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Some Remarks on Two-Step Exothermic Reactions with Arrhenius Kinetics and Reactants Consumption

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Abstract

Many reactions that are written as a single reaction equation in actual fact consist of a series of elementary steps. Even though a balanced chemical equation may give the ultimate result of a reaction, what actually happens in the reaction may take place in several steps. A chemical equation does not tell us how reactants become products. Knowledge about this process will become extremely important as we learn more about the theory of chemical reaction rates. This paper presents an analytical method for describing two-step exothermic reactions with Arrhenius kinetics and reactants consumption. We assume that the reaction is not stirred, that is, change depends on space variable and examines the properties of the solution of the model. We solve the equations using parameter-expanding method and eigenfunctions expansion technique. The results obtained revealed that the temperature of the medium, for a non-stirred reaction, is symmetric and monotonically increasing. Also, the temperature of the medium increases and reaches steady state as activation energies ratio increases, for a well-stirred reaction.

Keyword: Arrhenius kinetics, two-step exothermic reactions, reactants consumption, analytical solution.

1. Introduction

Chemical reaction kinetics deals with the rates of chemical processes. Any chemical process may be broken down into a sequence of one or more single-step processes known either as elementary processes, elementary reactions, or elementary steps. Elementary reactions usually involve either a single reactive collision between two molecules, which we refer to as a bimolecular step or dissociation/ isomerization of a single reactant molecule, which we refer to as a unimolecular step. Very rarely, under conditions of extremely high pressure, a termolecular step may occur, which involves the simultaneous collision of three reactant molecules. An important point to recognize is that many reactions that are written as a single

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reaction equation in actual fact consist of a series of elementary steps. This will become extremely important as we learn more about the theory of chemical reaction rates.

A two-step reaction is a chain reaction of the form $A \xrightarrow{Rate1} X \xrightarrow{Rate2} B$, where are the reactant and the intermediate product X generates the final product B. Although chain reaction involves multiple steps but the *initiation* (step where the chain carriers are initially formed), *propagation* (step where the chain carriers produced in the initiation step attack other molecules which results in the formation of a new carrier) and *termination* (step where the carriers combine and end the chain) steps are primarily involved (Folly, 2004). The reactions $A \to C$ and $A \to B \to C$ have different implications in terms of heat release which is our interest.

The study of mathematical equations describing some combustion problems has attracted the interest of many researchers. The study, in general, has led to the design of new or improved combustion devices. Although the research into reactions started a long time ago, for examples: Frank-Kamenetskii (1969), Ayeni (1982), William (1985), Buckmaster and Ludford (1992), Okoya (1999), Popoola and Ayeni (2003), Olanrewaju (2005), Olayiwola (2013), but there is need for new study.

Ayeni (1982) presented an asymptotic analysis of a spatially homogeneous model of non-isothermal branched-chain reaction. Of particular interest is the so-called explosion time and he provided an upper bound for it as a function of the activation energy. Okoya (1999) considered the spatially homogeneous form of a reactive system model and employed effective activation energy approach to obtain an analytic expression for the thermal ignition time. Popoola (2007) studied the mathematical theory of two-step Arrhenius reaction and investigated the influence of some rate parameters on the chain reaction. Recently, Makinde *et al*. (2013) studied two-step exothermic reactions with and without reactants consumption subject to Arrhenius kinetic model. They solved the system of equations numerically to account for the effect of various dimensionless parameters.

The objectives of this paper are to examine the properties of the solution of two-step exothermic reactions with Arrhenius kinetics and reactants consumption and obtain an analytical solution for describing the phenomenon.

2. Model Formulation

The basic model scheme follows from the simple chemistry of sequential reaction: $A \xrightarrow{k_1} B \xrightarrow{k_2} C$. We assume that the reaction is not stirred, that is, change depends on space variable and that the initial reactant A participated in two parallel reactions with activation energies E_1 and E_2, and heats of reaction Q_1 and Q_2 respectively. Under these assumptions, the equations describing two-step exothermic reactions with Arrhenius kinetics and reactants consumption are:

$$\frac{\partial X}{\partial t} = D_1 \frac{\partial^2 X}{\partial x^2} - A_1 X\, e^{-\frac{E_1}{RT}} \tag{1}$$

$$\frac{\partial Y}{\partial t} = D_2 \frac{\partial^2 Y}{\partial x^2} - A_2 Y\, e^{-\frac{E_2}{RT}} \tag{2}$$

$$\rho c_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} + A_1 Q_1 X\, e^{-\frac{E_1}{RT}} + A_2 Q_2 Y\, e^{-\frac{E_2}{RT}} \tag{3}$$

The initial and boundary conditions were formulated as follows:

$$\left.\begin{array}{lll} X(x,0) = X_0, & X(0,t) = 0, & X(L,t) = 0 \\ Y(x,0) = Y_0, & Y(0,t) = 0, & Y(L,t) = 0 \\ T(x,0) = T_0, & T(0,t) = T_1, & T(L,t) = T_0 \end{array}\right\}, \tag{5}$$

where X is the concentration of reactant A $(kg/kmol)$, Y is the concentration of reactant B $(kg/kmol)$, t is the time (s), R is the universal gas constant $(Jkmol^{-1}K^{-1})$, A_1, A_2 are the pre-exponential factors of the two reactions (s^{-1}), E_1, E_2 are the activation energies of the two reactions $(J/kmol)$, k is the thermal conductivity, Q_1, Q_2 are the heat of the reactions (J/kg), D_1, D_2 are the diffusion coefficients, c_p is the specific heat capacity at constant pressure $(JK^{-1}kg^{-1})$, ρ is the density (kg/m^3), T is the temperature (K), T_0 is the initial temperature (K), x is the distance (m), X_0 is the initial concentration of reactant A $(kg/kmol)$, Y_0 is the initial concentration of reactant B $(kg/kmol)$.

3. Method of Solution

3.1 Existence and Uniqueness of Solution

Theorem 1: Let $D_1 = D_2 = \dfrac{k}{\rho c_p} = \lambda$. Then the equations (1) – (3) with initial and boundary conditions (4) has a unique solution for all $t \geq 0$.

Proof: Multiply (1) by $\dfrac{Q_1}{\rho c_p}$, (2) by $\dfrac{Q_2}{\rho c_p}$ and adding, we obtain

$$\frac{\partial \varphi}{\partial t} = \lambda \frac{\partial^2 \varphi}{\partial x^2} \tag{5}$$

$$\varphi(x,0) = T_0 + \frac{1}{\rho c_p}(Q_1 X_0 + Q_2 Y_0), \qquad \varphi(0,t) = T_1, \qquad \varphi(L,t) = T_0, \tag{6}$$

where

$$\varphi(x,t) = T(x,t) + \frac{1}{\rho c_p}(Q_1 X(x,t) + Q_2 Y(x,t))$$

Using the eigenfunctions expansion method (where details can be found in Myint-U and Debnath (1987)), we obtain the solution of equations (5) and (6) as

$$\varphi(x,t) = \sum_{n=1}^{\infty} \frac{2}{n\pi}\left(1-(-1)^n\right)\left(T_0 + \frac{1}{\rho c_p}(Q_1 X_0 + Q_2 Y_0)\right)\exp\left(-\lambda\left(\frac{n\pi}{L}\right)^2 t\right)\sin\frac{n\pi}{L}x + \left(T_1 + \frac{x}{L}(T_0 - T_1)\right) \tag{7}$$

Then, we obtain

$$X(x,t) = \frac{\rho c_p}{Q_1}\left(\sum_{n=1}^{\infty} \frac{2}{n\pi}\left(1-(-1)^n\right)\left(T_0 + \frac{1}{\rho c_p}\left(Q_1 X_0 + Q_2 Y_0\right)\right)\exp\left(-\lambda\left(\frac{n\pi}{L}\right)^2 t\right)\sin\frac{n\pi}{L}x + \left(T_1 + \frac{x}{L}(T_0 - T_1)\right) - \left(T(x,t) + \frac{Q_2}{\rho c_p}Y(x,t)\right)\right) \tag{8}$$

$$Y(x,t) = \frac{\rho c_p}{Q_2}\left(T_0 + \sum_{n=1}^{\infty} \frac{2}{n\pi}\left(1-(-1)^n\right)\left(T_0 + \frac{1}{\rho c_p}\left(Q_1 X_0 + Q_2 Y_0\right)\right)\exp\left(-\lambda\left(\frac{n\pi}{L}\right)^2 t\right)\sin\frac{n\pi}{L}x + \left(T_1 + \frac{x}{L}(T_0 - T_1)\right) - \left(T(x,t) + \frac{Q_1}{\rho c_p}X(x,t)\right)\right) \tag{9}$$

$$T(x,t)=\begin{pmatrix} T_0+\sum_{n=1}^{\infty}\frac{2}{n\pi}\left(1-(-1)^n\right)\left(T_0+\frac{1}{\rho c_p}\left(Q_1X_0+Q_2Y_0\right)\right)\exp\left(-\lambda\left(\frac{n\pi}{L}\right)^2 t\right)\sin\frac{n\pi}{L}x+ \\ \left(T_1+\frac{x}{L}\left(T_0-T_1\right)\right)-\frac{1}{\rho c_p}\left(Q_1X(x,t)+Q_2Y(x,t)\right)\end{pmatrix} \tag{10}$$

Hence, there exists a unique solution of problem (1) – (3). This completes the proof.

3.2 Non-dimensionalisation

Here, we substituted equation (8) and equation (9) into equations (1) – (3) and non-dimensionalised, using the following dimensionless variables:

$$\left.\begin{array}{llll} t'=\frac{\lambda t}{L^2}, & x'=\frac{x}{L}, & \phi=\frac{X}{X_0}, & \psi=\frac{Y}{Y_0}, \\ \theta=\frac{(T-T_0)}{\in T_0}, & \gamma=\frac{E_2}{E_1}, & \in=\frac{RT_0}{E_e} & \end{array}\right\}, \tag{11}$$

and we obtain, after dropping prime

$$\frac{\partial\phi}{\partial t}=\frac{\partial^2\phi}{\partial x^2}-\sigma_1\left(\sum_{n=1}^{\infty}a\exp\left(-n^2\pi^2t\right)\sin n\pi x+h(1-x)-b\theta-c\psi\right)e^{\frac{\theta}{1+\in\theta}} \tag{12}$$

$$\frac{\partial\psi}{\partial t}=\frac{\partial^2\psi}{\partial x^2}-\sigma_2\left(\sum_{n=1}^{\infty}d\exp\left(-n^2\pi^2t\right)\sin n\pi x+h_1(1-x)-b_1\theta-f\phi\right)e^{\frac{\gamma\theta}{1+\in\theta}} \tag{13}$$

$$\begin{aligned}\frac{\partial\theta}{\partial t}=\frac{\partial^2\theta}{\partial x^2}&+\delta_1\left(\sum_{n=1}^{\infty}a\exp\left(-n^2\pi^2t\right)\sin n\pi x+h(1-x)-b\theta-c\psi\right)e^{\frac{\theta}{1+\in\theta}}+\\ &\delta_2\left(\sum_{n=1}^{\infty}d\exp\left(-n^2\pi^2t\right)\sin n\pi x+h_1(1-x)-b_1\theta-f\phi\right)e^{\frac{\gamma\theta}{1+\in\theta}}\end{aligned} \tag{14}$$

Together with initial and boundary conditions:

$$\left.\begin{array}{lll} \phi(x,0)=1, & \phi(0,t)=0, & \phi(1,t)=0 \\ \psi(x,0)=1, & \psi(0,t)=0, & \psi(1,t)=0 \\ \theta(x,0)=0, & \theta(0,t)=\theta_*, & \theta(1,t)=0 \end{array}\right\}, \tag{15}$$

where

$$a=\frac{2\rho c_p\left(1-(-1)^n\right)}{n\pi X_0Q_1}\left(T_0+\frac{1}{\rho c_p}\left(Q_1X_0+Q_2Y_0\right)\right),\quad b=\frac{\rho c_p\in T_0}{X_0Q_1},\quad c=\frac{Y_0Q_2}{X_0Q_1},\quad f=\frac{X_0Q_1}{Y_0Q_2},$$

$$d=\frac{2\rho c_p\left(1-(-1)^n\right)}{n\pi Y_0Q_2}\left(T_0+\frac{1}{\rho c_p}\left(Q_1X_0+Q_2Y_0\right)\right),\quad b_1=\frac{\rho c_p\in T_0}{Y_0Q_2},\quad \theta_*=\frac{T_1-T_0}{\in T_0},$$

$\delta_1 = \dfrac{A_1 X_0 Q_1 L^2 e^{-\frac{1}{\epsilon}}}{\rho c_p \in T_0 \lambda}$ = Frank-Kamenetskii parameter, $\delta_2 = \dfrac{A_2 Y_0 Q_2 L^2 e^{-\frac{\gamma}{\epsilon}}}{\rho c_p \in T_0 \lambda}$ = Frank-Kamenetskii parameter, $\sigma_1 = \dfrac{A_1 L^2}{\lambda} e^{-\frac{1}{\epsilon}}$, $\sigma_2 = \dfrac{A_2 L^2}{\lambda} e^{-\frac{\gamma}{\epsilon}}$, $h = \dfrac{\rho c_p (T_1 - T_0)}{X_0 Q_1}$, $h_1 = \dfrac{\rho c_p (T_1 - T_0)}{Y_0 Q_2}$

Equations (12) – (15) will be considered in three forms and we shall examine the properties of the solution of these problems.

3.3 <u>Problem</u> 1: *A non-stirred reactions with reactants consumption.*

For non-stirred reactions with reactants consumption, let equations (12) – (15) be written as

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} - \sigma_1 (ag + hq - b\theta - c\psi) e^{\frac{\theta}{1+\epsilon\theta}} \tag{16}$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2} - \sigma_2 (dg + h_1 q - b_1\theta - f\phi) e^{\frac{\gamma\theta}{1+\epsilon\theta}} \tag{17}$$

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2} + \delta_1 (ag + hq - b\theta - c\psi) e^{\frac{\theta}{1+\epsilon\theta}} + \delta_2 (dg + h_1 q - b_1\theta - f\phi) e^{\frac{\gamma\theta}{1+\epsilon\theta}} \tag{18}$$

where

$$g = g(x,t) = \sum_{n=1}^{\infty} \exp(-n^2 \pi^2 t) \sin n\pi x, \qquad q = q(x) = (1 - x)$$

3.3.1 Properties of Solution

Theorem 2: Let $\epsilon > 0$, $a = b = d = b_1 = h = h_1 = \gamma = 1$ and $c = f = 0$ in (18). Then $\theta(x,t) \geq 0$ for $(x,t) \in (0,\infty) \times (0,t_0)$, $t_0 > 0$. In the proof, we shall make use of the following Lemma of Kolodner and Pederson (1966).

Lemma (Kolodner and Pederson (1966)) Let $u(x,t) = 0\left(e^{\alpha |x|^2}\right)$ be a solution on $R^n \times [0,t)$ of the differential inequality $\dfrac{\partial u}{\partial t} - \Delta u + K(x,t)u \geq 0$, where K is bounded from below. If $u(x,0) \geq 0$, then $u(x,t) \geq 0$ for all $(x,t) \in R^n \times [0,t_0)$.

Proof of Theorem 2: Let $\epsilon > 0$, $a = b = d = b_1 = h = h_1 = \gamma = 1$ and $c = f = 0$ in (18). We obtain

$$\frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} + (\delta_1 + \delta_2) e^{\frac{\theta}{1+\epsilon\theta}} \theta = (\delta_1 + \delta_2)(g + q) e^{\frac{\theta}{1+\epsilon\theta}}$$

That is

$$\frac{\partial\theta}{\partial t}-\frac{\partial^2\theta}{\partial x^2}+(\delta_1+\delta_2)e^{\frac{\theta}{1+\epsilon\theta}}\theta\geq 0, \qquad \text{since} \quad (\delta_1+\delta_2)(g+q)e^{\frac{\theta}{1+\epsilon\theta}}\geq 0.$$

This can be written as

$$\frac{\partial\theta}{\partial t}-\frac{\partial^2\theta}{\partial x^2}+K(x,t)\theta\geq 0$$

where

$$K(x,t)=(\delta_1+\delta_2)e^{\frac{\theta}{1+\epsilon\theta}}$$

Hence, by Kolodner and Pederson's lemma $\theta(x,t)\geq 0$. This completes the proof.

Theorem 3: Let $\epsilon>0$, $a=b=d=b_1=h=h_1=\sigma_1=\sigma_2=\delta_1=\delta_2=\gamma=1$ and $c=f=0$ in (16) - (18). Then $\frac{\partial\phi}{\partial t}\geq 0$, $\frac{\partial\psi}{\partial t}\geq 0$ and $\frac{\partial\theta}{\partial t}\geq 0$.

Proof: Let $\epsilon>0$, $a=b=d=b_1=h=h_1=\sigma_1=\sigma_2=\delta_1=\delta_2=\gamma=1$ and $c=f=0$ in (16) - (18). We obtain

$$\frac{\partial\phi}{\partial t}-\frac{\partial^2\phi}{\partial x^2}+(g+q-\theta)e^{\frac{\theta}{1+\epsilon\theta}}=0$$

$$\frac{\partial\psi}{\partial t}-\frac{\partial^2\psi}{\partial x^2}+(g+q-\theta)e^{\frac{\theta}{1+\epsilon\theta}}=0$$

$$\frac{\partial\theta}{\partial t}-\frac{\partial^2\theta}{\partial x^2}-2(g+q-\theta)e^{\frac{\theta}{1+\epsilon\theta}}=0$$

Differentiating with respect to t, we have

$$\frac{\partial}{\partial t}\left(\frac{\partial\phi}{\partial t}\right)-\frac{\partial^2}{\partial x^2}\left(\frac{\partial\phi}{\partial t}\right)=\left(\frac{\partial\theta}{\partial t}-\frac{\partial g}{\partial t}+(\theta-g-q)\left(\frac{1}{1+\epsilon\theta}\right)^2\frac{\partial\theta}{\partial t}\right)e^{\frac{\theta}{1+\epsilon\theta}}$$

$$\frac{\partial}{\partial t}\left(\frac{\partial\psi}{\partial t}\right)-\frac{\partial^2}{\partial x^2}\left(\frac{\partial\psi}{\partial t}\right)=\left(\frac{\partial\theta}{\partial t}-\frac{\partial g}{\partial t}+(\theta-g-q)\left(\frac{1}{1+\epsilon\theta}\right)^2\frac{\partial\theta}{\partial t}\right)e^{\frac{\theta}{1+\epsilon\theta}}$$

$$\frac{\partial}{\partial t}\left(\frac{\partial\theta}{\partial t}\right)-\frac{\partial^2}{\partial x^2}\left(\frac{\partial\theta}{\partial t}\right)+2\left(1-(g+q-\theta)\left(\frac{1}{1+\epsilon\theta}\right)^2\right)e^{\frac{\theta}{1+\epsilon\theta}}\frac{\partial\theta}{\partial t}=2\frac{\partial g}{\partial t}e^{\frac{\theta}{1+\epsilon\theta}}$$

Let

$u=\frac{\partial\phi}{\partial t}$, $v=\frac{\partial\phi}{\partial t}$ and $w=\frac{\partial\theta}{\partial t}$

Then

$$\frac{\partial u}{\partial t}-\frac{\partial^2 u}{\partial x^2}\geq 0$$

$$\frac{\partial v}{\partial t}-\frac{\partial^2 v}{\partial x^2}\geq 0$$

$$\frac{\partial w}{\partial t}-\frac{\partial^2 w}{\partial x^2}+2\left(1-(g+q-\theta)\left(\frac{1}{1+\in\theta}\right)^2\right)e^{\frac{\theta}{1+\in\theta}}w\geq 0$$

This can be written

$$\frac{\partial u}{\partial t}-\frac{\partial^2 u}{\partial x^2}+K_1(x,t)u\geq 0$$

$$\frac{\partial v}{\partial t}-\frac{\partial^2 v}{\partial x^2}+K_2(x,t)v\geq 0$$

$$\frac{\partial w}{\partial t}-\frac{\partial^2 w}{\partial x^2}+K_3(x,t)w\geq 0$$

where

$$K_1(x,t)=0,\qquad K_2(x,t)=0,\qquad K_3(x,t)=2\left(1-(g+q-\theta)\left(\frac{1}{1+\in\theta}\right)^2\right)e^{\frac{\theta}{1+\in\theta}}$$

Clearly, K_1 and K_2 are bounded everywhere and K_3 is bounded from below. Hence by Kolodner and Pederson's lemma $u(x,t)\geq 0$, $v(x,t)\geq 0$ and $w(x,t)\geq 0$ i.e., $\frac{\partial\phi}{\partial t}\geq 0$, $\frac{\partial\psi}{\partial t}\geq 0$ and $\frac{\partial\theta}{\partial t}\geq 0$. This completes the proof.

3.4 <u>Problem</u> 2: *A steady-state reactions with reactants consumption.*

For steady-state reactions with reactants consumption, equations (12) – (15) reduce to

$$\frac{d^2\phi}{dx^2}-\sigma_1(ag+hq-b\theta-c\psi)e^{\frac{\theta}{1+\in\theta}}=0 \tag{19}$$

$$\frac{d^2\psi}{dx^2}-\sigma_2(dg+h_1q-b_1\theta-f\phi)e^{\frac{\gamma\theta}{1+\in\theta}}=0 \tag{20}$$

$$\frac{d^2\theta}{dx^2}+\delta_1(ag+hq-b\theta-c\psi)e^{\frac{\theta}{1+\in\theta}}+\delta_2(dg+h_1q-b_1\theta-f\phi)e^{\frac{\gamma\theta}{1+\in\theta}}=0 \tag{21}$$

where

$$g=g(x)=\sum_{n=1}^{\infty}\sin n\pi x,\qquad q=q(x)=(1-x)$$

3.4.1 Properties of Solution

Theorem 4: Let $\in \to 0,\ a = b = d = b_1 = h = h_1 = 0,\ \ c = f = -1$ and $\phi = \psi = \gamma = 1$ in (19) – (21). Then $\theta(x)$ is symmetric about $x = \frac{1}{2}$.

Proof: Let $\in \to 0,\ a = b = d = b_1 = h = h_1 = 0,\ \ c = f = -1$ and $\phi = \psi = \gamma = 1$ in (19) – (21). We obtain

$$\frac{d^2\theta(x)}{dx^2} + (\delta_1 + \delta_2)e^{\theta(x)} = 0, \qquad \theta(0) = 0, \qquad \theta(1) = 0$$

Let $y = 2x - 1$

Then

$$\frac{d^2}{dx^2} = 4\frac{d^2}{dy^2}$$

So the problem becomes

$$\frac{d^2\theta(y)}{dy^2} + \frac{(\delta_1 + \delta_2)}{4}e^{\theta(y)} = 0, \qquad \theta(-1) = 0, \qquad \theta(1) = 0.$$

It suffices to show that $\theta(-y) = \theta(y)$. Replace y by $-y$. We obtain

$$\frac{d^2\theta(-y)}{d(-y)^2} + \frac{(\delta_1 + \delta_2)}{4}e^{\theta(-y)} = 0$$

Hence θ is symmetric about $y = 0$ i.e. θ is symmetric about $x = \frac{1}{2}$. This completes the proof.

Theorem 5: Let $\in \to 0,\ a = b = d = b_1 = h = h_1 = 0,\ \ c = f = -1$ and $\phi = \psi = \gamma = 1$ in (19) – (21). Then $\theta'\left(\frac{1}{2}\right) = 0$.

Proof: Let $\in \to 0,\ a = b = d = b_1 = h = h_1 = 0,\ \ c = f = -1$ and $\phi = \psi = \gamma = 1$ in (19) – (21). We obtain

$$\frac{d^2\theta(x)}{dy^2} + (\delta_1 + \delta_2)e^{\theta(x)} = 0, \qquad \theta(0) = 0, \qquad \theta(1) = 0$$

Since $\theta(x)$ is symmetric about $x = \frac{1}{2}$. Then $\theta'\left(\frac{1}{2}\right) = 0$. This completes the proof.

Theorem 6: Let $\in \to 0,\ a = b = d = b_1 = h = h_1 = 0,\ \ c = f = -1$ and $\phi = \psi = \gamma = 1$ in (19) – (21). Then $\theta'(x) > 0$ for $x \in \left(0, \frac{1}{2}\right)$.

Proof: Let $\in \to 0,\ a = b = d = b_1 = h = h_1 = 0,\ \ c = f = -1$ and $\phi = \psi = \gamma = 1$ in (19) – (21). We obtain

$$\frac{d^2\theta(x)}{dx^2} = -(\delta_1 + \delta_2)e^{\theta(x)}, \qquad \theta(0) = 0, \qquad \theta(1) = 0$$

Using Ayeni (1978), we obtain

$$\theta(x) = (\delta_1 + \delta_2)\int_0^{\frac{1}{2}} k(x,t)e^{\theta(t)}dt,$$

where

$$k(x,t) = \begin{cases} x, & 0 \le x \le t \\ t, & t \le x \le \frac{1}{2} \end{cases}$$

So

$$\theta'(x) = (\delta_1 + \delta_2)\left[x e^{\theta(x)} + \int_x^{\frac{1}{2}} e^{\theta(t)}dt - x e^{\theta(x)} \right] = (\delta_1 + \delta_2)\int_x^{\frac{1}{2}} e^{\theta(t)}dt$$

Hence, $\theta(x)$ is strictly monotonically increasing for $x \in \left(0, \frac{1}{2}\right)$. This completes the proof.

3.5 <u>Problem</u> 3: *A well-stirred reactions with reactants consumption.*

For well-stirred reactions with reactants consumption, equations (12) – (15) reduce to

$$\frac{\partial \phi}{\partial t} = \sigma_1(b\theta + c\psi + h)e^{\frac{\theta}{1+\epsilon\theta}} \qquad (22)$$

$$\frac{\partial \psi}{\partial t} = \sigma_2(b_1\theta + f\phi + h_1)e^{\frac{\gamma\theta}{1+\epsilon\theta}} \qquad (23)$$

$$\frac{\partial \theta}{\partial t} = -\delta_1(b\theta + c\psi + h)e^{\frac{\theta}{1+\epsilon\theta}} - \delta_2(b_1\theta + f\phi + h_1)e^{\frac{\gamma\theta}{1+\epsilon\theta}} \qquad (24)$$

3.5.1 Properties of Solution

Theorem 7: Let $\epsilon \to 0$, $b = b_1 = h = h_1 = 0$, $c = f = -1$ and $\phi = \psi = \gamma = 1$ in (22) – (24). Then $t = \frac{1}{(\delta_1 + \delta_2)}$ for $\theta(t) \to \infty$.

Proof: Let $\epsilon \to 0$, $b = b_1 = h = h_1 = 0$, $c = f = -1$ and $\phi = \psi = \gamma = 1$ in (22) – (24). We obtain

$$\frac{d\theta(t)}{dt} = (\delta_1 + \delta_2)e^{\theta(t)}, \qquad \theta(0) = 0$$

Integrating with respect to t, we obtain the temperature of the reactants as

$$\theta(t) = -\ln(1 - (\delta_1 + \delta_2)t)$$

Then

$$t = \frac{1}{(\delta_1 + \delta_2)} \qquad as \qquad \theta(t) \to \infty$$

where t is the time for ignition to occur. This completes the proof.

3.6 Analytical Solution

Here, we consider problem 1 and 3 when $\in \to 0$. Ayeni (1982 has shown that $\exp(\theta)$ can be approximated as $1 + (e-2)\theta + \theta^2$. In our analysis, we are interested in an approximation of the form:

$$\exp(\theta) \approx 1 + (\exp(1) - 2)\theta = 1 + (e-2)\theta \tag{25}$$

Using parameter-expanding method (where details can be found in He (2006)) and eigenfunctions expansion technique (where details can be found in Myint-U and Debnath (1987)), we obtain the solution of problem 1 and 3 respectively as

Problem 1:

$$\theta(x,t) = \theta_*(1-x) + \sum_{n=1}^{\infty} \frac{2A\theta_*}{qn\pi}\left(e^{-q_0 t} - 1\right)\sin n\pi x +$$

$$(e-2)\sum_{n=1}^{\infty}\left(\begin{array}{l} \sum_{n=1}^{\infty} BB_{12}\left(e^{-q_1 t} - e^{-q_0 t}\right) + \frac{A_{12}}{q_0}\left(1 - e^{-q_0 t}\right) - \sum_{n=1}^{\infty} A_5 \left(\begin{array}{l} te^{-q_0 t} - \\ \frac{1}{q_0}\left(1 - e^{-q_0 t}\right)\end{array}\right) - \\ \sum_{n=1}^{\infty} A_6 \sum_{n=1}^{\infty} A_7 \left(\frac{1}{q_0} - \frac{1}{q_0} e^{-2q_0 t} - 2te^{-q_0 t}\right) - \\ \sum_{n=1}^{\infty}\left(\begin{array}{l} A_8\left(B_{12}\left(e^{-q_1 t} - e^{-q_0 t}\right) - \frac{1}{q_0}\left(1 - e^{-q_0 t}\right)\right) + A_9 B_{12}\left(e^{-q_1 t} - e^{-q_0 t}\right) + \\ \sum_{n=1}^{\infty}\left(A_{10}\left(te^{-q_0 t} - B_{12}\left(e^{-q_1 t} - e^{-q_0 t}\right)\right) - A_{11}\left(\begin{array}{l}\frac{1}{q_0}\left(1 - e^{-q_0 t}\right) - \\ B_{12}\left(e^{-q_1 t} - e^{-q_0 t}\right)\end{array}\right)\right)\end{array}\right)\end{array}\right)\sin n\pi x$$

(26)

$$\phi(x,t) = \sum_{n=1}^{\infty}\left(B_6 e^{-q_1 t} + B_9\left(e^{-q_1 t} - 1\right) + \sum_{n=1}^{\infty}\left(B_{10}\left(e^{-q_0 t} - e^{-q_1 t}\right) - B_{11}\left(1 - e^{-q_1 t}\right)\right)\right)\sin n\pi x +$$

$$(e-2)\left(\sum_{n=1}^{\infty}\left(e^{-q_1 t}\left(\begin{array}{l}\sum_{n=1}^{\infty}\frac{\sigma_1 s_2}{q_1}\left(1 - e^{q_1 t}\right) + \frac{2\sigma_1 s_5}{q_1 n\pi}\left(1 - e^{q_1 t}\right) + g_1(t) + \\ g_2(t) + g_3(t)\end{array}\right)\right)\sin n\pi x\right) \tag{27}$$

$$\psi(x,t)=\sum_{n=1}^{\infty}\left(B_6e^{-q_1t}+B_5\left(e^{-q_1t}-1\right)+\sum_{n=1}^{\infty}\left(B_7\left(e^{-qt}-e^{-q_1t}\right)-B_8\left(1-e^{-q_1t}\right)\right)\right)\sin n\pi x+$$
$$(e-2)\left(\sum_{n=1}^{\infty}\left(e^{-q_1t}\left(\begin{array}{l}\sum_{n=1}^{\infty}\frac{\sigma_2s_3}{q_1}\left(1-e^{q_1t}\right)+\frac{2\sigma_2s_6}{q_1n\pi}\left(1-e^{q_1t}\right)+g_4(t)+\\ g_5(t)+g_6(t)\end{array}\right)\right)\sin n\pi x\right) \quad (28)$$

where

$$g_1(t)=\sigma_1b\left(\begin{array}{l}\frac{B_1}{q_1}\left(e^{-q_1t}-1\right)+\sum_{n=1}^{\infty}B_2\left(B_{12}\left(1-e^{(q_1-q_0)t}\right)-\frac{1}{q_1}\left(e^{q_1t}-1\right)\right)+\\ \sum_{n=1}^{\infty}B_3\sum_{n=1}^{\infty}B_4\left(B_{13}\left(e^{(q_1-2q_0)t}-1\right)+2B_{12}\left(e^{(q_1-q_0)t}-1\right)+\frac{1}{q_1}\left(e^{q_1t}-1\right)\right)\end{array}\right)$$

$$g_2(t)=\sigma_1b\left(\sum_{n=1}^{\infty}\left(\begin{array}{l}\sum_{n=1}^{\infty}BB_{12}\left(t-B_{12}\left(1-e^{(q_1-q_0)t}\right)\right)+\frac{A_{12}}{q_0}\left(\frac{1}{q_1}\left(e^{q_1t}-1\right)-B_{12}\left(1-e^{(q_1-q_0)t}\right)\right)-\\ \sum_{n=1}^{\infty}\sum_{n=1}^{\infty}A_5\left(B_{12}^2\left(1-e^{(q_1-q_0)t}\right)-B_{12}te^{(q_1-q_0)t}-\frac{1}{q_0}\left(\begin{array}{l}\frac{1}{q_1}\left(e^{q_1t}-1\right)-\\ B_{12}\left(1-e^{(q_1-q_0)t}\right)\end{array}\right)\right)-\\ \sum_{n=1}^{\infty}A_6\sum_{n=1}^{\infty}A_7\left(\begin{array}{l}B_{14}\left(1-e^{(q_1-2q_0)t}\right)-2\left(B_{12}^2\left(1-e^{(q_1-q_0)t}\right)-B_{12}te^{(q_1-q_0)t}\right)+\\ \frac{1}{q_0q_1}\left(e^{q_1t}-1\right)\end{array}\right)-f(t)\end{array}\right)\right)$$

$$g_3(t)=\sigma_1s_1\left(\sum_{n=1}^{\infty}\left(B_5\left(t-\frac{1}{q_1}\left(e^{q_1t}-1\right)\right)+B_6t+\sum_{n=1}^{\infty}\left(\begin{array}{l}B_7\left(B_{12}\left(1-e^{(q_1-q_0)t}\right)-t\right)-\\ B_8\left(\frac{1}{q_1}\left(e^{q_1t}-1\right)-t\right)\end{array}\right)\right)\right)$$

$$g_4(t)=\sigma_2b_1\gamma\left(\begin{array}{l}\frac{B_1}{q_1}\left(e^{q_1t}-1\right)+\sum_{n=1}^{\infty}B_2\left(B_{12}\left(1-e^{(q_1-q_0)t}\right)-\frac{1}{q_1}\left(e^{q_1t}-1\right)\right)+\\ \sum_{n=1}^{\infty}B_3\sum_{n=1}^{\infty}B_4\left(B_{13}\left(e^{(q_1-2q_0)t}-1\right)+2B_{12}\left(e^{(q_1-q_0)t}-1\right)+\frac{1}{q_1}\left(e^{q_1t}-1\right)\right)\end{array}\right)$$

$$g_5(t) = \sigma_2 b_1 \left(\sum_{n=1}^{\infty} \left(\begin{array}{l} \sum_{n=1}^{\infty} BB_{12}\left(t - B_{12}\left(1 - e^{(q_1-q_0)t}\right)\right) + \frac{A_{12}}{q_0}\left(\frac{1}{q_1}\left(e^{q_1 t} - 1\right) - B_{12}\left(1 - e^{(q_1-q_0)t}\right)\right) - \\ \sum_{n=1}^{\infty} A_5 \left(B_{12}^2\left(1 - e^{(q_1-q_0)t}\right) - B_{12} t e^{(q_1-q_0)t} - \frac{1}{q_0}\left(\begin{array}{l} \frac{1}{q_1}\left(e^{q_1 t} - 1\right) - \\ B_{12}\left(1 - e^{(q_1-q_0)t}\right) \end{array} \right) \right) - \\ \sum_{n=1}^{\infty} A_6 \sum_{n=1}^{\infty} A_7 \left(\begin{array}{l} B_{14}\left(1 - e^{(q_1-2q_0)t}\right) - 2\left(B_{12}^2\left(1 - e^{(q_1-q_0)t}\right) - B_{12} t e^{(q_1-q_0)t}\right) + \\ \frac{1}{q_0 q_1}\left(e^{q_1 t} - 1\right) \end{array} \right) - f(t) \end{array} \right) \right)$$

$$g_6(t) = \sigma_2 s_4 \left(\sum_{n=1}^{\infty} \left(B_9\left(t - \frac{1}{q_1}\left(e^{q_1 t} - 1\right)\right) + B_6 t + \sum_{n=1}^{\infty} \left(\begin{array}{l} B_{10}\left(B_{12}\left(1 - e^{(q_1-q_0)t}\right) - t\right) - \\ B_{11}\left(\frac{1}{q_1}\left(e^{q_1 t} - 1\right) - t\right) \end{array} \right) \right) \right)$$

$$f(t) = \sum_{n=1}^{\infty} \left(A_8 \left(\begin{array}{l} B_{12}\left(t - B_{12}\left(1 - e^{(q_1-q_0)t}\right)\right) - \frac{1}{q_0}\left(\frac{1}{q_1}\left(e^{q_1 t} - 1\right) - B_{12}\left(1 - e^{(q_1-q_0)t}\right)\right) + \\ A_9 B_{12}\left(t - B_{12}\left(1 - e^{(q_1-q_0)t}\right)\right) + h(t) \end{array} \right) \right)$$

$$h(t) = \sum_{n=1}^{\infty} \left(\begin{array}{l} A_{10}\left(B_{12}^2\left(1 - e^{(q_1-q_0)t}\right) - B_{12} t e^{(q_1-q_0)t} - B_{12}\left(t - B_{12}\left(1 - e^{(q_1-q_0)t}\right)\right)\right) - \\ A_{11}\left(\frac{1}{q_0}\left(\frac{1}{q_1}\left(e^{q_1 t} - 1\right) - B_{12}\left(1 - e^{(q_1-q_0)t}\right)\right) - B_{12}\left(t - B_{12}\left(1 - e^{(q_1-q_0)t}\right)\right)\right) \end{array} \right)$$

$A=(\delta_1 b+\delta_2 b_1),\quad q_0=A+n^2\pi^2,\quad A_1=\sigma_1 b,\quad A_2=\sigma_2 b_1,\quad B_5=\frac{2A_2\theta_*}{n^3\pi^3},$

$B_6=\frac{2\left(1-(-1)^n\right)}{n\pi},\quad q_0=n^2\pi^2,\quad B_7=\frac{2AA_2\theta_*}{q_0 n\pi(q_1-q_0)},\quad B_8=\frac{2AA_2\theta_*}{q_0 n\pi q_1},\quad B_9=\frac{2A_1\theta_*}{n^3\pi^3},$

$B_{10}=\frac{2AA_1\theta_*}{q_0 n\pi(q_1-q_0)},\quad B_{11}=\frac{2AA_1\theta_*}{q_0 n\pi q_1},\quad B_{12}=\frac{1}{q_0-q_1},\quad B=(\delta_1 s_2+\delta_2 s_3),$

$C=(\delta_1 s_5+\delta_2 s_6),\quad D=(\delta_1 b+\delta_2 b_1\gamma),\quad A_3=\frac{2C}{n\pi},\ A_4=\frac{2D\theta_*^2\left(n^2\pi^2-2+2(-1)^n\right)}{n^3\pi^3},$

$A_5=\frac{4AD\theta_*^2\left(n^2\pi^2-1+(-1)^{2n}\right)}{2q_0 n^3\pi^3},\quad A_6=\frac{2AD}{q_0 n\pi},\quad A_7=\frac{4A\theta_*^2\left(2-3(-1)^n+(-1)^{3n}\right)}{3q_0 n^2\pi^2},$

$A_8=\frac{2\theta_*(A_2\delta_1 s_1+A_1\delta_2 s_4)}{n^3\pi^3},\quad A_9=B_6(\delta_1 s_1+\delta_2 s_4),\quad A_{10}=\frac{2A\theta_*(A_2\delta_1 s_1+A_1\delta_2 s_4)}{q_0 n\pi(q_1-q_0)},$

$A_{11}=\frac{2A\theta_*(A_2\delta_1 s_1+A_1\delta_2 s_4)}{q_0 n\pi q_1},\quad A_{12}=(A_3-A_4),\quad B_1=\frac{2\theta_*^2\left(n^2\pi^2-2+2(-1)^n\right)}{n^3\pi^3},$

$B_2=\frac{4A\theta_*^2\left(n^2\pi^2-1+(-1)^{2n}\right)}{2q_0 n^3\pi^3},\quad B_3=\frac{2A}{q_0 n\pi},\quad B_4=\frac{4A\theta_*^2\left(2-3(-1)^n+(-1)^{3n}\right)}{3q_0 n^2\pi^2},$

$B_{13}=\frac{1}{(q_1-2q_0)},\quad B_{14}=\frac{1}{q_0(q_1-2q_0)},\quad p=(e-2),\quad s_1=\frac{c}{p},\quad s_2=\frac{a}{p},\quad s_3=\frac{d}{p},\quad s_4=\frac{f}{p},$

$s_5=\frac{h}{p},\quad s_6=\frac{h_1}{p}$

Problem 2:

$$\theta(t)=\frac{B}{A}\left(e^{-At}-1\right)+(e-2)\begin{pmatrix} A_1\left(\frac{1}{A}\left(1-e^{-At}\right)-2te^{-At}-\frac{1}{A}\left(e^{-2At}-e^{-At}\right)\right)+ \\ B_1\left(\frac{1}{A}\left(1-e^{-At}\right)-te^{-At}\right)- \\ (A_2+B_2)\left(\frac{1}{A}\left(1-e^{-At}\right)-t+\frac{1}{A}\left(1-e^{-At}\right)-te^{-At}\right)- \\ (A_3+B_3)\left(\frac{1}{A}t-\frac{1}{A^2}\left(1-e^{-At}\right)\right) \end{pmatrix}, \tag{29}$$

$$\phi(t)=1+(e-2)\left(r(c+h)t+\frac{rbB}{A^2}\left(1-At-e^{-At}\right)\right) \tag{30}$$

$$\psi(t)=1+(e-2)\left(s(f+h_1)t+\frac{sb_1B}{A^2}\left(1-At-e^{-At}\right)\right) \tag{31}$$

where

$p=(e-2),\quad r=\frac{\sigma_1}{p},\quad s=\frac{\sigma_2}{p},\quad A=(\delta_1 b+\delta_2 b_1),\quad B=(\delta_1(c+h)+\delta_2(f+h_1)),$

$A_1=\frac{B^2(\delta_1 b+\delta_2 b_1\gamma)}{A^2},\quad B_1=\frac{B(\delta_1(c+h)+\delta_2(f+h_1)\gamma)}{A},\quad A_2=\frac{B\delta_1 scb_1}{A^2},$

$B_2=\frac{B\delta_2 frb}{A^2},\quad A_3=\delta_1 sc(f+h_1),\quad B_3=\delta_2 r(c+h)f$

The computations were done using computer symbolic algebraic package MAPLE.

4. Results and Discussion

The systems of coupled nonlinear partial differential equations governing two-step exothermic sequential reactions with Arrhenius kinetics and reactant consumption are solved analytically using parameter-expanding method, direct integration and eigenfunctions expansion technique. In particular, we prove the existence and uniqueness of the solution of the model by actual solution approach. The model formulated is considered in three forms and we examine the properties of the solution of each form. Analytical solutions given by equations (26) - (28) and (29) - (31) are computed using computer symbolic algebraic package MAPLE. The numerical results obtained from direct integration and eigenfunctions expansion technique are shown in Figures. 1 to 6. Figures 1 – 3 is for a non-stirred reaction while figures 4 – 6 is for a well-stirred reaction. The relation between temperature, time and distance is depicted in Figure 1. The relation among the concentration of reactants, time and distance are depicted in Figures 2 and 3. The temperature-time relationships are displayed in Figure 4. The concentration-time relationships are displayed in Figures 5 and 6.

Figure 1 depicts the graph of $\theta(x,t)$ against x and t for different values of γ. It is observed that the temperature of the medium is steady with time and increases and later decreases along distance but does not change much as the ratio of activation energy increases. Figure 2 shows the graph of $\phi(x,t)$ against x and t for different values of γ. It is observed that the concentration of reactant A is steady with time and increases and later decreases along distance but does not change much as the ratio of activation energy increases. Figure 3 displays the graph of $\psi(x,t)$ against x and t for different values of γ. It is observed that the concentration of reactant B is steady with time and increases and later decreases along distance but does not change much as the ratio of activation energy increases.

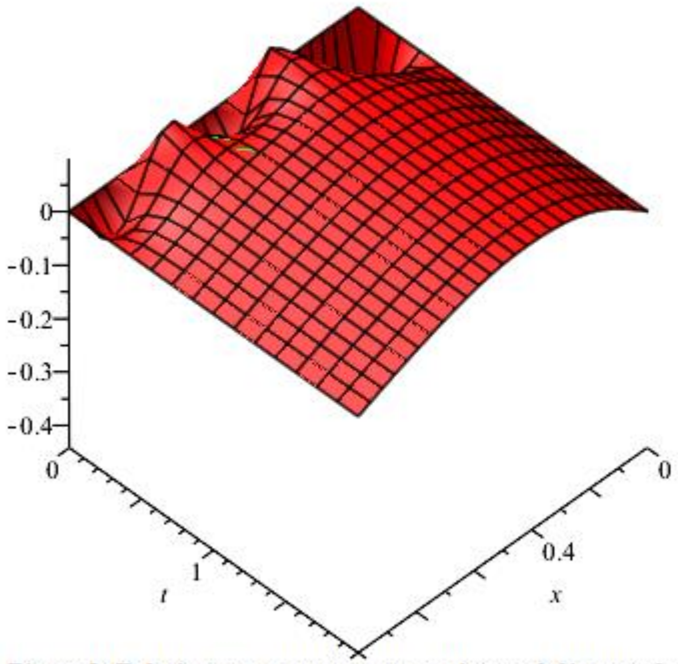

Figure 1: Relation among temperature, time and distance for difference values of γ

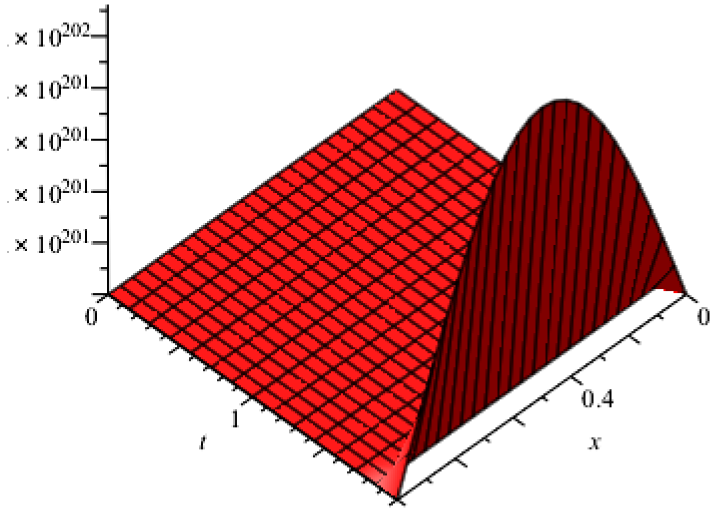

Figure 2: Relation among concentration of reactant A, time and distance for difference values of γ

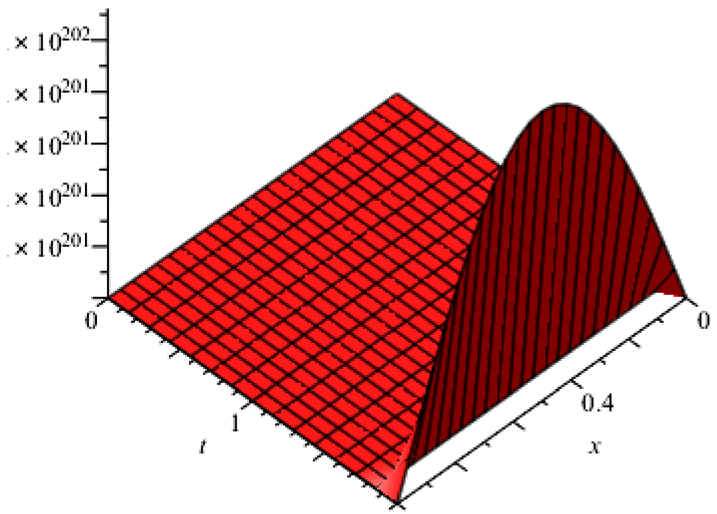

Figure 3: Relation among concentration of reactant B, time and distance for difference values of γ

Figure 4 depicts the graph of $\theta(t)$ against t for different values of γ. It is observed that the temperature of the medium increases and reached steady state with time but increases as the ratio of activation energy increase. Figure 5 shows the graph of $\phi(t)$ against t for different values of γ. It is observed that the concentration of reactant A decreases with time but does not change much as the ratio of activation energy increases. Figure 3 displays the graph of $\psi(t)$ against t for different values of γ. It is observed that the concentration of reactant B decreases with time but does not change much as the ratio of activation energy increases.

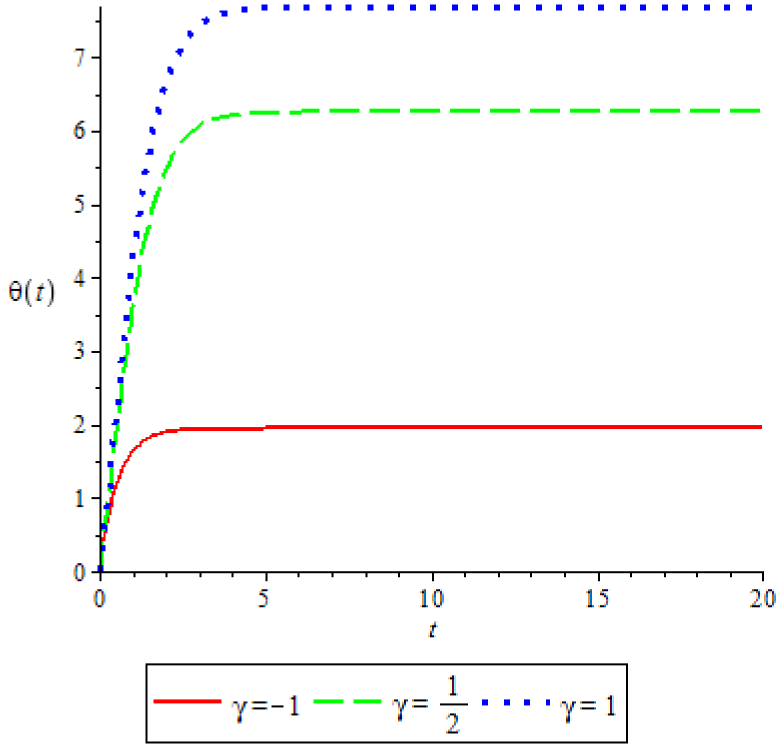

Figure 4: Temperature - time relationships for different values of γ

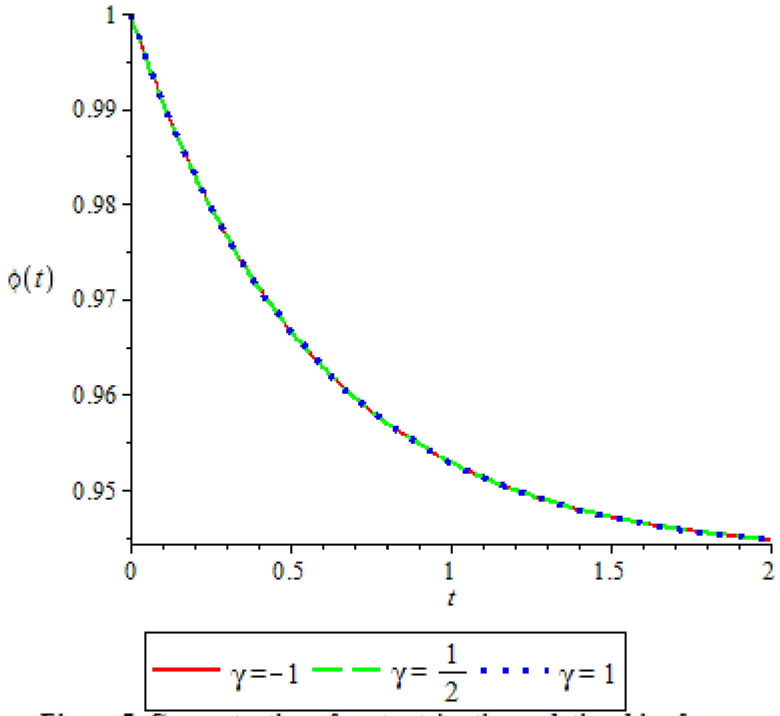

Figure 5: Concentration of reatant A - time relationships for different values of γ

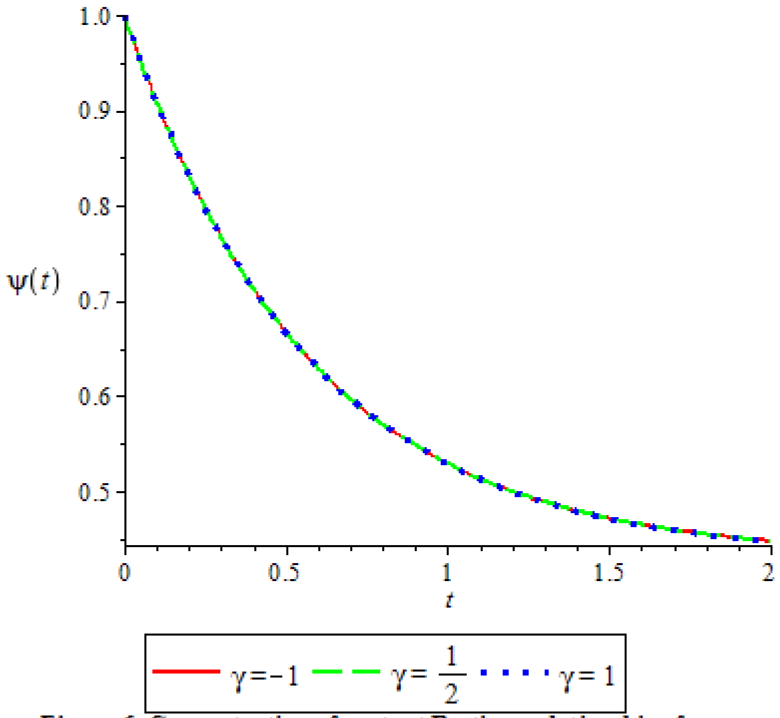

Figure 6: Concentration of reatant B - time relationships for different values of γ

5. Conclusion

This study had delved into the mathematical modeling of two-step exothermic sequential reactions with Arrhenius kinetics and reactant consumption. The governing parameters of the problem are the Frank-Kamenetskii numbers and the ratio of activation energies. The study revealed the following:

1. For non-stirred reactions: (i) temperature of the medium is symmetric about $x = \frac{1}{2}, \quad 0 \le x \le 1$. (ii) temperature of the medium is strictly monotonically increasing for $x \in \left(0, \frac{1}{2}\right)$. (iii) Ratio of activation energies has no significant effects on temperature of the medium and concentration of reactants.
2. For well-stirred reactions: (i) For a large temperature of the medium, when $E_1 = E_2$, the ignition time is equal to the inverse of the sum of Frank-Kamenetskii numbers, that is $t = \frac{1}{\delta_1 + \delta_2} \ \ as \ \ \theta(t) \to \infty$. (ii) the temperature of the medium increases and reached steady state as the ratio of activation energies increases while the ratio of activation energies has no effect on the concentration of reactants A and B.

The results highlighted above showed that the rate of reactants consumption and temperature of the medium could be controlled by activation energies ratio and activation energy parameters. These results are useful in both explosion and combustion industries for regulations and safety purposes.

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