Volume 3 No 2, February 2013 ISSN 2224-3577

International Journal of Science and Technology

http://www.ejournalofsciences.org

Modelling and Analytical Simulation of the Chemical Kinetics of a Laminar Premixed Flame

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ABSTRACT

In this paper we present a mathematical model of the flame dynamics. We assume that fuel is the limiting species, so that the combustion is lean. Under this assumption, we consider the steady equations describing the flame dynamics in a combustor. We prove the existence and uniqueness of solution by actual solution and examine the properties of solution by transforming the dimensionless equation from infinite domain to finite domain. The equations are solved analytically using asymptotic expansions. The steady-state temperature and concentration distributions profiles are presented and discussed. It is discovered that the Frank-Kamenetskii number plays a crucial role in the flame dynamics and the temperature is increased and species is consumed in the spatial direction.

Keywords : *Chemical kinetics, Combustion, Hydrocarbon fuel, Limiting species, Premixed flame.*

1. INTRODUCTION

Combustion includes many chemical chain reactions and many intermediate species are involved. To model this combustion process, we assume that the reaction satisfies the one-step reaction mechanism of a convectional hydrocarbon fuel

$$C_xH_y + \left(x + \frac{y}{4}\right)O_2 \rightarrow xCO_2 + \frac{y}{2}H_2O \tag{1}$$

The rate of fuel consumption is usually expressed using an Arrhenius term

$$\frac{d[C_xH_y]}{dt} = -A[C_xH_y]^m[O_2]^n e^{-\frac{E_a}{R_uT}} \tag{2}$$

For a premixed laminar flame, methane react with air in the form of

$$CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2, \tag{3}$$

where $m = 1,\ n = 1$.

Many gas-phase mixture or pure substances that react or decompose exothermically are capable of supporting a low-velocity subsonic decomposition wave, which is called a flame [1]. Zeldovitch et al. [2] were the first to model purely gaseous premixed flames with a chain mechanism using a two-step chemical mechanism. Other work followed using this non-linear mechanism (see, for example, a modified mechanism by Dold et al. [3]). The advantage of the latter mechanism is the fact that it takes the chain breaking or completion step to be linear in the concentration of some intermediate radical or species. This is completely consistent with the final state being an equilibrium one in a broader chemical system and bears the added advantage of enabling mathematical tractability. Hammoud and Souidi [4] presented a numerical method for the study of chemically reacting flow in laminar premixed flame of carbon monoxide / oxygen mixture in the region of the stagnation point. Hu et al. [5] conducted numerical study on laminar burning velocity and NO formation of the premixed methane–hydrogen–air flames at room temperature and atmospheric pressure. The unstretched laminar burning velocity, adiabatic flame temperature, and radical mole fractions of H, OH and NO are obtained at various equivalence ratios and hydrogen fractions. In another related paper, Hu et al. [6] conducted experimental and numerical study on the lean methane–hydrogen–air flames at elevated pressures and temperatures. The unstretched laminar burning velocities and Markstein lengths were obtained over a wide range of hydrogen fractions at elevated pressures and temperatures. Olayiwola et al. [7] considered a steady, adiabatic, premixed laminar flame in an approximation in which all species concentrations can be related to the temperature T as the single dependent variable. They provided an analytical solution for the model with variable thermal conductivity. .

In this paper we study mathematically the chemical kinetics of a laminar premixed flame. We assume that the fuel is the limiting species, so that combustion is lean. We examine the properties of solution. To simulate the flow, we assume that the incoming mixture is at the burner temperature.

2. MODEL FORMULATION

Here, we study lean premixed laminar flame, and equivalence ratio $\phi < 1$. Under this assumption, the governing equations that describe the flame dynamics in a combustor are

Conservation of mass

$$\rho\frac{du}{dx}=0 \qquad (4)$$

Conservation of momentum

$$u\frac{du}{dx}=-\frac{1}{\rho}\frac{dp}{dx}+\upsilon\frac{d^2u}{dx^2} \qquad (5)$$

Conservation of species

$$u\frac{dY_k}{dx}=\frac{1}{\rho}\frac{d}{dx}\left(\rho D_k\frac{dY_k}{dx}\right)-\frac{1}{\rho}R_kM_k \qquad (6)$$

Conservation of energy

$$u\frac{dT}{dx}=\frac{1}{\rho c_p}\frac{d}{dx}\left(\lambda\frac{dT}{dx}\right)+\frac{1}{\rho c_p}\sum_{k=1}^{N}R_kM_kh_k \qquad (7)$$

From the continuity equation (4), we obtain

$u=$ constant (8)

Here, we let

$u=-v_0,\quad v_0>0$ (9)

We make the additional assumptions that c_p, λ and D are constant and equal for all species. Although these assumptions could be relaxed in the future, they considerably simplify the equations. Thus the equations (4) – (9) can be simplified as

$$D\frac{d^2Y}{dx^2}+v_0\frac{dY}{dx}-\frac{1}{\rho}RM=0 \qquad (10)$$

$$\frac{\lambda}{\rho c_p}\frac{d^2T}{dx^2}+v_0\frac{dT}{dx}+\frac{1}{\rho c_p}RM\Delta h=0, \qquad (11)$$

where T is the temperature, Y is the mass fraction of the fuel (assumed to be the limiting species), ρ is the density, x is the position, λ is the thermal conductivity, c_p is the specific heat at constant pressure, Δh is the heat of reaction, D is the diffusion coefficients and R is the rate term in Arrhenius form

$$R=\upsilon_f k\rho^{\upsilon_f+\upsilon_o}M_o^{-\upsilon_o}M_f^{-\upsilon_f}Y_o^{\upsilon_o}Y_f^{\upsilon_f}e^{-\frac{E}{RT}}, \qquad (12)$$

where Y_f, Y_o are the mass fraction of the fuel and oxidizer, and M_f, M_o are molecular weights. υ_f, υ_o are the correspond stoichiometric coefficients and k is the pre exponential constant.

The boundary conditions were formulated as follows:

$$\left.\begin{array}{ll} T|_{x=0}=T_{burner}, & Y|_{x=0}=Y_0 \\ \lim_{x\to\infty}T(x)=T_0, & \lim_{x\to\infty}Y(x)=0 \end{array}\right\} \qquad (13)$$

3. METHOD OF SOLUTION

3.1 Existence and Uniqueness Solution |

Theorem 1 Let $D=\frac{\lambda}{\rho c_p}$. Then there exists a unique solution of problem (10) – (12) satisfy (13).

Proof: Let $D=\frac{\lambda}{\rho c_p}$ and $\phi=\left(T+\frac{\Delta h}{c_p}Y\right)$. Then (10) - (12) become

$$D\frac{d^2\phi}{dx^2}+v_0\frac{d\phi}{dx}=0 \qquad (14)$$

$$\phi(0)=T_{burner}+\frac{\Delta h}{c_p}Y_0,\ \phi(x)\to T_0\ as\ x\to\infty \qquad (15)$$

We obtain the solution of problem (14) as

$$\phi(x)=\left((T_{burner}-T_0)+\frac{\Delta h}{c_p}Y_0\right)e^{-\frac{v_0}{D}x}+T_0 \qquad (16)$$

Then, we obtain

Volume 3 No.2, February 2013 ISSN 2224-3577

International Journal of Science and Technology

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$$T(x)=\left[\left(\begin{array}{l}(T_{burner}-T_0)+\\ \frac{\Delta h}{c_p}Y_0\end{array}\right)e^{-\frac{v_0}{D}x}+T_0-\frac{\Delta h}{c_p}Y(x)\right] \quad (17)$$

$$Y(x)=\frac{c_p}{\Delta h}\left[\left(\begin{array}{l}(T_{burner}-T_0)+\\ \frac{\Delta h}{c_p}Y_0\end{array}\right)e^{-\frac{v_0}{D}x}+T_0-T(x)\right] \quad (18)$$

Hence, there exists a unique solution of problem (10) – (12). This completes the proof.

3.2 Non-dimensionalisation

We make the variables dimensionless by introducing

$$\theta=\frac{E}{RT_0^2}(T-T_0),\ Y^{*}=\frac{Y}{Y^{0}},\ x^{*}=\frac{x}{L},\ v_0=\frac{D}{L} \quad (19)$$

and using (18), equations (10) and (11) (after dropping prime) become

$$\frac{d^2Y}{dx^2}+\frac{dY}{dx}-\sigma\left(ae^{-x}-b\theta\right)^{v_f+v_o}e^{\frac{\theta}{1+\epsilon\theta}}=0 \quad (20)$$

$$\frac{d^2\theta}{dx^2}+\frac{d\theta}{dx}+\delta\left(ae^{-x}-b\theta\right)^{v_f+v_o}e^{\frac{\theta}{1+\epsilon\theta}}=0 \quad (21)$$

$$Y(0)=Y_0,\qquad Y(x)\rightarrow 0\ \text{as}\ x\rightarrow\infty \quad (22)$$

$$\theta(0)=\theta_0,\qquad \theta(x)\rightarrow 0\ \text{as}\ x\rightarrow\infty. \quad (23)$$

where

$$a=\frac{c_p}{\Delta h}(T_{burner}-T_0)+Y_0,\quad b=\frac{c_p\epsilon T_0}{\Delta h}$$

$$\delta=\frac{\Delta h M\upsilon_f k\rho^{v_f+v_o}M_o^{-v_o}M_f^{-v_f}\left(Y^0\right)^{v_f+v_o}e^{-\frac{E}{RT_0}}}{\rho c_p\epsilon T_0 v_0}$$ is the Frank-Kamenetskii parameter

$$\sigma=\frac{M\upsilon_f k\rho^{v_f+v_o}M_o^{-v_o}M_f^{-v_f}\left(Y^0\right)^{v_f+v_o-1}e^{-\frac{E}{RT_0}}}{\rho v_0}$$

When $\epsilon\rightarrow 0$, equations (20) and (21) become

$$\frac{d^2Y}{dx^2}+\frac{dY}{dx}-\sigma\left(ae^{-x}-b\theta\right)^{v_f+v_o}e^{\theta}=0 \quad (24)$$

$$\frac{d^2\theta}{dx^2}+\frac{d\theta}{dx}+\delta\left(ae^{-x}-b\theta\right)^{v_f+v_o}e^{\theta}=0 \quad (25)$$

3.3 Properties of Solution

We consider equation (25) when $\theta_0=0$ and transform the equation from infinite domain to finite domain, using $y=e^{-x}$ and we obtain

$$\frac{d^2\theta}{dy^2}+\frac{\delta}{y^2}\left(ay-b\theta\right)^{v_f+v_o}e^{\theta}=0 \quad (26)$$

$$\theta(0)=0,\qquad \theta(1)=0$$

Theorem 2 Let $b=0$ and $v_o=v_f=1$ in (26). Then $\theta(y)$ is symmetric about $y=\frac{1}{2}$.

Proof: Let $b=0$ and $v_o=v_f=1$ in (26). We obtain

$$\frac{d^2\theta(y)}{dy^2}+\delta_1 e^{\theta(y)}=0,\quad \theta(0)=0,\quad \theta(1)=0.$$

Let $z=2y-1$

Then

$$\frac{d^2}{dy^2}=4\frac{d^2}{dz^2}$$

So the problem becomes

$$\frac{d^2\theta(z)}{dz^2}+\frac{\delta_1}{4}e^{\theta(z)}=0,\quad \theta(-1)=\theta(1)=0$$

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It suffices to show that $\theta(-z)=\theta(z)$.

Replace z by $-z$. We obtain

$$\frac{d^2\theta(-z)}{d(-z)^2}+\frac{\delta_1}{4}e^{\theta(-z)}=0$$

Hence θ is symmetric about $z=0$ i.e. θ is symmetric about $y=\frac{1}{2}$. This completes the proof.

Theorem 3 Let $b=0$ and $v_0=v_f=1$ in (26). Then $\theta'\left(\frac{1}{2}\right)=0$.

Proof: Let $b=0$ and $v_0=v_f=1$ in (26). We obtain

$$\frac{d^2\theta(y)}{dy^2}+\delta_1 e^{\theta(y)}=0$$

$$\theta(0)=0, \qquad \theta(1)=0.$$

Since $\theta(y)$ is symmetric about $y=\frac{1}{2}$. Then $\theta'\left(\frac{1}{2}\right)=0$.

This completes the proof.

Theorem 4 Let $b=0$ and $v_0=v_f=1$ in (26). Then $\theta'(y)>0$ for $y\in\left(0,\frac{1}{2}\right)$.

Proof: Let $b=0$ and $v_0=v_f=1$ in (26). We obtain

$$\frac{d^2\theta(y)}{dy^2}=-\delta_1 e^{\theta(y)}$$

$$\theta(0)=0, \qquad \theta(1)=0.$$

Using Ayeni [8], we obtain

$$\theta(y)=\delta_1\int_0^{\frac{1}{2}}k(y,t)e^{\theta(t)}dt,$$

where

$$k(y,t)=\begin{cases} y, & 0\le y\le t \\ t, & t\le y\le \frac{1}{2}\end{cases}$$

So

$$\theta'(y)=\delta_1\left[ye^{\theta(y)}+\int_y^{\frac{1}{2}}e^{\theta(t)}dt-ye^{\theta(y)}\right]$$
$$=\delta_1\int_y^{\frac{1}{2}}e^{\theta(t)}dt$$

Hence, $\theta(y)$ is strictly monotonically increasing for $y\in\left(0,\frac{1}{2}\right)$. This completes the proof.

3.4 Analytical Solution

Here, we consider equations (24) and (25) when $v_0=v_f=1$. Ayeni [9] has shown that $\exp(\theta)$ can be approximated as $1+(e-2)\theta+\theta^2$. In this paper we are going to take an approximation of the form

$$\exp(\theta)\approx 1+(e-2)\theta \tag{27}$$

Using the asymptotic expansion

$$\theta=\theta_0+\in\theta_1+\in^2\theta_2+h.o.t. \tag{28}$$

$$Y=Y_0+\in Y_1+\in^2 Y_2+h.o.t., \tag{29}$$

where $h.o.t.$ read "higher order terms in $\in$. In our analysis we are interested only in the first three terms.

Let

$$a=\in a_0 \tag{30}$$

neglecting the nonlinear terms and equate the powers of $\in$, we have

$O(1)$:

$$\frac{d^2\theta_0}{dx^2}+\frac{d\theta_0}{dx}=0 \tag{31}$$

Volume 3 No.2, February 2013 ISSN 2224-3577

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$$\theta_0(0)=\theta_b, \qquad \theta_0(\infty)=0$$

$$\frac{d^2Y_0}{dx^2}+\frac{dY_0}{dx}=0 \tag{32}$$

$$Y_0(0)=Y_0, \qquad Y_0(\infty)=0$$

$O(\in)$:

$$\frac{d^2\theta_1}{dx^2}+\frac{d\theta_1}{dx}-2\delta a_0 b e^{-x}\theta_0=0 \tag{33}$$

$$\theta_1(0)=0, \qquad \theta_1(\infty)=0$$

$$\frac{d^2Y_1}{dx^2}+\frac{dY_1}{dx}+2\delta a_0 b e^{-x}\theta_0=0 \tag{34}$$

$$Y_1(0)=0, \qquad Y_1(\infty)=0$$

$O(\in^2)$:

$$\frac{d^2\theta_2}{dx^2}+\frac{d\theta_2}{dx}+\delta\begin{pmatrix} a_0^2e^{-2x}-2a_0be^{-x}\theta_1+ \\ a_0^2(e-2)e^{-2x}\theta_0\end{pmatrix}=0 \tag{35}$$

$$\theta_2(0)=0, \qquad \theta_2(\infty)=0$$

$$\frac{d^2Y_2}{dx^2}+\frac{dY_2}{dx}-\sigma\begin{pmatrix} a_0^2e^{-2x}-2a_0be^{-x}\theta_1+ \\ a_0^2(e-2)e^{-2x}\theta_0\end{pmatrix}=0 \tag{36}$$

$$Y_2(0)=0, \qquad Y_2(\infty)=0$$

We obtain the solution of (31) - (36) respectively as

$$\theta_0(x)=\theta_b e^{-x} \tag{37}$$

$$Y_0(x)=Y_0 e^{-x} \tag{38}$$

$$\theta_1(x)=\delta a_0 b\theta_b\left(e^{-2x}-e^{-x}\right) \tag{39}$$

$$Y_1(x)=-\sigma a_0 b\theta_b\left(e^{-2x}-e^{-x}\right) \tag{40}$$

$$\theta_2(x)=-\begin{pmatrix}-\frac{1}{2}\delta a_0^2-\frac{2}{3}\theta_b a_0^2 b^2\delta^2- \\ \frac{1}{6}\theta_b a_0^2 e\,\delta+\frac{1}{3}\theta_b a_0^2\delta\end{pmatrix}e^{-x}+ \\ \frac{1}{3}\delta^2 a_0^2 b^2\theta_b e^{-3x}-\delta^2 a_0^2 b^2\theta_b e^{-2x}- \\ \frac{1}{6}\delta a_0^2 e\,\theta_b e^{-3x}+\frac{1}{3}\delta a_0^2\theta_b e^{-3x}-\frac{1}{2}\delta a_0^2 e^{-2x} \tag{41}$$

$$Y_2(x)=-\frac{1}{6}\sigma a_0^2\left(3+4\delta b^2\theta_b+\theta_b e-2\theta_b\right)e^{-x} \\ -\frac{1}{3}\sigma a_0^2\delta b^2\theta_b e^{-3x}+\sigma a_0^2\delta b^2\theta_b e^{-2x}+ \\ \frac{1}{6}\sigma a_0^2 e\theta_b e^{-3x}-\frac{1}{3}\sigma a_0^2\theta_b e^{-3x}+\frac{1}{2}\sigma a_0^2 e^{-2x} \tag{42}$$

Therefore, we obtain

$$\theta(x)=\theta_b e^{-x}+a\delta b\theta_b\left(e^{-2x}-e^{-x}\right)+ \\ \begin{pmatrix} -\begin{pmatrix}-\frac{1}{2}\delta a^2-\frac{2}{3}\theta_b a^2b^2\delta^2- \\ \frac{1}{6}\theta_b a^2 e\,\delta+\frac{1}{3}\theta_b a^2\delta\end{pmatrix}e^{-x}+ \\ \frac{1}{3}\delta^2 a^2b^2\theta_b e^{-3x}-\delta^2a^2b^2\theta_b e^{-2x}- \\ \frac{1}{6}\delta a^2 e\,\theta_b e^{-3x}+\frac{1}{3}\delta a^2\theta_b e^{-3x}- \\ \frac{1}{2}\delta a^2 e^{-2x}\end{pmatrix} \tag{43}$$

$$Y(x) = Y_0 e^{-x} + \sigma ab\theta_b \left(e^{-x} - e^{-2x}\right) + \begin{pmatrix} -\frac{1}{6}\sigma a^2 \left(3 + 4\delta b^2\theta_b + \theta_b e - 2\theta_b\right) e^{-x} \\ -\frac{1}{3}\sigma a^2 \delta b^2 \theta_b e^{-3x} + \sigma a^2 \delta b^2 \theta_b e^{-2x} \\ +\frac{1}{6}\sigma a^2 e \theta_b e^{-3x} - \frac{1}{3}\sigma a^2 \theta_b e^{-3x} + \\ \frac{1}{2}\sigma a^2 e^{-2x} \end{pmatrix} \quad (44)$$

4. RESULTS AND DISCUSSION

The existence and uniqueness of solution of the Problem is proved by the actual solution. Under certain conditions, we have shown that (i) $\theta(x)$ is symmetric about $x = \frac{1}{2}$, (ii) $\theta'\left(\frac{1}{2}\right) = 0$ and (iii) $\theta(x)$ is strictly monotonically increasing for $x \in \left(0, \frac{1}{2}\right)$. Analytical solutions given by equations (43) and (44) are computed for the values of $a = 1.0,\ b = 1.0,\ \theta_b = 0.01,\ \in = 0.01,\ e = 2.718,\ v_o = v_f = 1$. The concentration and temperature values are depicted graphically in Figures 1 and 2.

The temperature distribution behavior along the spatial direction is shown in Figure 1. Figure 1 depicts the graph of $\theta(x)$ against x for different values of δ. It is observed that the temperature increases along spatial direction as Frank-Kamenetskii number increases. The concentration distribution behavior along the spatial direction is shown in Figure 2. Figure 2 depicts the graph of $Y(x)$ against x for different values of δ. It is observed that the concentration does not change much with increase in Frank-Kamenetskii number.

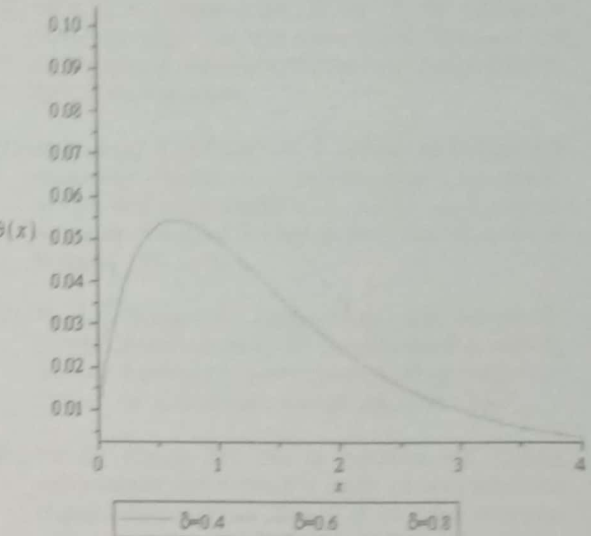

Figure 1: Plots of $\theta(x)$ against x for equation (25) for different values of δ and $a = 1,\ b = 1,\ \theta_b = 0.01,\ \epsilon = 0.01,\ e = 2.718,\ v_o = v_f = 1$

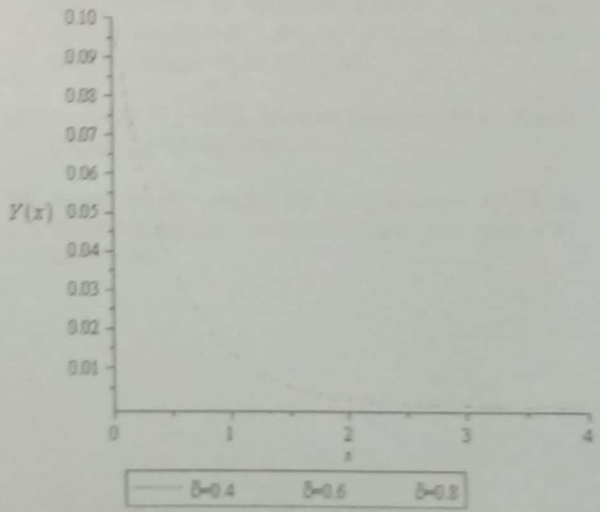

Figure 2: Plots of $Y(x)$ against x for equations (24) and (25), for different values of δ and $a = 1,\ b = 1,\ \theta_b = 0.01,\ \epsilon = 0.01,\ e = 2.718,\ v_o = v_f = 1$

It is worth pointing out that the effect of δ as shown in Figures 1 and 2 indicating that there is increase in heat of reaction Δh. When the heat of reaction is high, the rate of conversion of hydrocarbon fuel into water and gas is high. This is of great economic importance.

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5. CONCLUSION

To study the dynamic response of the heat release model, we used high activation energy asymptotics and analytical solution via asymptotic expansions is obtained for steady-state, also called equilibrium solutions of the flame model. The governing parameter for the problem under study is the Frank-Kamenetskii number. Considering the physical constraints, the temperature must increase and species be consumed in the positive spatial direction. The analytical method is used to search for steady state temperature and species mass fraction profiles. The temperature and species mass fraction profiles are significantly influenced by the parameter involved. The analytical solution of the problem may help model numerical solutions and codes. It may be used as a preliminary predictive tool to study mathematically the dynamics of a laminar premixed flame. The work may be extended to more complex cases such as transient state and two-dimensional cases and therefore, recommended for further research.

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