Journal of the Nigerian Association of Mathematical Physics
Volume 10 (November 2006), **403 - 408**
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On the existence and uniqueness result for a two-step reactive-diffusive equation with variable pre-exponential factor

P. O. Olanrewaju, **R. O. Ayeni,**A. O. Ajala,**O. Adebimpe, and *A. O. Ajayi
****Department of Pure and Applied Mathematics , Ladoke Akintola University of Technology, Ogbomoso, Nigeria.**
e-mail: Oladapo_anu@yahoo.ie
***Department of Computer Science and Engineering, Ladoke Akintola University of Technology, Ogbomoso, Nigeria.**

Abstract

We examine the existence and uniqueness result of the steady-state solutions for the exothermic chemical reactions taking the diffusion of the reactants in a slab into account and assuming Arrhenius dependence with variable pre-exponential factor. We establish the criteria's and conditions for existence and uniqueness of solution for the newly formulated problem. It is shown that if $\Gamma \succ o,\ 0 \le x_1 \le 1,\ 0 \le x_2 \le b,$ and $-c \le x_3 \le C,$ where $b, c\ and\ C$ positive constants are then the newly formulated model will have only one solution. We further discovered that there are certain values for n, m, r and β that the problem can accommodate for solution to be stable. Similarly, Frank-Kamenetskii parameters δ_1, δ_2 must not exceed some values for the solution to exist and at the same time stable. Finally, the Frank-Kamenetskii parameter must not exceed the critical value for the solution to have physical implication or application and r must not be large for convergence of the solution (i.e $r < 1$).

Keywords: Exothermic chemical reaction, variable pre-exponential factor, two-step Arrhenius reactions

1.0 Introduction

The present discipline of combustion draws on the field of chemical kinetics, thermodynamics, fluid mechanics, and transport processes. In nature, and particularly in industry, rapid exothermic reaction processes which take place with the evolution of large amount of heat are considerably important. Such processes have long been called combustion processes. The classical examples of combustion are those related to oxidation of organic substances or carbon with atmospheric oxygen i.e the combustion of wood, coal, and petroleum.

Olajuwon (2000) investigated the existence and uniqueness of a power law fluid flowing in a cylinder vessel. They examined the appropriate conditions for a similarity. Of particular interest are the questions of existence and uniqueness of solution.

Adegbie and Ayeni (2003) examined the existence and uniqueness of two-step Arrhenius combustion. They showed that a two-step Arrhenius combustion with finite activation energy has a unique solution. The conditions for the uniqueness of solution was stated and proved.

Olanrewaju and Ayeni (2003) investigated effects of the geometry of vessel on detonations. It is shown that in a non-uniform vessel, maximum temperature occurs at the centre. Also maximum temperature for diverging or converging channel is greater than that of a uniform vessel.

Okoya (2004) examined reactive-diffusive equation with variable pre-exponential factor. He considered the steady-state solutions for the exothermic chemical reaction, taking the diffusion of the reactant in a slab into account and assuming an Arrhenius temperature dependence with variable pre-exponential factor. He solved the resulting nonlinear boundary value problem using both numerical and analytical method. This new analytical solution for the Frank-Kamenetskii parameter δ, as it is in term of Bernoulli's numbers, is in accordance with the numerical integration provided the activation energy parameter ε (<<1) is very small and for ε→ 0 it goes to the well- known

Frank-Kamenetskii case. They determined numerically the transitional values of δ, ε and the dimensionless central temperature θ_m.

2.0 Mathematical formulation

The equation for the temperature $T(x)$ of a one – dimensional slab, with boundaries lying in the coordinate planes $x = \pm a$, may be written in terms of physical variables

$$\lambda \frac{d^2T}{dx^2} + \rho\, Q_1 A\left(\frac{kT}{\nu h\rho}\right)^n \exp\left(-E_1/RT\right) + \rho Q_2 B\left(\frac{kT}{\nu h\rho}\right)^m \exp\left(-\frac{E_2}{RT}\right) = 0 \qquad (2.1)$$

where all the variables and parameters are clearly defined in the nomenclature. We take as the boundary conditions:

$$T = T_0 \quad \text{on } x = \pm a \ ,$$

where T_0 is the initial temperature.

In this model, we neglect the consumption of the combustible material. If $Q_2 = 0$, it has been shown experimentally that the model is able to predict the critical ignition temperature for variety of combustible material (see for example, the data reviewed by Bowes, 1984; Dainton, 1966). By using the non dimensional variable defined by

$$\bar{x} = x/a, \quad \theta = (T - T_0)\left(E/RT_0^2\right), \ \beta = \frac{RT_0}{E_1}, \quad r = E_2/E_1 \qquad (2.2)$$

on equations (2.1) and (2.2) the governing equations are (bar dropped)

$$\frac{d^2\theta}{dx^2} + \delta_1 (1+\beta\theta)^n \exp\left(\theta/1+\beta\theta\right) + \delta_2 (1+\beta\theta)^m \exp\left(r\theta/1+\beta\theta\right) = 0 \qquad (2.3)$$

$$\theta = 0 \ \ on \ \ x = \pm 1 \qquad (2.4)$$

$$where \quad \delta_1 = \frac{a^2 Q_1 E_1\ A\left(kT_0/\nu h\rho\right)^n \exp\left(-E_1/RT_0\right)}{\lambda RT_0^2}, \ \ \delta_2 = \frac{a^2 Q_2\, r\, E_1\ B\left(kT_0/\nu h\rho\right)^m \exp\left(-rE_1/RT_0\right)}{\lambda RT_0^2}$$

In (2.3) δ_1 and δ_2 are the Frank-Kamenetskii parameters which are the measures of the exothermicity of the reactions.

We noted that the factors that control the thermal ignition of combustion materials consisting of the mathematical equations (2.3) and (2.4) is the fundamental importance in many industrial processes (see, for example, Bowes, 1984 for some special cases).

Infact, the greatest temperature for which a low temperature steady distribution is possible is known as the critical ignition temperature or criteria storage temperature (see, for example, Kenneth, 2005). At temperature higher than the critical ignition temperature, thermal ignition will occur (see, for example, Olanrewaju, 2005; Buckmaster and Ludford, 1982).

It has been shown for this problem when $Q_2 = 0$ in the limit of large activation energy ($\beta \to 0$) by Frank-Kamenetskii (1969) that equation (2.3) possesses simple closed – form solution in the form

$$\theta = \theta_m + In \sec h^2 \left(D \pm \sqrt{\delta_1 \exp\left(\theta_m/2x\right)}\right), \qquad (2.5)$$

where θ_m is the dimensionless temperature at the centre of the slab and D is a constant of integration. On employing the boundary condition (2.4), we have

$$\delta_1 = 2\exp\left(-\theta_m\right)\left\{\cosh^{-1}\left(\exp\left(\frac{\theta_m}{2}\right)\right)\right\}^2 \qquad (2.6)$$

In connection with equation (2.3) when $Q_2 = 0$, $\boldsymbol{n} = 0$, it in well known that the reactive – diffusive equation admits perturbation solutions under physically reasonable assumptions (Bowes, 1980; Ward and Van De Velde, 1992) and numerical solutions are available for some realistic conditions; for example, see Burnell et al. (1989). In Billingham (2000) a new set of asymptotic and numerical solutions were constructed for some Biot numbers. Within the admissible parameters range, asymptotic solutions and numerical solutions agree with each other.

Obviously a realistic mathematical description of thermal explosion needs to include the effects of Arrhenius temperature dependence with variable pre-exponential factor (see, for example, Ayeni, 1982, Okoya, 2002).

Here the principal aim of this paper is to extend the work of Okoya (2004) to a two–step reaction and to establish that the new problem has a unique solution when *n*, *m* =-2 corresponding to the sensitized reaction. Okoya (2004) becomes a special case of equation.(2.3). We also determine numerically the transitional values of δ_1 , δ_2, β, m, n and r.

3.0 Method of Solution

Equation (2.3) and (2.4) posses no closed form solution. We employ numerical method called shooting method so as to transform the boundary value problem to an initial value problem. We let

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x \\ \theta \\ \theta^1 \end{pmatrix} \quad (3.1)$$

By differentiating equation (3.1), we have

$$\begin{pmatrix} x_1^1 \\ x_2^1 \\ x_3^1 \end{pmatrix} = \begin{pmatrix} 1 \\ x_3 \\ -[\left[\delta_1 (1+\beta x_2)^n \exp(x_2/1+\beta x_2)\right] + \delta_2 (1+\beta x_2)^m \exp(rx_2/1+\beta x_2)] \end{pmatrix} \quad (3.2)$$

Satisfying the initial conditions

$$\begin{pmatrix} x_1(-1) \\ x_2(-1) \\ x_3(-1) \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ \Gamma \end{pmatrix} \quad (3.3)$$

where $\Gamma = \theta^1(-1)$, the guess values for shooting method.

4.0 Existence and uniqueness of solution

***Theorem* 4.1** (see, for example, Williams et al. 1978)

Let *D* denote the region (*n* (*n* + 1)) dimensional space, one dimension for *t* and *n* dimensions for vector [*x*] $|t - t_0| \leq a$, $\|x - x_0\| \leq b$, if

$$\begin{cases} x_1^1 = f_1(x_1, x_2, \ldots, xn, t), \; x_1(t_0) = x_{10} \\ x_2^1 = f_2(x_1, x_2, \ldots, xn, t), \; x_2(t_0) = x_{20} \\ \vdots \\ x_n^1 = f_n(x_1, x_2, \ldots, xn, t), \; x_n(t_0) = x_{n0} \end{cases} \quad (4.1)$$

Then, the system of equations (4.1) has a unique solution of $\frac{\partial f_i}{\partial x_j}$, $i, j = 1, 2, \ldots, n$ are continuous in *D*. (H1): $\Gamma > 0$, $0 \leq x_1 \leq 1$, $0 \leq x_2 \leq b$, and $c \leq x_3 \leq C$, where *b*, *c* and *C* are positive constants.

***Theorem* 4.2**

If (H1) holds then problem (2.1) has a unique solution satisfying (2.2).

Proof

We let

$$y^1 = \begin{pmatrix} x_1^1 \\ x_2^1 \\ x_3^1 \end{pmatrix} = \begin{pmatrix} g_1(x_1, x_2, x_3) \\ g_2(x_1, x_2, x_3) \\ g_3(x_1, x_2, x_3) \end{pmatrix} \quad (4.2)$$

where $g_1 = 1$, $g_2 = x_3$ and $g_3 = -\left[\delta_1 (1+\beta x_2)^n \exp(x_2/1+\beta x_2) + \delta_2 (1+\beta x_2)^m \exp(x_2/1+\beta x_2)\right]$

Clearly $\dfrac{\partial f_i}{\partial x_j}$ is bounded for i = 1, 2, 3. Thus, g_i, i = 1, 2, 3 are Lipschitz continuous. Hence there exists a unique solutions of equations. (2.1) and (2.2).

5.0 Discussion of numerically generated result.

The results of the numerical analysis generated were used to plot the curses below.

Figure 1 shows the curve of temperature against position x for δ_1 = 0.3064, δ_2 = 0.5721, β =0.001, r = 0.5 and the shooting guess value Γ = 1.18124 for equations (2.3) and (2.4). It is observed that the solution is symmetry and θ_m occur at the centre i.e θ_m = 0.6341 for prescribe Γ.

Figure 2 shows the graph of temperature θ(x) against position x for δ_1=0.3064, δ_2=0.5721, β =0.001, r = 0.8 and the shooting guess value for the solution to be unique is Γ= 1.3945. The solution is symmetry as well as the θ_m = 0.7751 for prescribe Γ.

Figure 3 shows the graph of temperature θ(x) against position x for the same values of δ_1 = 0.3064, δ_2 = 0.5721, β = 0.001 and various values of r. It was shown that at r = 0.8, we have the highest temperature (θ_m) for prescribe Γ. The temperature gradient increase as r increases.

Figure 4 gives the graph of temperature against position x for the same value of δ_1=0.3064, δ_2 = 0.5721, r = 0.5 and various values of β. It is shown that the solution is symmetry and we have the highest temperature. We observed that both have the same turning point. Similarly for β→0 we have the highest value of temperature gradient

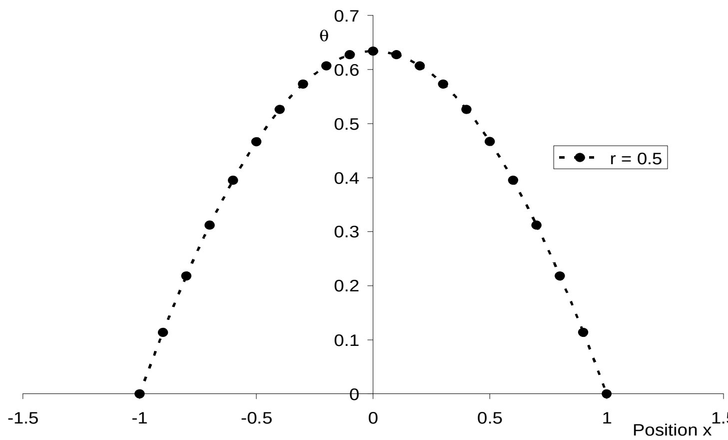

Figure 1: Graph of temperature against position x for δ1 = 0.3064 , δ2 = 0.5721 , β = 0.001 , r = 0.5

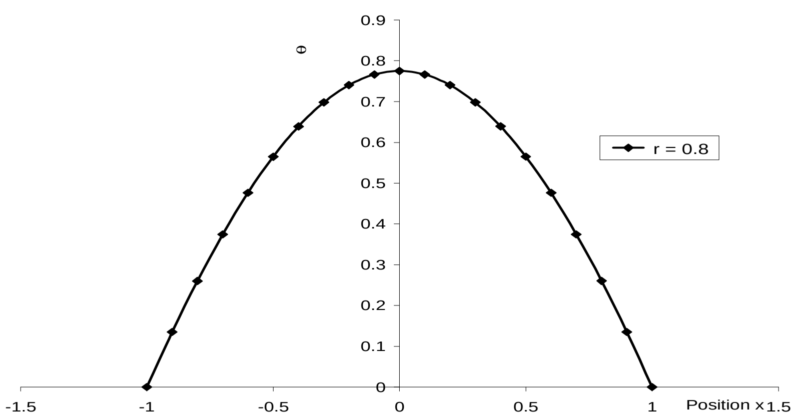

Figure 2: Graph of temperature against position x for δ1 = 0.3064, δ2 = 0.5721, β = 0.001 , r = 0.8

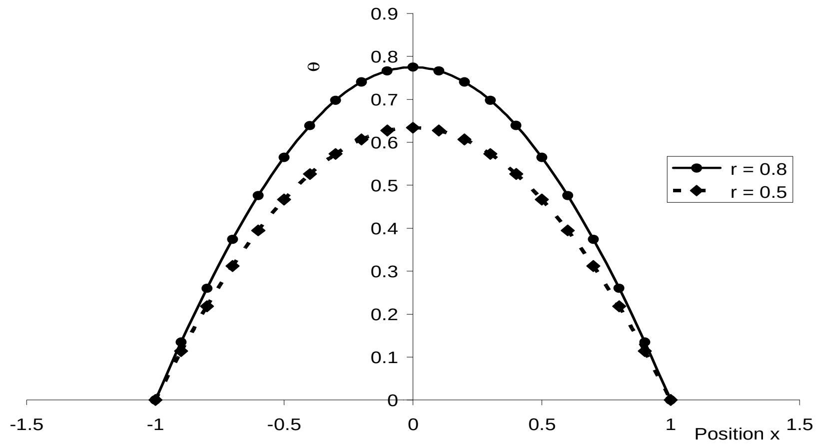

Figure 3: Graph of temperature against position x for the same values of δ1 = 0.3064 , δ2 = 0.5721 ,β = 0.001 and various values of r

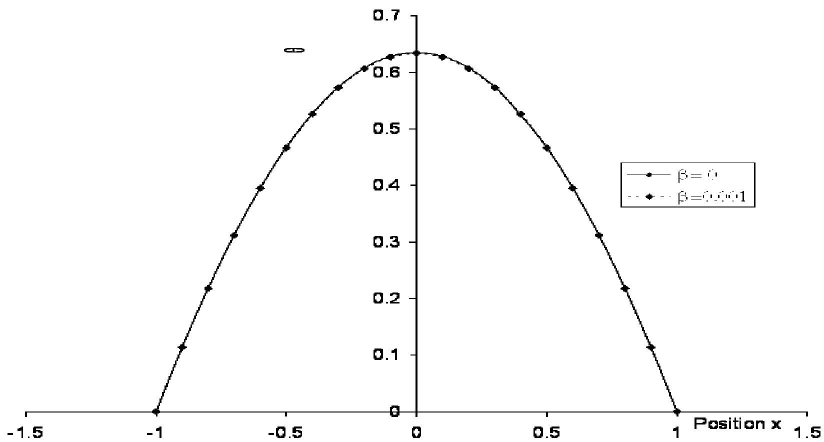

Figure 4: Graph of temperature against position x for the same value of δ1 = 0.3064 , δ2 = 0.5721 , r = 0.5 and various values of β

4.0 Conclusions

Reactive – diffusive equation with variable pre-exponential factor for two-step Arrhenius reactions was examined in this present work. The investigations were conducted numerically by using shooting technique. The method was used to convert the boundary value problem to an initial value problem.

We further established that the solution exists and is unique (when the derivative is prescribed) for some values of δ_1, δ_2, m, n, r and β. For sensitized reaction where m, n=-2, we established that for some r, the solution is not stable..

The results of this study will serve as baseline information to combustion engineering in designing combustion equipments or manufacturing of chemical to aid complete combustion reactions and to burn fuel more efficiently to avoid knocking of engines.

Nomenclature

λ = thermal conductivity of the material
Q_1 = the heat of reaction in step one
Q_2 = the heat of reaction in step two
A = the rate constant in step one
B = the rate constant in step two
m,n = the exponent
E_i; i = 1, 2 = the activation energies

r = the ratio of the activation energies

v = the vibration frequency
h = the Plank's constant
ρ = the density
R = the universal gas constant
a = characteristic length
δ_i, i =1,2 = the Frank-Kamenetskii parameter
β = activation energy parameter
θ_m = temperature maximum
Γ = shooting guess value

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