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Effect of power-law exponent in endothermic reactions

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Abstract

We present the solutions of a steady Arrhenious endothermic reaction. We reduced the exponential term to a power-law approximation. We solved the problem by using shooting method technique. It is shown that the heat generated by the endothermic reaction depends on the power-law exponent. The minimum temperature increases as the power-law index α increases, whereas the minimum temperature decreases as the Frank-Kamenestkii parameter β increases.

1.0 Introduction

Several works have been done in the past by scientists on reactions 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.

Quoting Williams (1985[5]), 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 [4]) 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 endothermic 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 simulation shows that there is a sharp increase in gas temperature and vapour concentration at times close to 2*ms*, 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.

The present work has its source from the work of Ayeni et al (2005 [1]) and Y.L Guo (2002 [6]). 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.

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2.0 Mathematical formulation

We consider a general chemical reaction of the form

$$\frac{\partial u}{\partial t} = K\frac{\partial^2 u}{\partial x^2} + h(x)u^{\alpha} \text{ , } 0 < \alpha < 1, -L \leq x \leq L, t > 0 \tag{2.1}$$

where

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

3.0 Materials and methods

Taking $h(x) = -\lambda$, $0 < \lambda \leq 1$ and for steady case

$$\frac{\partial u}{\partial t} = 0 \tag{3.1}$$

Then equation (2.1) becomes
$$\frac{d^2 u}{dx^2} - \beta u^{\alpha} = 0 \tag{3.2}$$

where $\lambda/K = \beta$, $0 < \beta < \infty$ with $u(-1) = u(1) = 1$, $0 < \alpha < 1$, $|x| \leq L$, $0 < K \leq 1$ (3.3)

Solving equation (3.2) subject to (3.3) numerically when $L = 1$. Equation (3.2) is resolved into system of first order differential equations as follows:

We let

$$Z = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = \begin{pmatrix} x \\ u \\ u' \end{pmatrix} \tag{3.4}$$

So,

$$\begin{pmatrix} X_1' \\ X_2' \\ X_3' \end{pmatrix} = \begin{pmatrix} 1 \\ u' \\ u'' \end{pmatrix} \tag{3.5}$$

$$E(Z) = \begin{pmatrix} X_1' \\ X_2' \\ X_3' \end{pmatrix} = \begin{pmatrix} 1 \\ X_3 \\ \beta X_2^{\alpha} \end{pmatrix} \tag{3.6}$$

Together with initial condition

$$\begin{pmatrix} X_1(-1) \\ X_2(-1) \\ X_3(-1) \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \\ \alpha_1 \end{pmatrix} \tag{3.7}$$

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

4.0 Results and discussion

4.1 Results

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

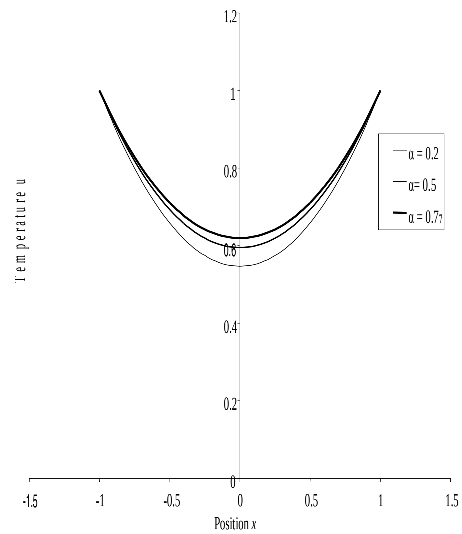

Figure 4.1: Graph of the minimum temperature u against position x at various values of α with β = 1

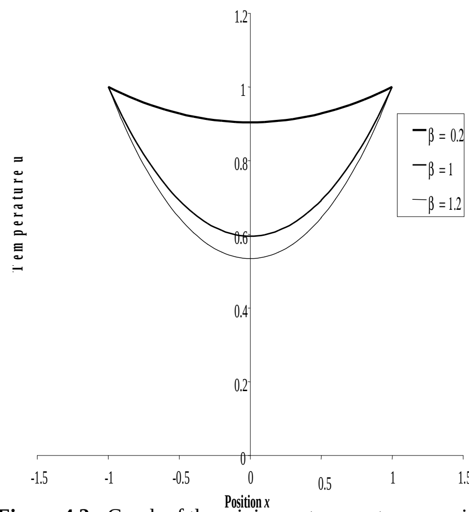

Figure 4.2 : Graph of the minimum temperature *u* against position *x* at various values of β with α = 0.5

Table 4.1: Table of values for various values of β with α=0.5

x	α = 0.2	α = 0.5	α = 0.7
-1	1	1	1
-0.9	0.9123	0.9201	0.9241
-0.8	0.8344	0.8497	0.8576
-0.7	0.7662	0.7886	0.8
-0.6	0.7074	0.7363	0.751
-0.5	0.6579	0.6926	0.7102
-0.4	0.6177	0.6572	0.6772
-0.3	0.5865	0.6299	0.6518
-0.2	0.5643	0.6105	0.6338
-0.1	0.551	0.5989	0.6231
0	0.5466	0.5951	0.6195
0.1	0.551	0.5989	0.6231
0.2	0.5643	0.6105	0.6338
0.3	0.5865	0.6299	0.6518
0.4	0.6177	0.6572	0.6772
0.5	0.658	0.6926	0.7102
0.6	0.7075	0.7363	0.751
0.7	0.7662	0.7886	0.8
0.8	0.8345	0.8497	0.8576
0.9	0.9124	0.9201	0.9241
1	1	1	1

Table 4.2: Table of values for various values of α with β=1

x	β = 0.2	β =1	β = 1.2
-1	1	1	1
-0.9	0.9817	0.9201	0.9072
-0.8	0.9653	0.8497	0.8259
-0.7	0.9509	0.7886	0.7554
-0.6	0.9385	0.7363	0.6954
-0.5	0.928	0.6926	0.6453
-0.4	0.9194	0.6572	0.6049
-0.3	0.9127	0.6299	0.5737
-0.2	0.908	0.6105	0.5517
-0.1	0.9051	0.5989	0.5385
0	0.9042	0.5951	0.5341
0.1	0.9051	0.5989	0.5385
0.2	0.908	0.6105	0.5517
0.3	0.9127	0.6299	0.5737
0.4	0.9194	0.6572	0.6048
0.5	0.928	0.6926	0.6453
0.6	0.9385	0.7363	0.6954
0.7	0.951	0.7886	0.7554
0.8	0.9654	0.8497	0.8259
0.9	0.9817	0.9201	0.9072

5.0 Discussion

The figure 4.1 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 exponent α increases, the minimum temperature of the system

increases. While figure 4.2 shows that as the value of scaled Frank–Kamenetskii parameter β increases, the minimum temperature also decreases.

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