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A Note on a Two-Step Reactive-Diffusive Equation with Variable Pre-Exponential Factor

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Abstract: To study the steady-state solutions for the exothermic chemical reactions (two-step Arrhenius reactions), taking the diffusion of the reactions in a slab into account and assuming an Arrhenius dependence with variable pre-exponential factor to determine the effects of Frank-Kamenetskii parameter and some thermo physical properties on temperature of a giving system. Steady state energy equation was transformed to non-dimensional form. Numerical solutions of the resulting equation were done by the use of shooting method. We discovered that there are certain values for n, m, r and β can accommodation for solution to be stable. Similarly, Frank-Kamenetskii parameter 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). 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.

Key words: Exothermic chemical reaction, variable pre-exponential factor, two-step, arrhenius reactions

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.

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

$$\lambda\frac{d^2T}{dx^2} + \rho Q_1 A\left(\frac{kT}{\nu h\rho}\right)^n \exp\left(-E_1/RT\right) + \rho Q_2 B\left(\frac{kT}{\nu h\rho}\right)^m \exp\left(-E_2/RT\right) = 0 \qquad (1)$$

Where all the variables and parameters are clearly defined in the nomenclature.

We take as the boundary conditions:

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

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 (Bowes, 1984; Dainton, 1966). By using the non dimensional variable defined by

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

on Eq. 1 and 2 the governing equation are (bar dropped)

$$\frac{d^2\theta}{dx^2} + \delta_1(1+\beta\theta)^n \exp(\theta/1+\beta\theta) + \delta_2(1+\beta\theta)^m \exp(r\theta/1+\beta\theta) = 0 \qquad (3)$$

$$\theta = 0 \qquad \text{on} \qquad x = \pm 1$$

$$\text{where} \quad \delta_1 = \frac{a^2 Q_1 E_1 A\left(kT_0/\nu h\rho\right)^n \exp\left(-E_1/RT_0\right)}{\lambda RT_0^2}, \qquad (4)$$

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

In Eq. 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 Eq. 3 and 4 is the fundamental importances in many industrial processes (Bowes, 1984).

Infact, the greatest temperature for which a low temperature steady distribution is possible is known as the critical ignition temperature or criteria storage temperature (Kenneth, 2005). At temperature higher than the critical ignition temperature, thermal ignition will occur (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 (1969) that Eq. 3 possesses simple closed-form solution in the form

$$\theta = \theta_m + \ln \operatorname{sech}^2\left(D \pm \sqrt{\delta_1 \exp(\theta_m/2x)}\right), \qquad (5)$$

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 (4), we have

$$\delta_1 = 2\exp(-\theta_m)\left\{\cosh^{-1}\left(\exp\left(\frac{\theta_m}{2}\right)\right)\right\}^2 \qquad (6)$$

In connection with Eq. 3 when $Q_2 = 0$, $n = 0$, it in well known that the reactive-diffusive equation admits perturbation solutions under physically reasonable assumptions (Bowes, 1984; Ward and Velde, 1992) and numerical solutions are available for some realistic conditions (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 (Ayeni, 1982; Okoya, 2002).

Here the principal aim of this study 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 Eq. 3.We also determine numerically the transitional values of δ_1, δ_2, β, m, n and r.

MATERIALS AND METHODS

Equation 3 and 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

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x \\ \theta \\ \theta^1 \end{pmatrix} \qquad (7)$$

By differentiating Eq. 7, we have

$$\begin{pmatrix} x_1^1 \\ x_2^1 \\ x_3^1 \end{pmatrix} = \begin{pmatrix} 1 \\ x_3 \\ -[\left[\delta_1(1+\beta x_2)^n \exp(x_2/1+\beta x_2)\right] \\ \qquad +\delta_2(1+\beta x_2)^m \exp(rx_2/1+\beta x_2)] \end{pmatrix} \qquad (8)$$

Satisfying the initial conditions

$$\begin{pmatrix} x_1(-1) \\ x_2(-1) \\ x_3(-1) \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ \Gamma \end{pmatrix} \qquad (9)$$

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

RESULTS AND DISCUSSION

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 $\delta_1 = 0.3064$, $\delta_2 = 0.5721$, $\beta = 0.001$, $r = 0.5$ and the shooting guess value $\Gamma = 1.18124$ for Eq. 3 and 4. It is observed that the solution is symmetry and θ_m occur at the centre i.e $\theta_m = 0.6341$.

Figure 2 shows the graph of temperature $\theta(x)$ against position x for $\delta_1 = 0.3064$, $\delta_2 = 0.5721$, $\beta = 0.001$, $r = 0.8$

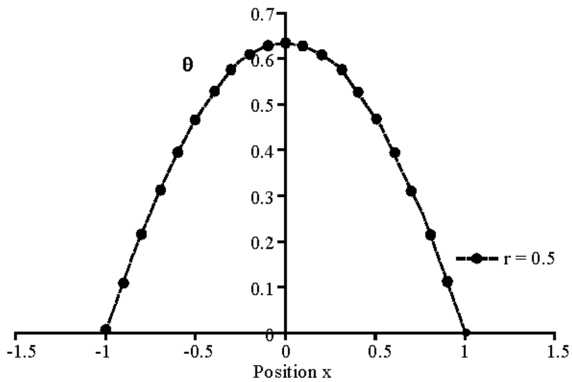

Fig. 1: Graph of temperature against position x for δ_1 = 0.3064, δ_2 = 0.5721, β = 0.001, r = 0.5

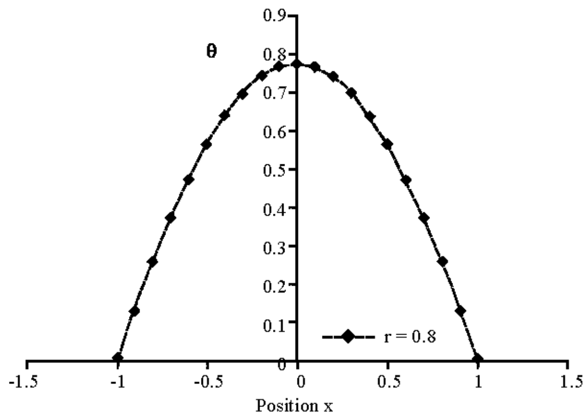

Fig. 2: Graph of temperature against position x for δ_1 = 0.3064, δ_2 = 0.5721, β = 0.001, r = 0.8

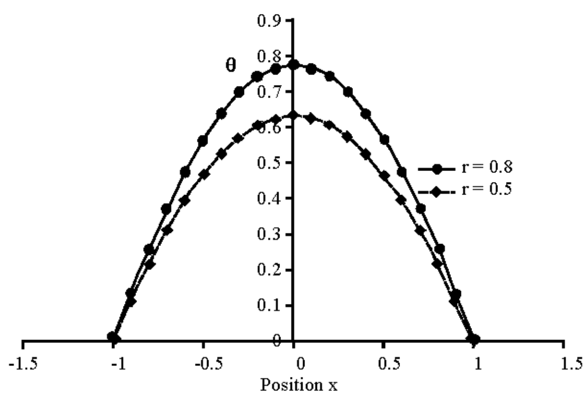

Fig. 3: Graph of temperature against position x for δ_1 = 0.3064, δ_2 = 0.5721, β = 0.001 and various values of r

and the shooting guess value for the solution to be unique is ⌈ = 1.3945. The solution is symmetry as well as the θ_m = 0.7751.

Figure 3 shows the graph of temperature $\theta(x)$ against position x for the same values of δ_1 = 0.3064, δ_2 = 0.5721,

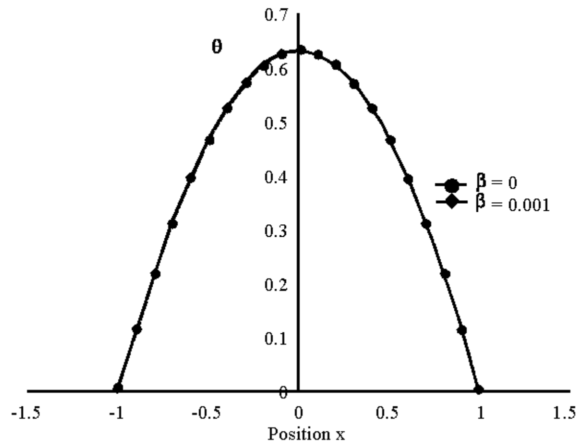

Fig. 3: Graph of temperature against position x for δ_1 = 0.3064, δ_2 = 0.5721, β = 0.001 and various values of β

β = 0.001 and various values of r. It was shown that at r = 0.8, we have the highest temperature ($\theta_{m)}$. 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 (i.e θ_m at $\beta \to 0$ and β = 0.001), we observed that both have the same turning point. Similarly for $\beta \to 0$ we have the highest value of temperature gradient.

CONCLUSION

Reactive-diffusive equation with variable pre-exponential factor for two-step Arr3henius reactions was exarmened in this research. 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 exist and is unique (when the derivative is presenbed) 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.

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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