COUNTERFLOW COMBUSTION OF MICRO ORGANIC PARTICLES

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ABSTRACT

The structure ofcounterflowpremixed flames in an axisymmetric configuration, containing uniformly distributed volatile fuel particles, with nonunity Lewis number of the fuel are examined. It is presumed that the gaseous fuel, produced from vaporization of the fuel particles, oxidizes in the gas phase and the fuel particles do not participate in the reaction. The analysis is carried out in the asymptotic limit for large values of Zeldovich number.A one-step reaction $v_F[F] + v_{O_2}[O_2] \rightarrow v_{product}[P]$ is assumed. The flame position is determined andthe effect of Lewis number change on the gaseous fuel mass fraction distribution is investigated.

KEYWORDS: Lapping, grinding, surface roughness, micro, nano scale.

1.0   INTRODUCTION

Many studies of dust clouds combustion have been published over the last few years; see, for example, introduction of the article on flame propagation through micro-organic dust particles (Bidabadi *et.al.*, 2010). But from the fact that in many practical applications the flow field is appreciably strained, to yield realistic flame prediction under such conditions, counterflow configuration is suitable for studying these cases. Over the last few decades, the counterflow configuration has been extensively adopted in theoretical, experimental and numerical studies as a means to investigate various physical effects on real flames on real flames, such as stretch, preferential diffusion, radiation and chemical kinetics (Daou, 2011), (Thatcher *et.al.*) and (Wang *et.al.*, 2007). But these studies are done for gaseous fuels. Eckhoff clarified the differences and similarities between dust and gases (Eckhof, 2006). It has been concluded that there are two basic differences between

dusts and gases which are of substantially greater significance in design of safety standards than these similarities. Firstly, the physics of generation and up-keeping of dust clouds and premixed gas/vapor clouds are substantially different. Secondly, contrary to premixed gas flame propagation, the propagation of flames in dust/air mixtures is not limited to the flammable dust concentration range of dynamic clouds. Thus here we modeled counterflow combustion of dust clouds and the effect of Lewis number on gaseous fuel mass fraction distribution is investigated.

A model is developed for describing a one dimensional, axisymmetric, premixed flame in a counterflow configuration. Uniformly distributed volatile fuel particles in air are considered as the entering materials. The initial number density of the particles, n_u (number of particles per unit volume) and the initial radius r_u are presumed to be known.

In the analysis it is presumed that the fuel particles vaporize to form a known gaseous compound which is then oxidized. In other words particles do not participate in the reaction. The kinetics of vaporization are presumed to be of the form:

$$w_v = An_s 4\pi r^2 T \tag{1}$$

Where the units of w_v are mass of gaseous fuel vaporized per unit volume per second. The quantity A is constant which is presumed to be known, and T denotes the gas temperature. For simplicity it is assumed that gas and particle have same temperature.

The combustion process is represented by one–step irreversible reaction of the form

$$v_F[F] + v_{O_2}[O_2] \rightarrow v_{product}[P] \tag{2}$$

Where the symbols F, O_2 and P denote the fuel, oxygen and product, respectively, and the quantities v_F, v_{O2}, and $v_{product}$ denote their respective stoichiometric coefficients. The Zeldovich number is presumed to be large and is defined as

$$Z_e = \frac{E(T_f - T_u)}{RT_f^2} \tag{3}$$

In this paper subscript f denotes conditions in the flame and the subscript

u denotes conditions at the inlet. The quantities *E* and *R* represent respectively the activation energy and the universal gas number.
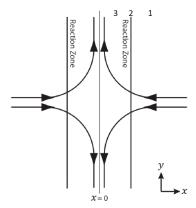

Figure 1 The counterflow configuration and twin planar premixed flames

In Figure 1 we have illustrated the considered configuration including the planar twin flames. Reactants enter from ±x direction and exhaust gases exit in the ±y direction. The flame structure consists of a broad preheat-vaporization zone, a thin reaction zone and a post flame zone. In the formulation,subscripts1, 2 and 3are respectively used to show these zones. To determine the structure of these zones, a number of approximations are introduced in the conservation equations governing their structure.In the preheat-vaporization zone the rate of reaction between the fuel andoxidizer is presumed to be small and the structure of this layer is determined from a balance between the convective, diffusive, and vaporization terms in the conservation equation. In the thin reaction zone the convective and vaporization terms are presumed to be small in comparison with the diffusive and reactive terms.It is assumed that all of the particles vaporizes just before the flame, thus in the post flame zone the vaporization term is not considered.

As it has been mentioned in (Seshadri *et.al,*. 1992) for large values of n_u, φ_u>0.7, where φ_u is equivalence ratio based on fuel available in the particles in the ambient reactant stream, the standoff distance of the envelope flame surrounding each particle is much larger than the characteristic separation distance between the particles. Thus, the analysis developed here is only valid for φ_u>0.7.

The velocity field has components (-*ax*,*ay*,0)in the Cartesian directions, where *a* is the (dimensional) strain rate. For small values of strain rate we can consider the problem as one dimensional. All external forces are

assumed to be negligible. Also diffusion caused by pressure gradient is neglected.

It is also assumed that the ratio $\frac{n_s}{\rho}$ is constant, where ρ is the density of the mixture of gas and the fuel particles.
The one dimensional governing equations are

$$-ax\frac{dT}{dx} = D_T\frac{d^2T}{dx^2} + \omega_F\frac{Q}{\rho C} - \omega_v\frac{Q_v}{\rho C}$$

(4)

$$-ax\frac{dY_F}{dx} = D_F\frac{d^2Y_F}{dx^2} - \frac{\omega_F}{\rho} + \frac{\omega_v}{\rho}$$

(5)

$$-ax\frac{dY_s}{dx} = -\frac{\omega_v}{\rho}$$

(6)

$$\rho T = constant$$

(7)

In Eqs. 4-7, ϱ denotes density, D_T and D_F represent diffusion coefficients for heat and fuel respectively, ω_F is the reaction rate and it's unit is mass of gaseous fuel consumed per unit volume per second, Q stands for the heat release per unit mass of the fuel burned, Q_v is the heat associated with vaporizing unit mass of the fuel, Y_F is the mass fraction of the fuel, C is the combined heat capacity of the gas and of the particles and Y_s denotes mass fraction of the particles. Further approximation introduced in Eqs. 4-7 are that the mean molecular weight do not vary and that the thermal conductivity of the mixture, λ, is constant and the diffusion coefficient, D, is proportional to T. Also particles diffusion is neglected and the density of a fuel particle, ρ_s, is presumed to be constant.

Given the symmetry of the configuration about the plane $x=0$, we only solve the problem for $x>0$ with the boundary conditions

$$T = T_u \ , \qquad Y_F = 0 \ , \ Y_s = Y_{Fu} \qquad as \ x \to \infty$$

$$\frac{dT}{dx} = 0 \ , \quad \frac{dY_F}{dx} = 0 \ , \quad \frac{dY_s}{dx} = 0 \qquad at \ x = 0$$

Where Y_{Fu} denotes the mass fraction of fuel available in the particles.

Nondimensionalization of governing equations

we define the following rescaled variables

$$\theta = \frac{T - T_u}{T_f - T_u} \quad , \quad y_F = \frac{Y_F}{Y_{FC}} \quad , \quad y_s = \frac{Y_s}{Y_{FC}}, \quad x' = \frac{x}{L}$$

(8)

where T_f is the maximum temperature attained in the reaction zone, calculated neglecting the heat of vaporization of the particles. The quantity Y_{FC} is chosen such that

$$Y_{FC}Q = C(T_f - T_u)$$

(9)

In Eq. 8, L is mixing layer thickness and is defined by $L = \sqrt{\frac{2D_T}{a}}$.

With introducing Eqs. 8 and 9 into governing equations, we obtain their non-dimensional form

$$-2x'\frac{d\theta}{dx'} = \frac{d^2\theta}{dx'^2} + \frac{\omega}{\rho} - q\gamma(y_s)^{\frac{2}{3}}\theta$$

(10)

$$-2x'\frac{dy_F}{dx'} = \frac{1}{Le}\frac{d^2y_F}{dx'^2} - \frac{\omega}{\rho} + \gamma y_s^{\frac{2}{3}}\theta$$

(11)

$$2x'\frac{dy_s}{dx'} = \gamma y_s^{\frac{2}{3}}\theta$$

(12)

Where the radius r has been rewritten in terms of y_s using the relation

$$y_s = \frac{4\pi r^3 n_s \rho_s}{3\rho Y_{FC}}$$

(13)

Further assumption used in Eqs. 10-12 is that the rate of vaporization is expected to be dominant near the reaction zone, for $\frac{T_f - T_u}{T_u} \gg 1$, the vaporization rate shown in Eq. 1 was presumed to be proportional to $(T - T_u)$. The quantities γ and ω used above are given by

$$\gamma = \frac{9.67An_u^{\frac{1}{3}}(T_f - T_u)}{aY_{FC}^{\frac{1}{3}}\rho_u^{\frac{1}{3}}\rho_s^{\frac{2}{3}}}$$

(14)

$$\omega = \frac{2\omega_F}{aY_{FC}}$$

(15)

$$q = \frac{Q_v}{Q}$$

(16)

Where the quantity q is the ratio of the heat required to vaporize the fuel particles to the overall heat release in the flame and is presumed to be small in this analysis. If θ^0 represents the nondimensionalized temperature for $q=0$, then non-dimensional equations transform into

$$-2x' \frac{d\theta^0}{dx'} = \frac{d^2\theta^0}{dx'^2} + \frac{\omega}{\rho}$$

(17)

$$-2x' \frac{dy_F}{dx'} = \frac{1}{Le} \frac{d^2 y_F}{dx'^2} - \frac{\omega}{\rho} + \gamma y_s^{\frac{2}{3}} \theta^0$$

(18)

$$2x' \frac{dy_s}{dx'} = \gamma y_s^{\frac{2}{3}} \theta^0 \quad [19]$$

With the boundary conditions

$$y_F = 0 \ , \ \theta^0 = 0 \ , \ y_s = \alpha \qquad as \ x' \to \infty$$

$$\frac{d\theta^0}{dx'} = 0 \ , \ \frac{dy_F}{dx'} = 0 \ , \ \frac{dy_s}{dx'} = 0 \qquad at \ x' = 0$$

Where

$$\alpha = \frac{Y_{Fu}}{Y_{FC}}$$

(19)

2.0   ASYMPTOTIC ANALYSIS

2.1   Preheat-vaporization zone

In the asymptotic limit $Z_e \to \infty,$, we can neglect chemical reaction between the gaseous fuel and oxidizer in the preheat-vaporization zone. Thus the energy equation in this zone reduces to

$$-2x' \frac{d\theta^0{}_1}{dx'} = \frac{d^2\theta^0{}_1}{dx'^2}$$

(20)

Since, by definition T_f is the flame temperature in the reaction zone, $\theta^0 = 1$ at $x' = x'^*$ is the flame position. Using boundary condition we have

$$\theta^0{}_1 = \frac{1 - \text{erf}(x')}{1 - \text{erf}(x'^*)}$$

(21)

Introducing Eq. 21 into the Eq. 19 using the boundary condition yields

$$y_{s_1} = \left(\int_{x'^*}^{x'} \frac{\gamma}{6x'} \left(\frac{1 - \text{erf}(x')}{1 - \text{erf}(x'^*)} \right) dx' \right)^3$$

(22)

Introducing Eqs. 21 and 22 into Eq. 18 and integratingit once, results in

$$\int_{x'^*}^{\infty} 2y_{F_1} dx' = \frac{1}{Le} \left(\left(\frac{dy_{F_1}}{dx'} \right)_{\infty} - \left(\frac{dy_{F_1}}{dx'} \right)_{x'^*+} \right)$$
$$+ \left(\frac{\gamma}{1 - \text{erf}(x'^*)} \right) \int_{x'^*}^{\infty} \left(\int_{x'^*}^{x'} \frac{\gamma}{6x'} \left(\frac{1 - \text{erf}(x')}{1 - \text{erf}(x'^*)} \right) dx' \right)^2 (1 - \text{erf}(x')) dx'$$

(23)

Where boundary conditions are used in writing Eq. 23. Also as the value of T_f is sufficiently high, it is assumed that $y_{Ff} = 0$, where y_{Ff} is gaseous fuel mass fraction in the reaction zone.

In the post flame zoneas we have assumed that all of the particles vaporizes just before the flame, the reaction and vaporization terms are not considered. Thus

$$\left(\frac{d\theta^0}{dx'} \right)_{x'^*-} = \left(\frac{dy_F}{dx'} \right)_{x'^*-} = 0$$

Where the subscript, - denotes conditions at the interface between post flame zone and the reaction zone.

The jump conditions across the reaction zone which are used in finding flame position are

$$\left(\frac{d\theta^0}{dx'} \right)_{x'^*+} + \frac{1}{Le} \left(\frac{dy_F}{dx'} \right)_{x'^*+} = \left(\frac{d\theta^0}{dx'} \right)_{x'^*-} + \frac{1}{Le} \left(\frac{dy_F}{dx'} \right)_{x'^*-}$$

(24)

Where the subscript + denotes conditions at the interface between preheat-vaporization zone and the reaction zone.

3.0   RESULTS AND DISCUSSION

For purpose of illustration it will be assumed that the gaseous fuel that evolves from the fuel particles is methane. The values of A, n_u, ρ_u, ρ_s and T_u are considered to be $3.4 \times 10^{-5} \frac{kg}{m^2 Ks}$, $3.9 \times 10^9 m^{-3}$, $1.135 \frac{kg}{m^3}$, $1000 \frac{kg}{m^3}$ and $300K$ respectively, based on (Seshadri *et.al,*. 1992).

Also $T_f = 1450K$, $C = 0.33 \frac{cal}{gK} = 1386 \frac{kJ}{kgK}$ and $Y_{FC} = 28.6$ are chosen from (Seshadri *et.al,*. 1992) based on φ_u=1 and r_u=20μm assumption. Where φ_u is equivalence ratio based on fuel available in the ambient reactant stream and r_u is radius of fuel particle in the ambient reactant stream.

The value of x'^{*} is calculated with trial and error method. A value is guessed. Then equation 22 is solved and the answer is substituted in 18 neglecting reaction term. This equation is solved numerically to find the first term of equation 23. At last Eq. 24 is used to find the next guess. This is done until convergence. The value that is obtained is x'^{*} =1.71, which results in

$$\theta^0{}_1 = 64.1313(1 - \text{erf}(x'))$$

(25)

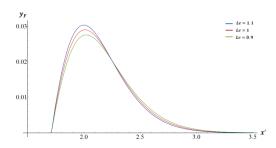$$y_{s_1} = (199.8759 \int_{1.71}^{x'} \frac{erfc(x')}{x'} dx')^3$$

(26)

Figure 2 effect of Lewis number on gaseous mass fraction distribution in preheat-vaporization zone

Eqs. 25 and 26 are used to find gaseous fuel mass fraction distribution in the preheat-vaporization zone, which the result is plotted in Figure 2. This Figure shows that Lewis number has a dual effect on gaseous fuel mass fraction distribution. First, since heat diffusion increases with increasing values of Lewis number, gaseous fuel mass fraction can be expected to become larger near the reaction zone, as Lewis number increases, because pyrolysis phenomena is increased. On the other side,

larger Lewis number means lower mass diffusion, which decreases gaseous fuel mass fraction far from the reaction zone.

4.0   CONCLUSIONS

In this work the structure of a one dimensional, axisymmetric, premixed flame in a counterflow configuration containing uniformly distributed volatile fuel particles is examined. Effect of Lewis number on gaseous mass fraction distribution in preheat-vaporization zone is investigated, which shows increasing in Lewis number has dual effect on gaseous mass fraction distribution based on increasing in heat diffusion and decreasing in mass diffusion. This dual effect results a higher value of gaseous mass fraction near the reaction zone and a lower value far from the reaction zone, in a higher Lewis number value.

5.0   REFERENCES

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