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# On the Influence of Frank-Kamenetskii Parameter and Numerical Exponents on Temperature Field of Two-Step Arrhenius Reactions

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**Abstract:** In this study, we investigate the effect of Frank-Kamenetskii parameter and numerical exponents on temperature of two-step Arrheniun reactions to give further insight into the theory of combustion under reasonable and physical conditions. Numerical solutions are constructed for the governing non linear boundary value problem using shooting technique and influence of Frank-kamenetskii parameter and numerical exponent are discussed.

**Key words:** Frank-kamenetskii parameter, numerical exponents, two-step arrhenius reactions, physical conditions, non linear boundary

## INTRODUCTION

The present discipline of combustion draws on the field of chemical kinetics, thermodynamics, fluid mechanics and transport processes. These four subject, particularly the first and last did not begin to flourish until the middle of the 19th century. Therefore, the seeds of the modern science of combustion were not sown until half of the 19th century, notably by the experiment of Rebert Bunsen, of clands louis Le chatelier on the propagation of combustion waves and by the theoretical explanation offered by David Leohard chapman and Emile Jouguest combustion as a scientific discipline has grown steady in the 20th century (The Encyclopedia American, 1990).

Olanrewau and Ayeni (2001) investigated the effect of Frank-Kamenetskii parameter on strong detonations in converging vessels in which they established the fact that there is an appreciable difference in the temperature along the vessel when Frank-Kamenetskii parameter differ only by 1/30.

Other contributions include Ayeni *et al*. (2005) examined the effect of radiation on the critical Frank-kamenetskii parameter of thermal ignition in a combustible gas containing fuel droplets. Previous researches show that radiation delays ignition in a well stired reactor. In their paper they showed that even in a non-homogeneous reaction,the critical frank-Kamenetskii parameter increase as the radiation parameter increases when the activation energy is high. This confirms the experimented observation in diesel engines.

Similarly Gbolagade and Makinde (2005) investigated thermal ignition in a reactive variable viscosity poiseuille flow. They investigated the thermal ignition in a strongly exothermic reaction of a variable viscosity combustible material flowing through a channel with isothermic walls under Arrhenius kinetic, neglecting the consumption of the material. Analytical solutions are contracted for the governing nonlinear boundary value problem using perturbation technique together with a special type of Hermite pade approximations and important properties of the temperature field including bifurcations and thermal criticality are discussed.

Gbolagade and Makinde (2005) examined the effect of Biot number of thermal critically in a coutte flow. Analytical solution are considered for the governing nonlinear boundary value problem using perturbation technique together with a special type of Hermite-pade approximation and thermal criticality are discussed.

In this study, we extend the research of the above researchers by considering two-step Arrhenius reactions instead of one-step Arrhenius reactions to give further insight into the theory of combustion.

## MATERIALS AND METHODS

In this study, we consider a two-step reaction of the form:

$$A \rightarrow B \rightarrow C \tag{1}$$

Where A is the reactant, B in the first unstable product and C in the final product. Equation 1 is an exothermic reaction. Equation 1 can be written as:

$$\rho c_p \; u\frac{dT}{dx} = k\frac{d^2T}{dx^2} + A_1Q_1 \; X^a \; T^n \; e^{-E_1/RT} + A_2Q_2 \; Y^b \; T^m \; e^{-E_2/RT} \tag{2}$$

and Eq. 2 is called steady state energy equation

Where
k = Thermal conductivity
R = Universal gas constant
T = Temperature
ρ = Density
$c_p$ = Specific heat at constant pressure
$A_i$ = Pre-exponential factors, I = 1,2
x = Mass fraction of species $A_1$
Y = Mass fraction of species $A_2$
a = Order of reaction of species $A_1$
b = Order of reaction of species $A_2$
x = Space variable
$Q_i$ = Heat release/unit mass
m,n = Numerical exponents
$E_i$ = Activation energies, i = 1, 2

Equation 2 takes it roots from Navier-stokes equations.

**Method of solution:** We non dimensionlize Eq. 2. The resulting equations is solved under physically reasonable assumption and reasoned physical conditions so as to represent the physical problems with physical implications.
Suitable dimensionless parameters

$$\left.\begin{aligned} \theta &= \frac{T-T_0}{\beta T_0} \\ \beta &= \frac{RT_0}{E_1} \\ r &= \frac{E_2}{E_1} \\ u^1 &= u/v_0 \end{aligned}\right\} \quad (3)$$

We take advantage of Eq. 3 and 2 becomes

$$\frac{d\theta}{dx} = \lambda\frac{d^2\theta}{dx^2} + \delta_1 (1+\beta\theta)^n\ e^{\theta/1+\beta\theta} + \delta_2 (1+\beta\theta)^m\ e^{r\theta/1+\beta\theta} \quad (4)$$

under the conditions

$$\theta(-1)=\theta(1)=0 \quad (5)$$

Where

$$\lambda = \frac{k\beta T_0}{\rho c_p u' v_0}$$

$$\delta_1 = \frac{A_1 Q_1 x^a\ e^{-E_2/RT_0}}{\rho c_p u' v_0 T_0 \beta}$$

$$\delta_2 = \frac{A_2 Q_2 Y^b\ e^{-E_2/RT_0}}{\rho c_p u' v_0 T_0 \beta}$$

($\delta_1$ and $\delta_2$ are Frank-kamenetskii parameters) (Olanrewaju and Ayeni, 2001) m and n are the numerical exponents.

By applying shooting method, Eq. 4 and 5 were transformed to an initial value problem of the form

$$\begin{pmatrix} x_1^{\ 1} \\ x_2^{\ 1} \\ x_3^{\ 1} \end{pmatrix} = \begin{pmatrix} 1 \\ x_3 \\ 1/\lambda \begin{pmatrix} x_3 - \delta_1 (1+\beta x_2)^n\ e^{x_2/1+\beta x_2} - \\ \delta_2 (1+\beta x_2)^m\ e^{\frac{rx_2}{1+\beta x_2}} \end{pmatrix} \end{pmatrix} \quad (6)$$

Satisfying

$$\begin{pmatrix} x_1(-1) \\ x_2(-1) \\ x_3(-1) \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ \Gamma \end{pmatrix} \quad (7)$$

Where $\theta^1(-1) = \Gamma$ (shooting guess value) for $\theta(1) = 0$.

## EXISTENCE AND UNIQUENESS OF SOLUTION

**Theorem 1 (Williams *et al.*, 1978):** Let D denote the region (n (n+1))

Dimensional space,one dimension for t and n dimensions for vector x] $|t-t_0| \le a$, $\|x-x_0\| \le b$.
if

$$\begin{cases} x_1^1 = f_1(x_1,x_2,....,xn,t)\ ,\ x_1(t_0) = x_{10} \\ x_2^1 = f_2(x_1,x_2,....,xn,t)\ ,\ x_2(t_0) = x_{20} \\ . \\ . \\ . \\ x_n^1 = f_n(x_1,x_2,....,xn,t)\ ,\ x_n(t_0) = x_{n0} \end{cases} \quad (8)$$

Then, the system of Eq. 10 has a unique solution of

$$\frac{\partial f_i}{\partial x_j},\quad i,j=1,2,...,n$$

are continuous in D.
($H_1$): $\Gamma > 0$, $0 \le x_1 \le 1$, $0 \le x_2 \le b$ and $c \le x_3 \le C$, where b, c and C are positive constants.

**Theorem 2:** IF ($H_1$) holds then problem (6) has a unique solution satisfying (7).

**Proof:** We let

$$y^1 = \begin{pmatrix} x_1^1 \\ x_2^1 \\ x_3^1 \end{pmatrix} = \begin{pmatrix} g_1(x_1, x_2, x_3) \\ g_2(x_1, x_2, x_3) \\ g_3(x_1, x_2, x_3) \end{pmatrix} \quad (9)$$

Where

$$g_1 = 1, \; g_2 = x_3$$

and

$$g_3 = 1/\lambda\Big[x_3 - \delta_1\,(1+\beta x_2)^n \exp\,(x_2/1+\beta x_2) - \delta_2(1+\beta x_2)^m \exp\,(r x_2/1+\beta x_2)\Big]$$

Clearly

$$\frac{\partial f_i}{\partial x_j}$$

is bounded for i = 1, 2, 3.

Thus, $g_i$, i= 1, 2, 3 are lipschitz continuous. Hence there exists a unique solutions of Eq. 6 and 7.

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