Effect Of Flame Velocity On Unsteady Endothermic Reaction With Power-Law Exponent

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Abstract—**The focus of present research paper is to analyze the flame velocity effect on unsteady endothermic reaction with power-law exponent and heat Source/Sink conditions, through numerical technique, under which consistency and convergence criterion exist. The theoretical non-linear model for the system has been derived by employing the Gibbs function, reaction rate and Fick's laws. Maple pdsolve/numeric routine that uses finite difference methods is used to obtain numerical solutions to the partial differential system of equations. From our analysis, we deduced that, concentration decreases as diffusion coefficient increases. Also, temperature increases with an increase power-law exponent while increase in Frank-Kamentskii parameter increases temperature.**

> *Keywords—Gibbs function; non-Newtonian fluid; Frank-Kamenestkii parameter; Fick's law, Heat Source/Sink, Maple pdsolve/numeric*

Subject Classification: 76D05, 76V05, 80A32

1. INTRODUCTION

Each type of non-Newtonian fluid behaviour has been illustrated via experimental data on real materials. as well as discussion on how to engineer non-Newtonian flow characteristics of a product for its satisfactory end use by manipulating its microstructure by controlling physico-chemical aspects of the system. The thermal theory was formulated on the basis of breakdown in thermal equilibrium, when heat loss due to conduction can no longer keep pace with the heat released due to exothermic reaction. The phenomenon of thermal explosion is not only relevant to the development of physics of combustion and explosions, which include the theory of thermal explosion as its subdivisions, but also to fundamental branches of knowledge such as chemical kinetics and theory of heat transfer.

Studies show that internal combustion and thermal explosions are increasingly becoming popular and its qualitative treatment were in agreement with experimental investigations, The thermal theory of ignition came into existence on the premise of breakdown in thermal equilibrium.

The breakdown is as a result of heat loss due to conduction no longer keep pace with the heat released due to exothermic reaction. The interest in combustion and thermal explosion are not only relevant to the development of physics of combustion and explosion but also to fundamental branches of knowledge such as chemical kinetics and theory of heat transfer. As a result of the imbalance in the thermal explosion processes, addition of heat source which result to either initiate early ignition point or delay it has been investigated theoretically and experimentally.

Thermal explosion in a combustible gas mixture containing fuel droplets with Arrhenius power law model was studied by [1]. Also, [2] – [6] carried out similar and related studies. Ajadi and Gol'dshtein [7], studied the thermal explosion characteristics in the presence of an additional heat source and opined the contributions of the heat release due to the forces of internal friction on the Frank- Kamenestkii parameter and Semenov parameter.

Ayeni [8], and [9], [10], all reported in their studies that decrease in temperature is caused by increase in the Frank-Kamenestkii parameter. Ngiangia [11], took a critical look at the approximation of flow behaviour index to Newtonian fluids in reaction pathway and deduced that Frank-Kamenestkii parameter and Semenov parameter decrease the minimum temperature of the reaction, thereby slowing down the initiation of thermal explosion. Recently, [12] analyzed the effect of Frank-Kamenestkii parameter on Newtonian fluids and non-Newtonian fluids and showed that for Newtonian and non-Newtonian fluids

cases, a decrease in temperature is observed as a result of increase in Frank-Kamenestkii parameter. Numerical investigation of the effects of a harmonic volume forcing of prescribed frequency on the turbulent pipe flow at a Reynolds number was carried out by [13], based on bulk velocity and pipe diameter, of 5900. Their study focuses on the analysis of the time- and space-averaged statistics of the first- and second-order moments, vorticity fluctuations and Reynolds stress budgets, and provide information about the statistics of the fluctuations about the mean.

Exothermic and endothermic chemical reactions and its application to processes of ignition and combustions has been a subject of intense study by scientists. In a study carried out by [14], a three-component model of a system is considered which includes exothermic oxidation and endothermic evaporation process. They concluded that 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. In another study, [3] examined delayed thermal explosion in inflammable gas and assumed 300k for initial temperature for droplets and 600k for initial temperature for gas.

The contributions of the heat release due to the forces of internal friction on the Frank-Kamenestkii parameter in the stationary theory and the semenov parameter in the non-stationary theories was investigated, in addition to the influence of frictional contribution on the rate of reaction and ignition time have been investigated and a departure from known results is observed.

For most elementary reactions, the rearrangement of atoms in going from reactants to products via a transition state proceeds through the movements of atomic nuclei that experience a potential energy field that is generated by the rapid motions of the electrons in the system. On this potential energy surface there will be a path of minimum energy expenditure for the reaction to proceed from reactants to products (reaction coordinate). The low energy positions of reactants and products on the potential energy surface will be separated by a higher energy region. The highest energy along the minimum energy pathway in going from reactants to products defines the transition state [15].

The present research is to derived theoretical non-linear model for the system by employing the reaction rate and Fick's laws and analyze the unsteady endothermic reaction with power-law exponent and heat Source/Sink through numerical technique, that guarantee consistency and convergence criterion.

2. MATHEMATICAL FORMULATION OF THE PHYSICAL PROBLEM

Consider the unimolecular reaction:

$$A \rightarrow \text{products} \tag{1}$$

Using Guldberg-Waage form of the reaction rate to describe this reaction gives:

$$-r = kC_A \tag{2}$$

Then,

$$\frac{1}{v_i}\frac{dn_i}{dt} = -\frac{dn_A}{dt} \tag{3}$$
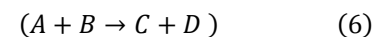
From equation (3), the differential form of (2) is written

$$r = \frac{1}{v_i V}\frac{dn_i}{dt} = -\frac{1}{V}\frac{dn_A}{dt} = kC_A \tag{4}$$

or

$$\frac{df_A}{dt} = k(1 - f_A) \tag{5}$$

Where f_A fractional conversion based on species A, n_A flux of species A, n_i number of moles of species i

If we consider also a reaction in which stoichiometric coefficients are the same as the individual reaction order of each species, such as,

$$(A + B \rightarrow C + D) \tag{6}$$

the rate law would be

$$-r_A = kC_A C_B \tag{7}$$

The basic criterion for equilibrium with a single reaction is:

$$\Delta G = \sum_{i=1}^{2} v_i \mu_i \tag{8}$$

where ΔG is the Gibbs function, v_i is the stoichiometric coefficient of species i, and μ_i is the chemical potential of species i. The chemical potential is:

$$\mu_i = \mu_i^0 + R_g T \ln a_i \tag{9}$$

where R_g is the universal gas constant, μ_i^0 is the standard chemical potential of species i in a reference state such that $a_i = 1$, and a_i is the activity of species i.

Therefore

$$\Delta G - \Delta G^0 = \sum_{i=1}^{2} v_i(\mu_i - \mu_i^0) \tag{10}$$

Using equations (9) and (10)

$$\Delta G - \Delta G^0 = \sum_{i=1}^{2} v_i(\mu_i - \mu_i^0) = R_g T \ln a_i$$

$$= R_g T \left(\ln \prod_i a_j^{v_i} \right)$$

$$\Delta G - \Delta G^0 = R_g T \left(\ln \prod_i a_j^{v_i} \right) \tag{11}$$

Equations (10) and (11) provides the functional form for the temperature dependence of the equilibrium constant:

$$K_a = \bar{K} \exp(-\frac{\Delta H^0}{R_g T}) \qquad (12)$$

Recall that when the reaction is exothermic (ΔH^0 is negative), K_a increases with decreasing T. For endothermic reactions the opposite is true.

For a channel filled with an isobaric binary gas mixture of components A and B. When component A moves it exerts a force on B. This frictional force, ff_{AB}, can be described as:

$$ff_{AB} = \left.\begin{array}{c} \text{proportionality constant} \\ \underbrace{\text{(concentration of A) (concentration of B)}}_{number\ of\ collision} \\ \times \underbrace{\text{(relative velocity of A to B)}}_{\substack{momentum\ excahange \\ per\ collision}} \end{array}\right\}$$

or

$$ff_{AB} = (\text{const})_{AB} C_A C_B (V_A - V_B) \qquad (13)$$

where V_i is the molecular velocity of species i. The total frictional losses have to equal the driving force.

$$-\frac{dP_A}{dz} = (\text{const})_{AB} C_A C_B (V_A - V_B) \qquad (14)$$

Multiply Equation (14) by C (total concentration) and rearrange to give:

$$-CP\frac{dX_A}{dz} = (\text{const})_{AB} C C_A C_B (V_A - V_B) \qquad (15)$$

$$\Rightarrow -\frac{CP}{(\text{const})_{AB} C_A C_B}\frac{dX_A}{dz} = C(V_A - V_B)$$

$$\Rightarrow -\frac{R_g T}{(\text{const})_{AB} X_A X_B}\frac{dX_A}{dz} = C(V_A - V_B) \qquad (16)$$

If the proportionality factor is defined as:

$$(\text{const})_{AB} = \frac{R_g T}{C D_{AB}}$$

then Equation (16) can be written as follows:

$$-\frac{C D_{AB}}{X_A X_B}\frac{dX_A}{dz} = C(V_A - V_B) \qquad (17)$$

Equation (17) is Fick's First Law. To see this, rearrange Equation (17) as shown below:

$$C X_A X_B (V_A - V_B) = -C D_{AB}\frac{dX_A}{dz}$$

$$C_A (X_B V_A - X_B V_B) = -C D_{AB}\frac{dX_A}{dz} \qquad (18)$$

Recall that Fick's First Law is:

$$\bar{J}_A = -C D_{AB}\frac{dX_A}{dz} = C_A(V_A - V_{total})$$

where $\bar{J}_A$ is the flux of A with respect to a coordinate system that is moving at V_{total} and:

$$V_{total} = X_A V_A - X_B V_B$$

Combining equations (16) to (18), fuel concentration, oxygen concentration and Temperature fields could be expressed as

$$\rho\frac{\partial X}{\partial t} = D_1\frac{\partial^2 X}{\partial x^2} - AXY e^{-E/_{RT}} \qquad (19)$$

$$\rho\frac{\partial Y}{\partial t} = D_2\frac{\partial^2 Y}{\partial x^2} - AXY e^{-E/_{RT}} \qquad (20)$$

$$\frac{\partial T}{\partial t} = \frac{K}{\rho c_p}\frac{\partial^2 T}{\partial x^2} + \frac{QA}{\rho c_p}XY e^{-\frac{E}{RT}} - \frac{Q_0(T - T_0)}{\rho c_p} \qquad (21)$$

The appropriate initial and boundary conditions are

$$\left.\begin{array}{c} T(x,0) = T_w(x), X(x,0) = X_w(x), \\ Y(x,0) = Y_w(x), T(-L,t) = T_w(t), \\ X(-L,t) = X_0(t), Y(-L,t) = Y_0(t) \\ T(L,t) = T_w(t), X(L,t) = X_0(t), \\ Y(L,t) = Y_0(t) \end{array}\right\} \qquad (22)$$

Where all the variables and parameters have their usual meaning.

3. METHOD OF SOLUTION

Without loss of generality, $e^{-E/_{RT}}$ is approximated as T^α (see [9]), where $\alpha < 1$ implies non-Newtonian fluids, $\alpha > 1$ dilatant fluids non- $\alpha = 0$ Newtonian fluids

Using the following dimensional quantities

$$\frac{T - T_w}{\epsilon T_w} = \theta, \frac{X}{X_w} = \phi, \frac{Y}{Y_w} = \psi, \epsilon = \frac{R T_0^2}{E}, t = \frac{v}{v_0^2}t', x = \frac{v}{v_0}x'$$

Equations (19) to (21) becomes

$$Sc\frac{\partial\phi(x,t)}{\partial t} = \frac{\partial^2\phi(x,t)}{\partial t^2}$$
$$-Sc\beta_1\phi(x,t)\psi(x,t)(1 + \epsilon\theta(x,t))^\alpha \qquad (23)$$

$$Sc\frac{\partial\psi(x,t)}{\partial t} = \frac{\partial^2\psi(x,t)}{\partial t^2}$$
$$-Sc\beta_2\phi(x,t)\psi(x,t)(1 + \epsilon\theta(x,t))^\alpha \qquad (24)$$

$$Pr\frac{\partial\theta(x,t)}{\partial t} = \frac{\partial^2\theta(x,t)}{\partial t^2}$$
$$+Pr\delta\lambda\phi(x,t)\psi(x,t)\big(1 + \epsilon\theta(x,t)\big)^\alpha - \delta\theta(x,t) \qquad (25)$$

where

$$Sc = \frac{\mu}{D_i}, i = 1,2, \beta_1 = \frac{Av^2 Y_0 T_w{}^\alpha}{\mu v_0^2}, \beta_2 = \frac{Av^2 X_0 T_w{}^\alpha}{\mu v_0^2}, \lambda$$
$$= \frac{AX_0 T_w{}^\alpha}{\epsilon T_0}, Pr = \frac{\mu c_p}{k}, \delta = \frac{v Q_0}{v_0^2 c_p}$$

The boundary condition (22) also becomes

$$\left.\begin{array}{l} \theta(x,0)=0, \phi(x,0)=1, \psi(x,0)=1 \\ \theta(-L,t)=0, \phi(-L,t)=0, \psi(-L,t)=0 \\ \theta(L,t)=0, \phi(L,t)=0, \psi(L,t)=0 \end{array}\right\} \quad (26)$$

Now, we make use of moving grid defined by $\varepsilon = x - vt$, (where v is the flame velocity) to transform equations (23) to (25), we have

$$\frac{d^2\phi(\varepsilon)}{d\varepsilon^2} + v\,Sc\,\frac{d\phi(\varepsilon)}{d\varepsilon}$$
$$-Sc\beta_1\phi(\varepsilon)\psi(\varepsilon)\big(1+\epsilon\theta(\varepsilon)\big)^{\alpha} = 0 \quad (27)$$

$$\frac{d^2\psi(\varepsilon)}{d\varepsilon^2} + v\,Sc\,\frac{d\psi(\varepsilon)}{d\varepsilon}$$
$$-Sc\beta_2\phi(\varepsilon)\psi(\varepsilon)\big(1+\epsilon\theta(\varepsilon)\big)^{\alpha} = 0 \quad (28)$$

$$\frac{d^2\theta(\varepsilon)}{d\varepsilon^2} + v\,Pr\,\frac{d\theta(\varepsilon)}{d\varepsilon}$$
$$+Pr\delta\lambda\phi(\varepsilon)\psi(\varepsilon)\big(1+\epsilon\theta(\varepsilon)\big)^{\alpha} - \delta\theta(\varepsilon) = 0 (29)$$

The above system of coupled ordinary differential equations is solved numerically using finite difference scheme (for detail about the scheme, see [16] and [17]) executed by Maple module for partial differential equations.

4. RESULTS AND DISCUSSION

For the purpose discussing the effect of various parameters on the reaction behavior, calculation have been carried out for different values of $v, \delta, \lambda, \alpha, \beta_1,$ β_2 and t and for fixed values of Sh, Pr and ϵ. In order to point out the effects of various parameters on flow characteristic, to be realistic, the values of Schmidt number (Sc) are chosen for plasma $(Sc = 0.62)$, at temperature 25^oC and one atmospheric pressure. The values of Prandtl number is chosen to be $Pr = 0.71$ which represents air at temperature 25^oC and one atmospheric pressure. Attention is focused on positive values of the heat generation ($\delta > 0$ heat is generated in the system and $\delta < 0$ imply heat is removed from the system) corresponding to source or sink. All parameters are primarily chosen as follows: $\beta_1 = 0.2$, $\beta_2 = 0.15$, $v = 0.4, \delta = 1.0, \alpha = 0.2$ and $\lambda = 0.4$ for a fixed value of $Sc = 0.62, Pr = 0.71$ and $\epsilon = 0.2$ unless otherwise stated.
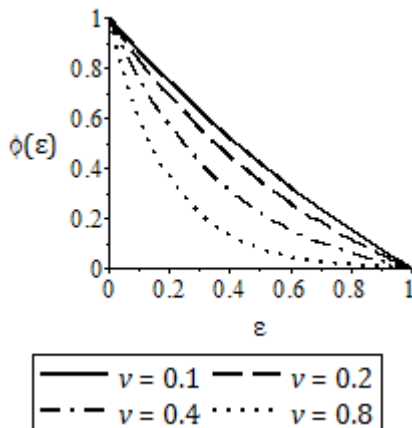

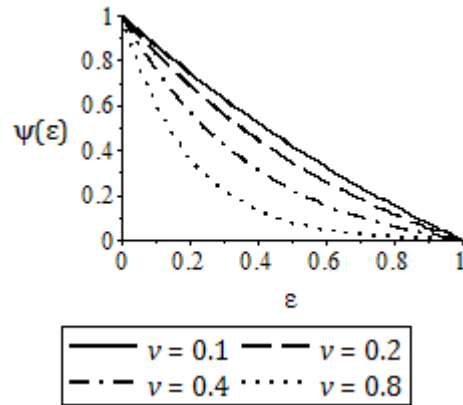Figure 1: Fuel Concentration Profile

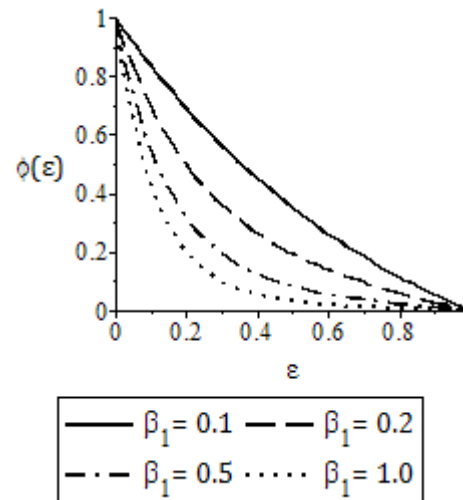Figure 2: Oxygen Concentration Profile

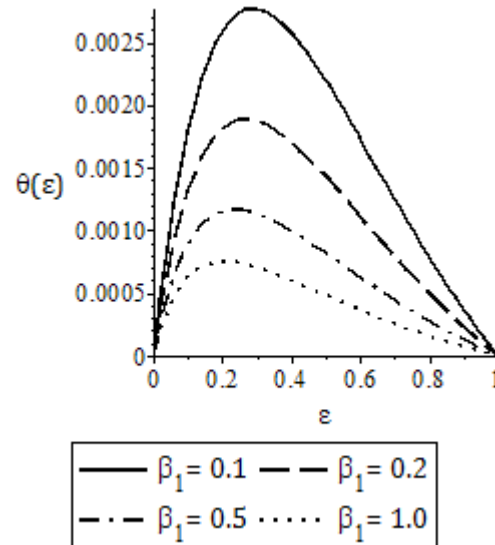Figure 3: Concentration profile for various diffusion coefficients

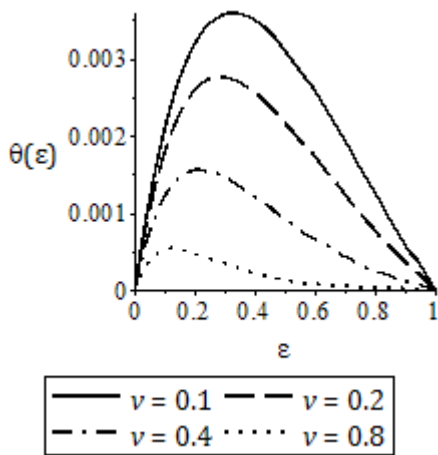Figure 4: Temperature profile for various diffusion coefficient

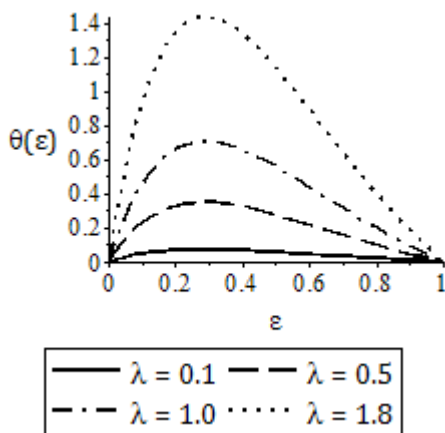Figure 5: Temperature distribution for various values of flame velocity

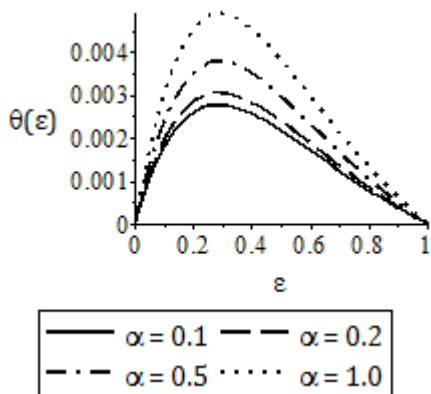Figure 6: Temperature profile for various values of Frank-Kamnetskii parameter

Figure 7: Temperature distribution for different values of power-law exponent

4.1. Species distribution.

The concentration distribution for fuel and oxygen are displayed in figures (1) to (3). We know that the behaviours of both species are similar in the sense that diffusion coefficient and pre-exponential factor of oxidation are the same. The diffusion coefficient of oxygen is taken to be higher than that of fuel, that is $\beta_1 > \beta_2$, however, the properties exhibited are similar. Hence we use either of the fuel or oxygen for our

discussion. Figure (1), (2) and (3) shows the distributions of Fuel and Oxygen. From this figures we could see that concentration decreases as either flame velocity or diffusion coefficient increases. We also observed from these figures that the closer the species to the plate the faster the rate of consumption.
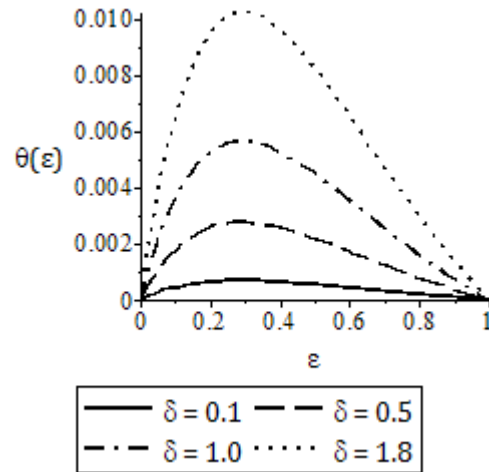

Figure 8: Temperature distribution for different values of heat generation or absorption coefficient

4.2. Temperature field.

In figure (4), we displayed the concentration distribution for various values of diffusion coefficient. We observed that concentration decreases as diffusion coefficient increases. This is in line with what has been reported previously in the literature. Thus, this validates our results. It should also be mentioned that our results also confirmed that concentration of species increases with an increase power-law exponent till a steady state is reached where further increase in power-law exponent becomes insignificant.

The effects of flame velocity, Frank-Kamnetskii parameter, power-law exponent and heat generation on the temperature field are shown graphically in figures (5 – 8). Fig. 5 shoe that increase in flame velocity generally reduces the bulk temperature while an increase in Frank-kamnetskii parameter increases the temperature as shown in fig. 6. We observe from Fig. 7 that increase in power–law exponent increases the temperature exponent till a steady state is reached where further increase in power-law exponent does not affect the generated heat while the effect of heat generation or absorption is shown in figure 8. From this figure, we observed that increase in heat absorption (sink) reduces the bulk temperature, while increase in heat generation (source) brings about increase in temperature.

7. CONCLUSION

The motivation of present research paper is to analyze the flame velocity effect on unsteady endothermic reaction with power-law exponent and

heat Source/Sink conditions, through numerical technique, under which consistency and convergence criterion exist. The theoretical non-linear model for the system has been derived by employing the reaction rate and Fick's laws. From our analysis, the following deductions were made:

- that the closer the species to the plate the faster the rate of consumption.
- concentration decreases as diffusion coefficient increases.
- temperature increases with an increase power-law exponent
- increase in Frank-Kamentskii parameter increases temperature.
- increase in heat absorption (sink) decreases temperature, while increase in heat generation (source) increase in temperature.

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