Influence of power-law index on an unsteady exothermic reaction

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Abstract

This study presents the solution of an unsteady Arrhenius exothermic reaction where we reduced the exponential term to a power-law approximation. A numerical solution of the problem is obtained using shooting technique with second order Runge-Kuta scheme. It is shown that the temperature of the reactant depends on the power-law index. The temperature of the reactant increases as the power-law index increases.

1.0   Introduction

Several works have been done in the past by scientists on reacting problems due to its wider useful application in the area of combustion. The study of chemical reaction involving exothermic and endothermic reactions has attracted the interest of chemical engineers and scientists over the past decades. (Truscott et al (1996 [5])).

Quoting Williams (1985 [6]), ignition is 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.

Truscott et al (1996 [5]) discussed the effect of diffusion on the auto-ignition of combustible fluids in insulation materials. In their paper, a three-component model of this system is considered which includes exothermic oxidation and endothermic evaporation process. By assuming a slow rate of consumption of fuel and oxygen, the behaviour 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 are discussed.

Goldfarb et al (2004 [2]) examined delayed thermal explosion in inflammable gas, which contains fuel droplets. Also Ayeni et al (2005 [1]) examined the effect of thermal radiation on the critical Frank-Kamenetskii parameter of a thermal ignition in a combustion gas containing fuel droplets. Goldfarb et al (2004[2]) assumed different initial temperature for gas and droplets. The initial temperature for droplets is 300k while the initial temperature of the gas is 600k.

The numerical simulations show that there is a sharp increase in gas temperature and vapour concentration at times close to 2ms, which indicates 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 evaporating.

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The present work has its source from the work of Ayeni et al (2005 [1]), Guo (2002) and Lamidi et al (2007 [[4]). 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 a general chemical reaction of the form

$$\frac{\partial u}{\partial t} = K\frac{\partial^2 u}{\partial x^2} + h(x)u^{\alpha} \ , 0 < \alpha < 1, 0 \le x < \infty, t > 0 \qquad (2.1)$$

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

3.0   Materials and methods
Taking $h(x) = \lambda, 0 < \lambda \le 1$ and for unsteady case

$$\frac{\partial u}{\partial t} = K\frac{\partial^2 u}{\partial x^2} + \lambda u^{\alpha} , \qquad (3.1)$$

with $u(x,t) = 0, t < 0, u(x,t) > 0, t > 0, u(x,vt) = 1$
$u(x- vt = 2) = 1.5, 0< \alpha < 1, 0 \le x < \infty, 0 < K \le 1$ (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

$$\frac{\partial}{\partial t} = \frac{d}{d\varepsilon}.\frac{\partial\varepsilon}{\partial t} = -v\frac{d}{d\varepsilon}$$

$$\frac{\partial}{\partial x} = \frac{d}{d\varepsilon}.\frac{\partial\varepsilon}{\partial x} = \frac{d}{d\varepsilon}$$

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

Then equation (3.1) becomes $\dfrac{d^2 w}{d\varepsilon^2} = -\left(\gamma\dfrac{dw}{d\varepsilon} + \beta w^{\alpha}\right)$ (3.3)

with $w(0) = 1, w(2) = 1.5, 0 < \alpha < 1,$
where $\beta = \lambda/K, \gamma = v/K, 0 < \beta < \infty, 0 < \gamma < \infty$ (3.4)
Solving equation (3.3) subject to (3.4) numerically, equation (3.3) is resolved into system of first order differential equations as follows. We let

$$Z = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = \begin{pmatrix} \varepsilon \\ w \\ w' \end{pmatrix} \qquad (3.5)$$

So,

$$\begin{pmatrix} X_1' \\ X_2' \\ X_3' \end{pmatrix} = \begin{pmatrix} 1 \\ w' \\ w'' \end{pmatrix} \qquad (3.6)$$

$$E(Z) = \begin{pmatrix} X_1{}' \\ X_2{}' \\ X_3{}' \end{pmatrix} = \begin{pmatrix} 1 \\ X_3 \\ -(\gamma X_3 + \beta X_2{}^{\alpha}) \end{pmatrix} \tag{3.7}$$

Together with initial condition

$$\begin{pmatrix} X_1(0) \\ X_2(0) \\ X_3(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ \alpha_1 \end{pmatrix} \tag{3.8}$$

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

4.0   Results and discussion

The numerical solution of equation (3.7) is computed for various values of power-law index α and values of Frank-Kamenetskii parameter $\beta = \lambda/K$ with $\gamma = v/K$ and used to plot the graphs in figures 1 and 2 below:
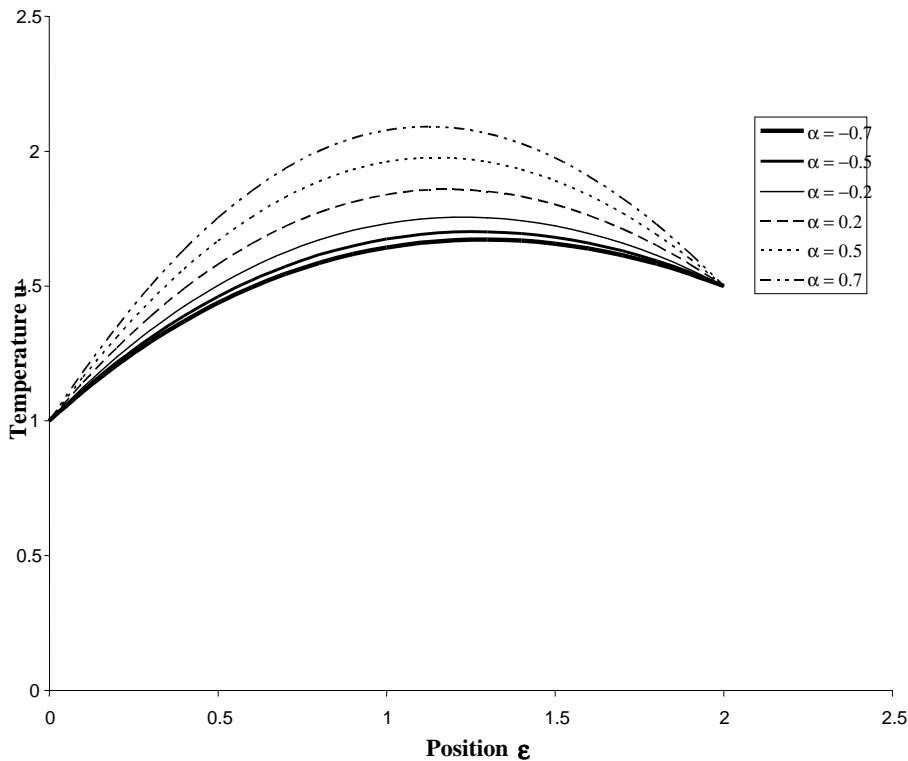

Figure 1: Graph of the temperature u against position ε at various values of α with $\beta = 1$, $\lambda = 0.2$
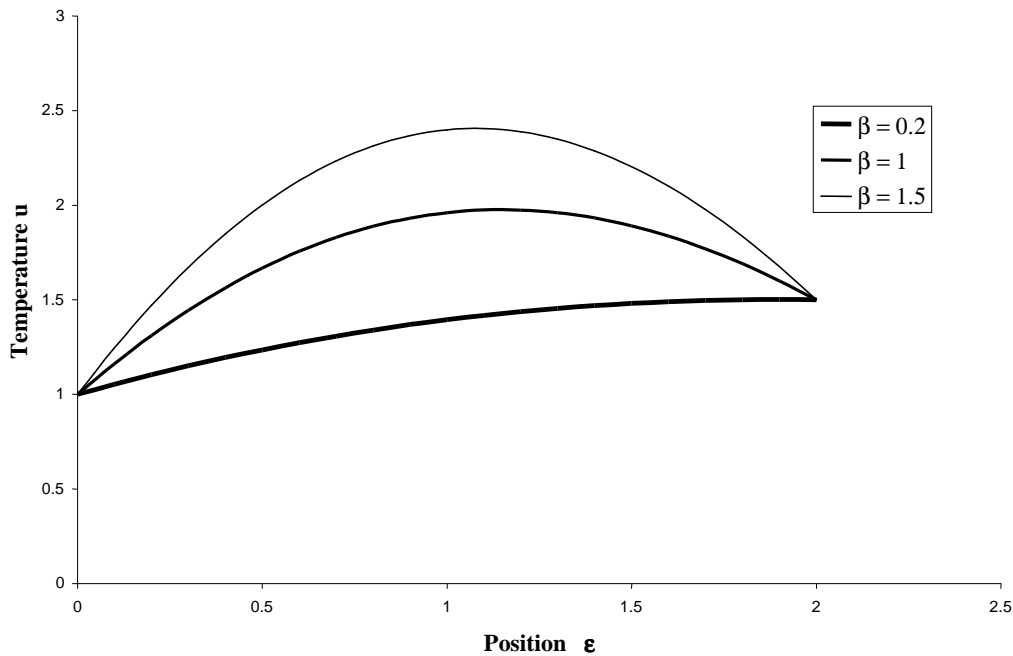
Figure 2: Graph of the temperature u against position ε at various values of β with α=0.5, $\lambda = 0.2$

5.0 Discussion

The Figure 1 above shows the steady profile of α. The temperature profile was studied for different values of α . It was shown that as the power-law index α increases, the maximum temperature experienced by the reacting system increases. While Figure 2 shows that as the value of scaled Frank–Kamenetskii parameter β increases, the maximum temperature attained by the reacting system also increases.

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