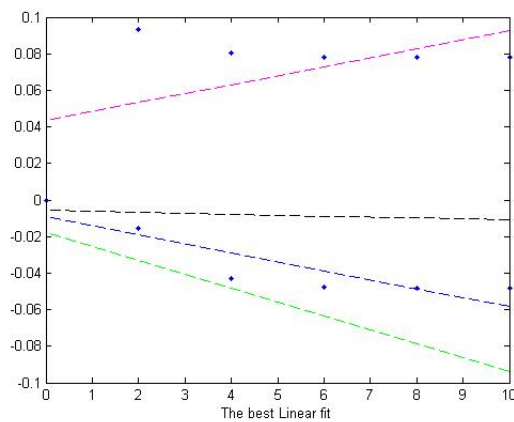

(a)

(b)

Figure 4.6. The concentration of enzyme–substrate $v(\tau)$ are plotted using Eq. (3.2) for the values $k = 8$, $\lambda = 6$, $h = -0.25$, (a) $\varepsilon = 0.5$, (b) $\varepsilon = 1$, (c) $\varepsilon = 1.5$ and (d) $\varepsilon = 2$.
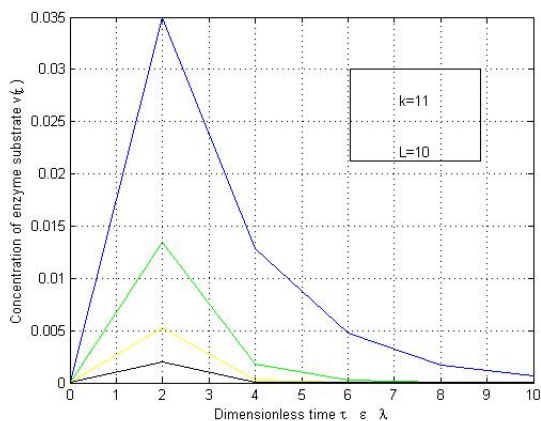
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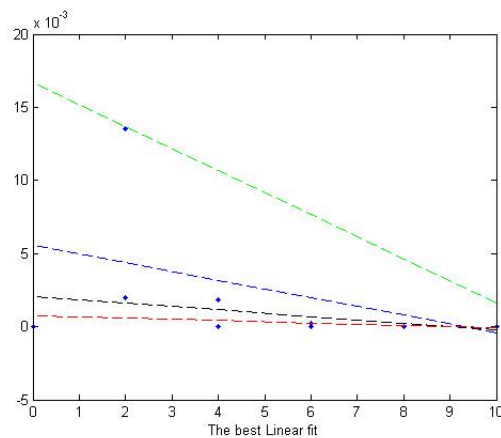
(b)

Figure 4.7. The concentration of enzyme–substrate $v(\tau)$ are plotted using Eq. (3.2) for the values $k = 11$, $\lambda = 10$, $h = -0.01$, (a) $\varepsilon = 0.5$, (b) $\varepsilon = 1$, (c) $\varepsilon = 1.5$ and (d) $\varepsilon = 2$.
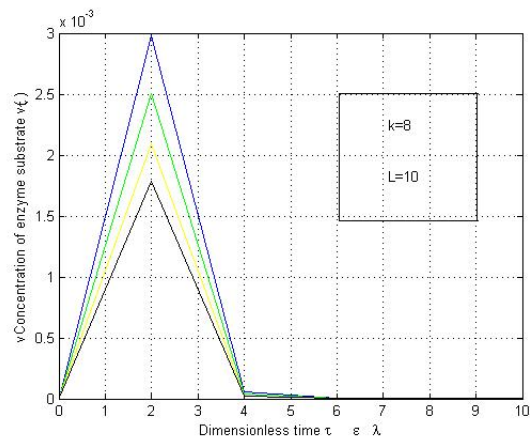
(a)

(b)

Figure 4.8. The concentration of enzyme-substrate $v(\tau)$ are plotted using Eq. (3.2) for the values $k = 8$, $\lambda = 4$, $h = -0.01$, (a) $\varepsilon = 2$, (b) $\varepsilon = 2.1$, (c) $\varepsilon = 2.2$ and (d) $\varepsilon = 2.3$.
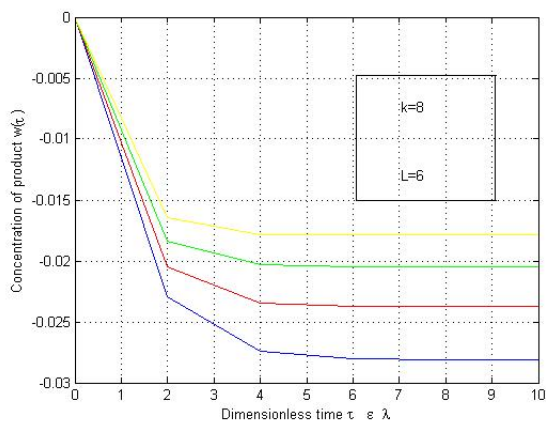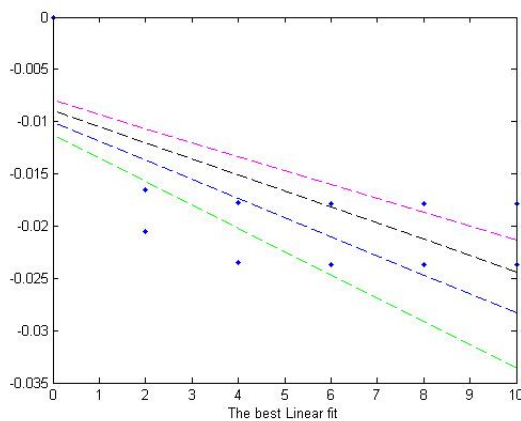

(a)

(b)

Figure 4.9. The concentration of product $w(\tau)$ are plotted using Eq. (3.3) for the values $k = 2$, $\lambda = 1$, $h = -0.25$, (a) $\varepsilon = 1.2$, (b) $\varepsilon = 1.4$, (c) $\varepsilon = 1.6$ and (d) $\varepsilon = 1.8$.
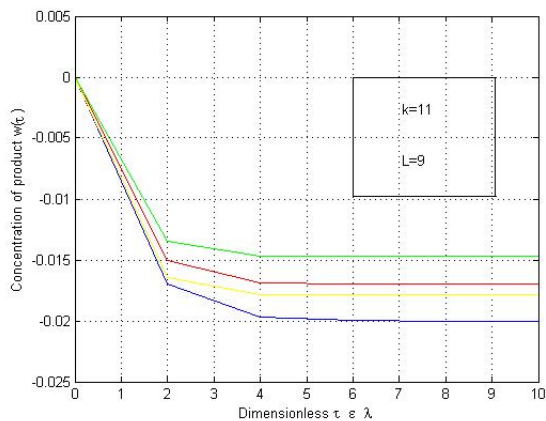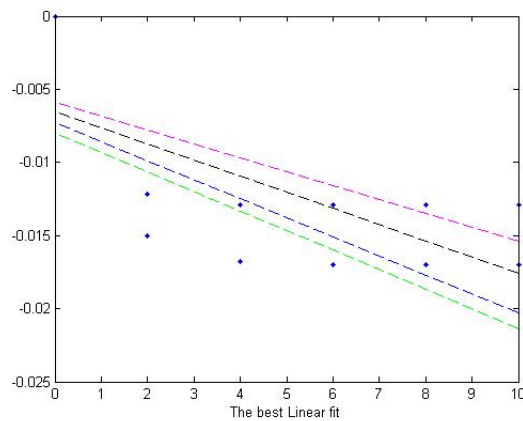

(a)

(b)

Figure 4.10. The concentration of product $w(\tau)$ are plotted using Eq. (3.3) for the values $k = 8$, $\lambda = 6$, h =-0.25, (a) $\varepsilon = 1.2$, (b) $\varepsilon = 1.4$, (c) $\varepsilon = 1.6$ and (d) $\varepsilon = 1.8$.
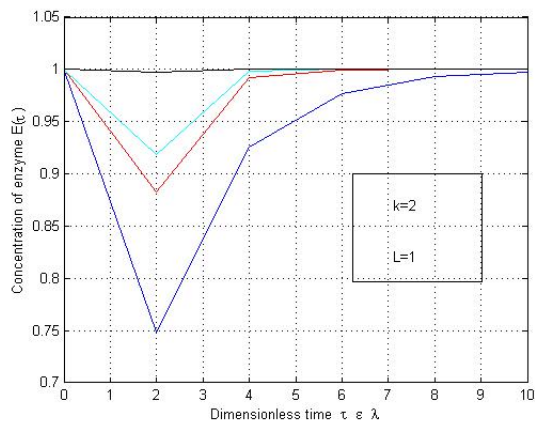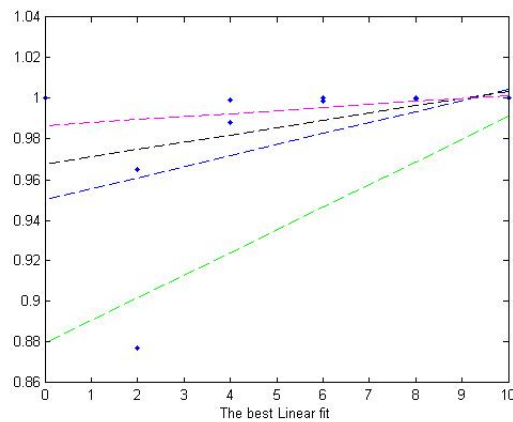
(a)   **(b)**

Figure 4.11. The concentration of product $w(\tau)$ are plotted using Eq. (3.3) for the values $k = 11$, $\lambda = 9$, h =-0.01, (a) $\varepsilon = 1.2$, (b) $\varepsilon = 1.4$, (c) $\varepsilon = 1.6$ and (d) $\varepsilon = 1.8$.

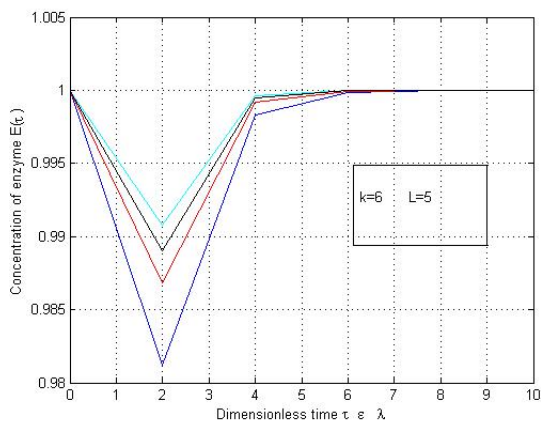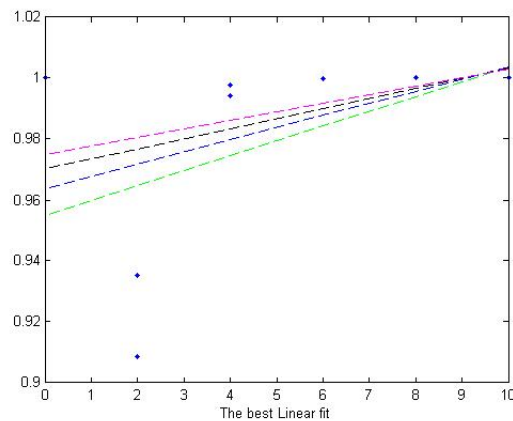**(a)**   **(b)**

Figure 4.12. The concentration of enzyme $E(\tau)$ are plotted using Eq. (3.4) for the values $k = 2$, $\lambda = 1$, $h = -0.15$, (a) $\varepsilon = 0.5$, (b) $\varepsilon = 1.1$, (c) $\varepsilon = 1.5$ and (d) $\varepsilon = 2.1$.

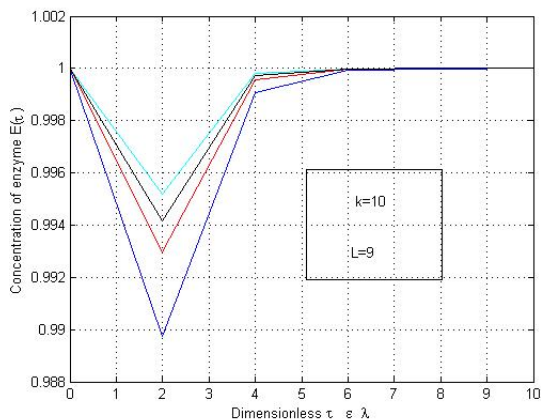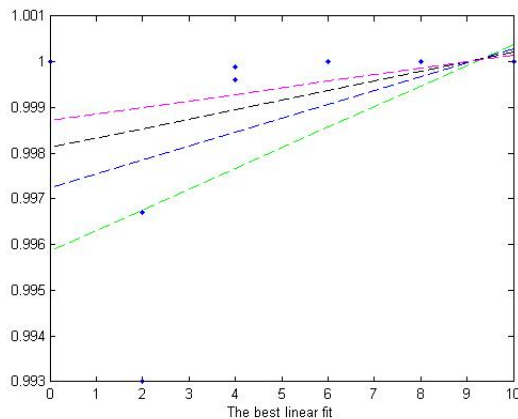**(a)**   **(b)**

Figure 4.13. The concentration of enzyme $E(\tau)$ are plotted using Eq. (3.4) for the values $k = 66$ $\lambda = 5$, $h = -0.01$, (a) $\varepsilon = 1.2$, (b) $\varepsilon = 1.4$, (c) $\varepsilon = 1.6$ and (d) $\varepsilon = 1.8$.

(a) **(b)**

Figure 4.14. The concentration of enzyme $E(\tau)$ are plotted using Eq. (3.4) for the values $k = 10$, $\lambda = 9$, $h = -0.01$, (a) $\varepsilon = 1.2$, (b) $\varepsilon = 1.4$, (c) $\varepsilon = 1.6$ and (d) $\varepsilon = 1.8$.
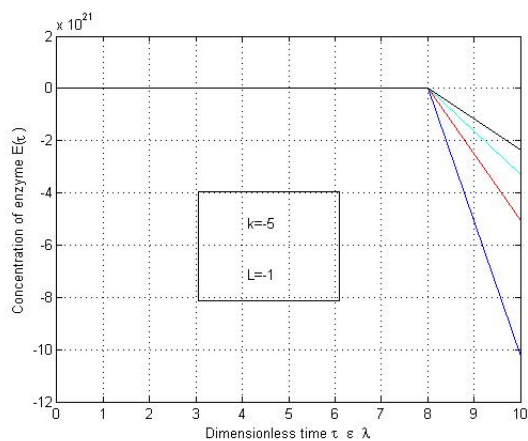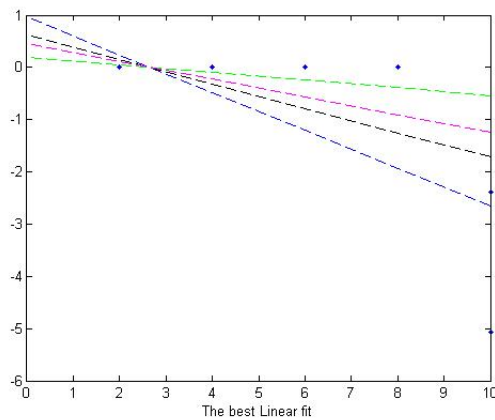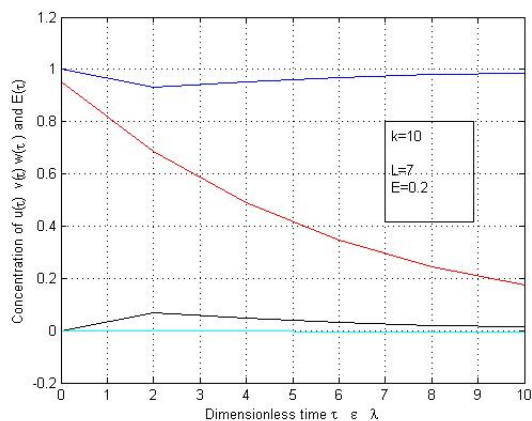

(a) **(b)**

Figure 4.15. The concentration of enzyme $E(\tau)$ are plotted using Eq. (3.4) for the values $k = -5$, $\lambda = -1$, $h = -0.01$, (a) $\varepsilon = 0.5$, (b) $\varepsilon = 1$, (c) $\varepsilon = 1.5$ and (d) $\varepsilon = 2$.

(a) **(b)**
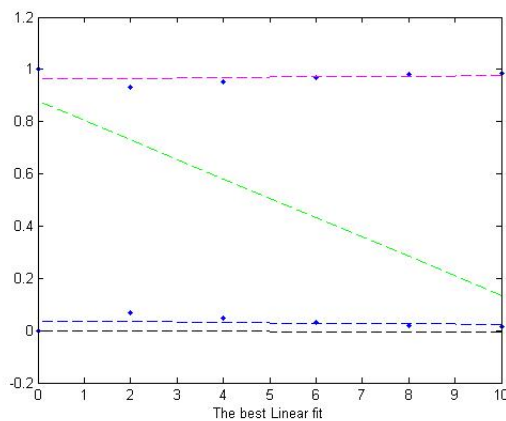
Figure 4.16. The concentration of the substrate $u(\tau)$, enzyme-substrate $v(\tau)$, enzyme $E(\tau)$ and product $w(\tau)$ are plotted using Eqs. (3.1)–(3.4) for the values $k = 10$, $\lambda = 5$, $h = -0.01$, and $\varepsilon = 0.2$.

(a) $\tau = 0$ to 10, $k = 2$, $h = 0.01$, $\lambda = 1$

(b) $k = -1$, $\lambda = 1$, $h = -0.001$

Figure 4.17. The concentration of the substrate $u(\tau)$, enzyme-substrate $v(\tau)$, enzyme $E(\tau)$ and product $w(\tau)$ are plotted using Eqs. (3.1)–(3.4) for the values $k = 10$, $\lambda = 5$, $h = -0.01$, and $\varepsilon = 0.2$.
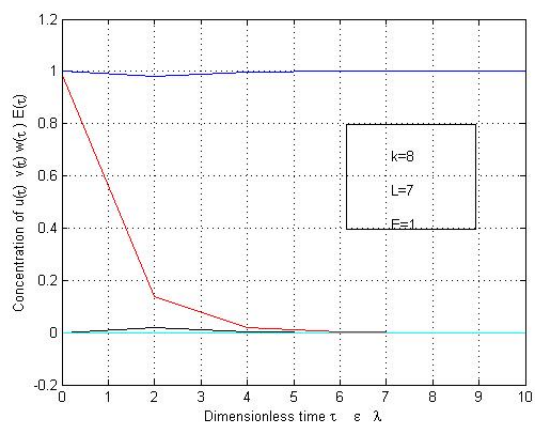

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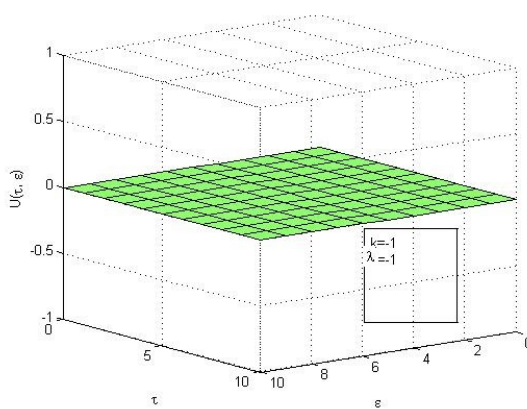
(b)

Figure 4.18. The concentration of the substrate $u(\tau)$, enzyme-substrate $v(\tau)$, enzyme $E(\tau)$ and product $w(\tau)$ are plotted using Eqs. (3.1)–(3.4) for the values $k = 8$, $\lambda = 7$, $h = -0.01$, and $\varepsilon = 1$.
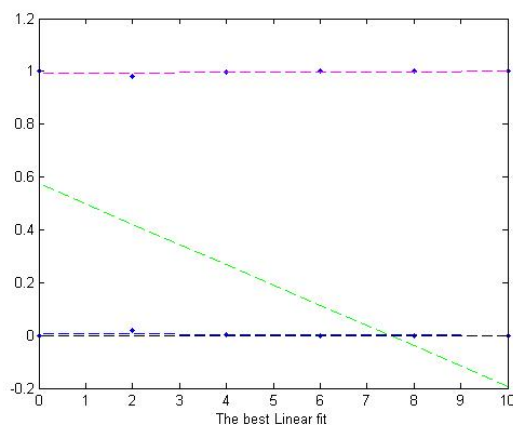

(a)

(b)

Figure 4.19. The concentration of the substrate $u(\tau)$, enzyme-substrate $v(\tau)$, enzyme $E(\tau)$ and product $w(\tau)$ are plotted using Eqs. (3.1)–(3.4) for the values $k = 8$, $\lambda = 7$, $h = -0.01$, and $\varepsilon = 1$.
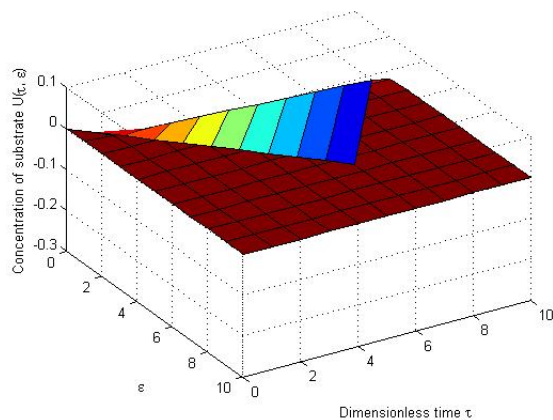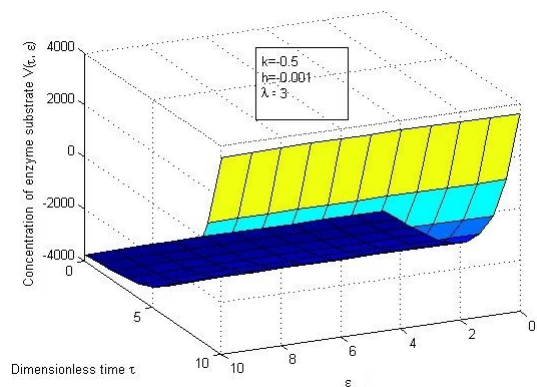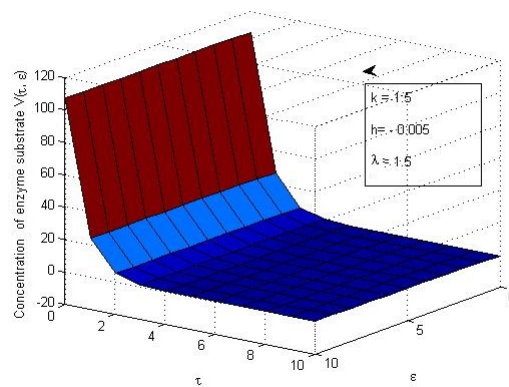
4.1 Results and Discussion

Figures 4.13–4.15 shows that the concentrations of substrate u, enzyme E, enzyme-substrate complex v and product w are shown in blue, green, red and sky blue colors respectively. In these figures, u and E decreases slowly and reaches the constant values but v and w increases slowly and reaches the constant value for greater values of τ. Figures 4.16–4.19 give us the confirmation for the above discussion in three-dimensional graphs also.

Eqs. (3.1)–(3.4) demonstrates the basic surmised analytical expression of concentrations of substrate u, enzyme E, enzyme-substrate complex v and item w for different estimations of dimensionless response parameters k, λ and ε. In Figures 4.1–4.3, the concentration of subtract gradually abatements and achieves the steady qualities for some settled estimations of k, λ and distinctive estimations of ε. The centralizations of substrate ends up zero for substantial estimations of τ. From the Figures 4.4–4.6, it is derived that the estimation of the concentration of the catalyst– substrate increments at $\tau < 1$ and diminishes gradually at $\tau \geqslant 1$ for various estimations of k, λ and ε. The convergence of the compound substrate ends up zero for more noteworthy qualities τ. Figures 4.7–4.9 demonstrates that the centralization of the item increments gradually from the underlying fixation and achieves the steady qualities for extensive estimations of τ. In Figures 4.10–4.12, the estimations of centralizations of catalyst diminish gradually and achieve consistent qualities for more prominent estimations of τ.

Figures 4.13–4.15 demonstrates that the convergences of substrate u, compound E, catalyst substrate complex v and item w are appeared in blue, green, red and sky blue hues individually. In these figures,u and E diminishes gradually and achieves the consistent qualities yet u expands gradually and achieves the steady an incentive for more prominent estimations of τ. Figures 4.16–4.19 give us the affirmation for the above exchange in three-dimensional charts too.

5. Conclusion

In this work, an induced methodical response for non-linear reaction equations has been displayed using homotopy analysis method. An incredible and essential system for evaluating the concentration of substrate, item, chemical substrate and catalyst are determined. In view of the consequence of this work, it can be easily contacted an extensive variety of course of action of coupled non-linear equation with various complex boundary conditions in chemical substrate reaction dispersal frames and our results are differentiated and numerical results and are seen to be in incredible understanding.

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