

Influence of power-law exponent on an unsteady endothermic reaction

¹O. T. Lamidi, ²A. M. Okedoye and ³R. O. Ayeni

¹*Department of Physical Sciences,*

Bells University of Technology, Ota, Nigeria

^{2,3}*Department of Pure and Applied Mathematics,*

Ladoke Akintola University of Technology, Ogbomosho, Nigeria

Abstract

In [6], the solution of a steady Arrhenius endothermic chemical reaction where the exponential term was reduced to a power-law approximation was studied. A numerical solution obtained using a shooting technique with second order Runge-Kutta scheme showed that the minimum temperature of the reactant increases as the power-law index increases. In this paper, the scope of the work was extended to a solution of an unsteady Arrhenius endothermic reaction using shooting technique [3]. The result showed that the temperature of the reactant depends greatly on the power-law exponent. The temperature of the reactant increases as the power-law exponent α increase, whereas the temperature decreases as the Frank-Kamenestkii parameter β increases.

Keywords

Power-law exponent, endothermic reactions, shooting technique,
Frank-Kamenestkii parameter.

1.0 Introduction

Over the years, many research works had been carried out by both the chemical engineers and scientists on reacting problems in chemical reactions due to its wider application in the area of combustion [7].

Most existing works had discussed extensively chemical reactions involving exothermic and endothermic reactions. In [8], ignition was defined as the process whereby a material capable of reacting exothermically is brought to a state of rapid combustion when the solid fuel which has been oxidized reaches the ignition temperature, the reaction occurs and the gas-solid interface changes position in forward direction until the whole fuel is consumed or the gaseous oxidizer is exhausted. As the burning continues, the temperature rises as the concentration reduces. This results in heat liberation by the reactants during chemical reactions.

In [7], the effect of diffusion on the auto-ignition of combustible fluids in insulating materials was investigated. In the paper, a three-component model of this system is considered

¹Corresponding author

¹e-mail address: tamumeji@yahoo.com

¹Telephone: +234-0803-332-9956

which includes exothermic oxidation and endothermic evaporation process. By assuming a slow rate of consumption of fuel and oxygen, the behavior of the full system can be approximated and the safe and dangerous regions of parameter space can be identified. The effect of changes in parameters such as the size and the endothermicity were discussed.

The delayed thermal explosion in inflammable gas, which contains fuel droplets was examined in [2]. Also in [1], the effect of thermal radiation on the critical Frank-Kamenestkii parameter of a thermal ignition in a combustible gas containing fuel droplets was examined. In [2], different initial temperature for gas and droplets was assumed. The initial temperature for droplets is 300k while the initial temperature of the gas is 600k. The temperature and vapour concentration at times close to 2ms indicate the explosion behaviour of the system when the droplets concentration is small. As expected, the liquid evaporates before explosion occurs. In the case of high droplets concentration, the thermal explosion of gas almost coincides with the time of droplet heating and evaporation.

In [4], the effect of power-law index on a steady Arrhenious exothermic chemical reaction was discussed. In the paper, it was shown that the maximum temperature attained by the reacting system decreases as the power-law exponent increases while in [5], the temperature increases as the power-law exponent increases in an unsteady Arrhenious exothermic chemical reaction.

The source of inspiration for the present study could be found in [1, 6, 9]. When the activation energy is not large we can approximate the heat term by $\pm QT^\alpha$ where Q is the heat released or heat absorbed, T is the temperature and α is the power-law exponent.

2.0 Mathematical formulation

We consider an Arrhenious chemical reaction of the form:

$$\rho \frac{\partial X}{\partial t} = D_1 \frac{\partial^2 X}{\partial x^2} - AXYe^{-E/RT} \quad (2.1)$$

$$\rho \frac{\partial Y}{\partial t} = D_2 \frac{\partial^2 Y}{\partial x^2} - AXYe^{-E/RT} \quad (2.2)$$

$$\rho c_p \frac{\partial T}{\partial t} = K \frac{\partial^2 T}{\partial x^2} + QAXYe^{-E/RT} \quad (2.3)$$

With boundary and initial conditions

$$T(x, 0) = T_0(x), X(x, 0) = X_0(x), Y(x, 0) = Y_0(x) \quad (2.4)$$

$$T(-L, t) = T_1(t), X(-L, t) = X_1(t), Y(-L, t) = Y_1(t) \quad (2.5)$$

$$T(L, t) = T_2(t), X(L, t) = X_2(t), Y(L, t) = Y_2(t) \quad (2.6)$$

where

$X = X(x, t)$ = fuel concentration, $Y = Y(x, t)$ = oxygen concentration,

$T = T(x, t)$ = temperature, D_1 = diffusion coefficient for fuel,

D_2 = diffusion coefficient for oxygen, K = thermal conductivity,

A = pre-exponential factor of oxidation, Q = heat released or heat absorbed per unit mass, ρ = density, c_p = specific heat capacity, E = activation energy,

R = ideal gas constant, t = time.

Dividing (2.1) and (2.2) by ρ and (2.3) by ρc_p and then non-dimensionalizing the temperature

$$\text{using } \frac{\partial X}{\partial t} = \frac{D_1}{\rho} \frac{\partial^2 X}{\partial x^2} - \frac{A}{\rho} XY e^{-E/RT_0} e^{E/RT_0} e^{-E/RT} \quad (2.7)$$

$$\frac{\partial Y}{\partial t} = \frac{D_2}{\rho} \frac{\partial^2 Y}{\partial x^2} - \frac{A}{\rho} XY e^{-E/RT_0} e^{E/RT_0} e^{-E/RT} \quad (2.8)$$

$$\frac{\partial T}{\partial t} = \frac{K}{\rho c_p} \frac{\partial^2 T}{\partial x^2} + \frac{QA}{\rho c_p} XY e^{-E/RT_0} e^{E/RT_0} e^{-E/RT} \quad (2.9)$$

we get

$$\frac{\partial X}{\partial t} = B_1 \frac{\partial^2 X}{\partial x^2} - A_1 XY e^{\theta/1+\epsilon\theta} \quad (2.10)$$

$$\frac{\partial Y}{\partial t} = B_2 \frac{\partial^2 Y}{\partial x^2} - A_1 XY e^{\theta/1+\epsilon\theta} \quad (2.11)$$

$$\frac{\partial \theta}{\partial t} = K_1 \frac{\partial^2 \theta}{\partial x^2} + Q_1 XY e^{\theta/1+\epsilon\theta} \quad (2.12)$$

with the boundary and initial conditions

$$\begin{aligned} \theta(x, 0) = 0, X(x, 0) = X_0(x), Y(x, 0) = Y_0(x) \\ \theta(-L, t) = \theta_1(t), X(-L, t) = X_1(t), Y(-L, t) = Y_1(t) \\ \theta(L, t) = \theta_2(t), X(L, t) = X_2(t), Y(L, t) = Y_2(t) \end{aligned} \quad (2.13)$$

where

$$\epsilon = \frac{RT_0}{E}, T = \epsilon T_0 \theta + T_0, B_1 = \frac{D_1}{\rho}, B_2 = \frac{D_2}{\rho}, K_1 = \frac{K}{\rho c_p}, A_1 = \frac{1}{\rho} A e^{-E/RT_0}, Q_1 = \frac{Q}{\rho c_p \epsilon T_0} A e^{-E/RT_0}$$

In this paper, it was assumed that the final form of $e^{\theta/1+\epsilon\theta}$ could be written as θ^α [1] and when X and Y are known, the problem below could be solved.

$$\frac{\partial u}{\partial t} = K \frac{\partial^2 u}{\partial x^2} + h(x) u^\alpha, 0 < \alpha < 1, -L \leq x \leq L, t > 0 \quad (2.14)$$

where

- $u(x, t)$ = temperature of the reaction
- $h(x)$ = heat released or heat absorbed
- α = power-law exponent
- K = thermal conductivity

such that $h(x)$ is greater than or less than zero depending on whether the reaction is exothermic or endothermic.

3.0 Method of solution

Taking $h(x) = -\lambda$ and for unsteady case we have

$$\frac{\partial u}{\partial t} = K \frac{\partial^2 u}{\partial x^2} - \lambda u^\alpha, 0 < \lambda \leq 1, 0 < K \leq 1 \quad (3.1)$$

with

$$\begin{aligned} u(x,t) &= 0, \quad t < 0, \quad u(x,t) > 0, \quad t > 0, \quad u(x,vt) = 1, \\ u(x-vt=2) &= 0.05, \quad 0 < \alpha < 1, \quad 0 \leq x < \infty, \quad 0 < K \leq 1 \end{aligned} \quad (3.2)$$

We apply a moving grid $\varepsilon = x - vt$, then $u(x,t) = w(\varepsilon)$, where v is the flame velocity. Using the chain rule with $\varepsilon = x - vt$, we have

$$\frac{\partial}{\partial t} = \frac{d}{d\varepsilon} \frac{\partial \varepsilon}{\partial t} = -v \frac{d}{d\varepsilon} \quad (3.3)$$

$$\frac{\partial}{\partial x} = \frac{d}{d\varepsilon} \frac{\partial \varepsilon}{\partial x} = \frac{d}{d\varepsilon} \quad (3.4)$$

$$\frac{\partial^2}{\partial x^2} = \frac{d^2}{d\varepsilon^2} \left(\frac{\partial \varepsilon}{\partial x} \right)^2 = \frac{d^2}{d\varepsilon^2} \quad (3.5)$$

Equation (2.2) becomes

$$\frac{d^2 w}{d\varepsilon^2} = - \left(\gamma \frac{d^2}{d\varepsilon^2} - \beta w^\alpha \right) \quad (3.6)$$

with $w(0) = 1, w(2) = 0.05, 0 < \alpha < 1,$ (3.7)
 where $\beta = \lambda/K, \gamma = v/K, 0 < \beta < \infty, 0 < \gamma < \infty.$ Solving equation (3.6) subject to (3.7) numerically, Equation (3.6) is resolved into system of first order differential equations as follows:

We let

$$Z = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = \begin{pmatrix} \varepsilon \\ w \\ w' \end{pmatrix} \quad (3.8)$$

so,

$$\begin{pmatrix} X_1' \\ X_2' \\ X_3' \end{pmatrix} = \begin{pmatrix} 1 \\ w' \\ w'' \end{pmatrix} \quad (3.9)$$

$$E(Z) = \begin{pmatrix} X_1' \\ X_2' \\ X_3' \end{pmatrix} = \begin{pmatrix} 1 \\ X_3 \\ -(\gamma X_3 - \beta X_2^\alpha) \end{pmatrix} \quad (3.10)$$

together with initial condition

$$\begin{pmatrix} X_1(0) \\ X_2(0) \\ X_3(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ \alpha_1 \end{pmatrix} \quad (3.11)$$

The constant α_1 is the initial guessed of the temperature gradient of the system.

4.0 Results and discussion

4.1 Results

The numerical solution of equation (3.6) was computed for various values of power-law exponent α and values of Frank-Kamenetskii parameter $\beta = \lambda/K$ with $\gamma = \nu/K$ and used to plot the graphs in figures 4.1 and 4.2.

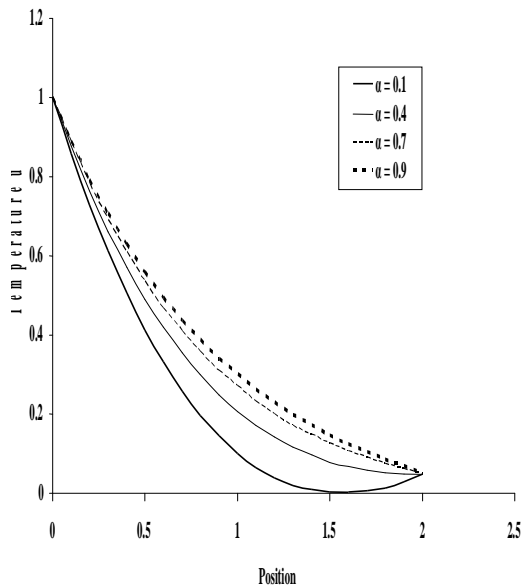


Figure 4.1: Graph of the temperature u against position ϵ at various values of α with $\beta = 1.0$ and $\gamma = 0.2$

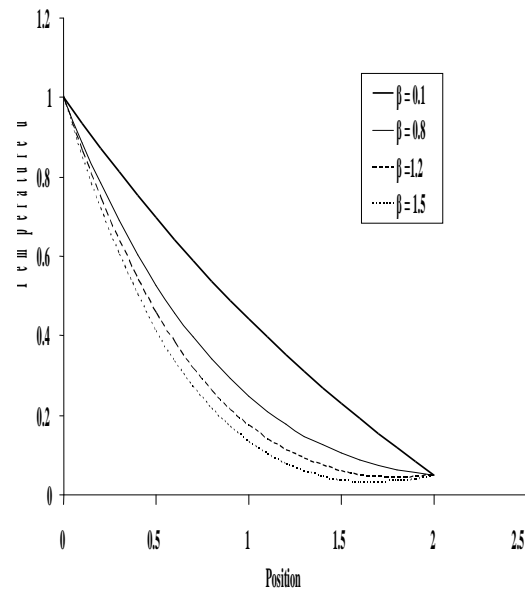


Figure 4.2: Graph of the temperature u against position ϵ at various values of β with $\alpha = 0.4$ and $\gamma = 0.2$

5.0 Discussion

The unsteady profile of α is shown in the figure 4.1. The temperature profile was studied for various values of α . It was shown that the temperature attained by the reacting system increases as the power-law exponent increases, while figure 4.2 shows that the temperature experienced by the reacting system also decreases as the Frank-Kamenetskii parameter β increases.

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