

COMBUSTION MODELING OF THE PREMIXED FLAME PROPAGATION

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ABSTRACT

In this paper, the effect of temperature difference between gas and particle in the structure of premixed flames propagation in combustible system, containing uniformly distributed volatile fuel particle, in an oxidizing gas mixture, is analyzed. In the present work, Equations based on the premixed flames of organic dust are used and then required relations for gas and particle are derived. Consequently, governing Equations and needed boundary conditions are applied and an analytical method is used for solving these Equations. It must be said that the structure of the flame consists of a preheat zone, a reaction zone and a convection zone. Finally, the variation of dimensionless temperature of gas and particle, particle mass friction, equivalence ratio of gas and particle, flame temperature and burning velocity of gas and temperature are shown in figures.

Nomenclature

A Rate of vaporization of fuel particle
 a Defined in Eq. 26
 B Frequency factor characterizing rate of gas phase oxidation of gaseous fuel
 $b = y_{Ff} / \varepsilon$, scaled mass fraction of fuel at the boundary between the reaction zone and the convection zone
 b' Heat transfer coefficient
 C Heat capacity of mixture, Eq. 8
 C_F Molar concentration of fuel
 C_p Heat capacity of the gas
 C_s heat capacity of a fuel particle
 D Diffusion coefficient
 E Activation energy characterizing the gas phase reaction
 k Rate constant of the gas-phase reaction
 m Defined in Eq. 7
 n Constant number for the temperature exponent
 n_s Local number density of particles

n_u Number density of particles in ambient stream
 Q Heat release per unit mass of gaseous fuel consumed
 Q_L Heat transfer from the walls
 Q_v Heat associated with vaporizing unit mass of fuel
 q Defined in Eq. 18
 R Gas constant
 r Radius of fuel particles
 T Temperature
 v Velocity
 v_u Burning velocity calculated neglecting heat of vaporization of fuel particles
 v_v Burning velocity calculated including heat of vaporization of fuel particles
 W_F Molecular weight of gaseous fuel
 w_v Rate of vaporization
 w_F Reaction rate characterizing consumption of gaseous fuel
 Y Mass fraction
 Y_{FC} Defined in Eq. 7
 Y_{Fu} Gaseous fuel available in the particles in the ambient reactant stream
 y_F Mass fraction of fuel
 y_s Mass fraction of particle
 Z_e Zeldovich number
 z Scaled independent variable

Greek Symbols

γ Defined in Eq. 17
 $\varepsilon = 1/Z_e$, expansion parameter
 ξ Independent variable
 κ Dimensionless burning velocity
 θ Dimensionless temperature

- θ° Dimensionless temperature neglecting vaporization heat of particles
 Λ Defined in Eq. 35
 λ Thermal conductivity
 ρ Density of the reactant mixture
 ρ_s Density of a fuel particle
 ν Stoichiometric coefficient
 ϕ_u Equivalence ratio based on fuel available in the particles in the ambient reactant stream
 ϕ_s Effective equivalence ratio in the reaction zone

1 INTRODUCTION

Dust explosions are the phenomena that flame propagates through dust clouds in air with increasing degree of subdivision of any combustible solids. They have been a recognized threat to humans and property for the last 150 years [1]. Recently, with the advancement of powder technology and the increase of powder handling processes, hazard assessment and the establishment of preventive methods for dust explosions have become more important from the viewpoint of industrial loss prevention. In spite of significant efforts to obtain information on the explosibility of dusts, the fundamental mechanisms of flame propagation in dust suspension have not been sufficiently studied. This is mainly due to experimental difficulties in the generation of a uniform dust suspension, as well as the fact that particle size and size distributions [1] can significantly influence the combustion mechanisms. Thus the limited experimental results known in literature are often apparatus dependent and contradict each other. To investigate the burning velocity of laminar flames of lycopodium, Kaesche-Krischer and Zelv [2] fed lycopodium into the lower end of a vertical 2 cm diameter tube, where it was dispersed into a stationary dust cloud by an upward-moving stream of air. This arrangement made it possible to obtain stable flames in the concentration range of dust between 200 and 500 g/m³. Mason and Wilson [3], who also studied the burning velocity of stationary flames of lycopodium, described a dispersing arrangement where the lycopodium was elutriated from a fluidized bed. They obtained stable dust flames in the concentration range 125-190 g/m³. Ross [4], working with clouds of lycopodium in air, was able to significantly reduce electrostatic agglomeration of particles, as well as electrostatic adhesion to the wall of an experimental flame tube, when the air was ionized by means of an alpha emitter mounted on the flame tube wall. Proust [5] described other experimental studies of laminar burning velocities and maximum flame temperatures in clouds of starch, lycopodium, and sulfur in air, whereas Seshadri, Berlad, and Tangirala [6] studied the inherent structure of laminar dust flames.

Bradley et al. [7] investigated the burning of clouds of fine graphite dust (4 μm) in premixed methane/air in a flat laminar flame. Several studies on the properties of flame propagation of dusts in a vertical duct have been reported; e.g. the laminar burning velocity, flame thickness and quenching distance in starch clouds [8] and the mechanism of flame acceleration in starch particles [9]. The experimental study has been conducted to elucidate the structure of flame propagating through lycopodium dust clouds in a vertical duct [10]. Nevertheless fundamental information such as the structure and movement of the combustion zone in a dust particles cloud in vertical duct is still ambiguous [11, 12].

In the present study, the aspects of flame propagation and the structure of combustion zone have been examined analytically to clarify the mechanisms of flame propagation through dust clouds in a vertical duct. The structure of the flame consists of preheat, reaction and convection zone. Finally, the variation of dimensionless temperature of gas and particle, particle mass friction, flame temperature and burning velocity of gas and particle is shown in figures.

2 THEORY

The structure of flame propagation is composed of three zones as follow:

In the preheat zone ($-\infty < y < 0^-$), particles are heating till they reach to the ignition temperature. In this zone, z_e is considered to be large so chemical reaction between the gaseous fuel and oxidizer is negligible and due to the different temperature between gas and particle, the heat exchanger between them is considered.

The next region in this research is the reaction zone in which particles are oxidized and burnt. In this region ($0^- < y < 0^+$), the convective terms and vaporization terms in the conservation Equations are presumed to be small in comparison with diffusive and reactive terms.

The last region is the convection zone ($0^+ < y < \infty$) which the diffusive terms in the conservation Equations are assumed to be small in comparison with other parameters.

3 ASSUMPTIONS

1. The structure of premixed flames propagation in a uniform cloud of fuel particles is considered.
2. The effect of gravity and radiative heat transfer has been surrendered.
3. The Biot number is assumed to be small so that particle temperature is monotonous.
4. Thermal conductivity is presumed constant for different temperature.

4 GOVERNING EQUATIONS

The combustion process is modeled as a one step overall reaction $\nu_F [F] + \nu_{O_2} [O_2] \rightarrow \nu_{Prod} [P]$. Where the symbols F, O_2, P : denote the fuel, oxygen and product respectively and the quantities $\nu_F, \nu_{O_2}, \nu_{Prod}$ denote their stoichiometric coefficients.

The constant rate of the overall reaction is written in the Arrhenius form $k = B \exp(-E/RT)$ where B represents the frequency factor, E the activation energy of the reaction and R is the gas constant.

Governing Equations can be written as:

Mass conservation:

$$\rho v = \text{const} \quad (1)$$

Energy conservation:

$$\rho v C \frac{dT}{dx} = \lambda_u \frac{d^2 T}{dx^2} + w_F \frac{\rho_u}{\rho} Q - w_v \frac{\rho_u}{\rho} Q_v \quad (2)$$

Where Q, Q_v are the heat release per unit mass of the burnt fuel and the heat associated with vaporizing unit mass of the fuel respectively. Gaseous fuel conservation:

$$\rho v \frac{dY_F}{dx} = \rho_u D_u \frac{d^2 Y_F}{dx^2} - w_F \frac{\rho_u}{\rho} + w_v \frac{\rho_u}{\rho} \quad (3)$$

The Equation governing the mass fraction of the particles neglecting diffusion can be written as:

$$\rho v \frac{dY_s}{dx} = -w_v \frac{\rho_u}{\rho} \quad (4)$$

Equation of state:

$$\rho T = \text{const} \quad (5)$$

The energy conservation Equation for particles is:

$$\left(\frac{4}{3} \pi r^3 \rho_s C_s \right) v_u \frac{dT_s}{dx} = \left(4 \pi r^2 \right) \frac{\lambda_u}{r} (T - T_s) \quad (6)$$

5 NONDIMENSIONALIZATION OF GOVERNING EQUATIONS

The nondimensional parameters are as follow

$$\theta = \frac{T - T_u}{T_f - T_u}, \theta_s = \frac{T_s - T_u}{T_f - T_u}, y_f = \frac{Y_F}{Y_{FC}} \quad (7)$$

$$m = \frac{\rho v}{\rho_u v_u}, z = \frac{\rho_u v_u C}{\lambda_u} x,$$

$$Y_{FC} = \frac{C}{Q} (T_f - T_u), \zeta = \frac{3 \lambda_u \lambda}{r^2 \rho_u v_u C \rho_s v_u C_s}$$

If these parameters are applied in Equations (2), (3), (4), (6) the nondimensionalized Equations (8-11) can be written as follow:

$$m \frac{d\theta}{dz} = \frac{d^2 \theta}{dz^2} + \omega \frac{\rho_u}{\rho} - q \gamma_s \frac{2}{3} \theta^n \quad (8)$$

$$m \frac{dy_F}{dz} = \frac{d^2 y_F}{dz^2} - \omega \frac{\rho_u}{\rho} + \gamma_s \frac{2}{3} \theta^n \quad (9)$$

$$m \frac{dy_s}{dz} = -\gamma_s \frac{2}{3} \theta^n \quad (10)$$

$$\frac{d\theta_s}{dz} = \xi (\theta - \theta_s) \quad (11)$$

In this research due to the fact that the quantity q , which is the ratio of heat required to vaporize the fuel particles to the overall heat release by the flame, is too small, it is neglected in the above Equation. Also the quantity m can be considered unity so the governing Equations are simplified and rewritten as:

$$\frac{d\theta^0}{dz} = \frac{d^2 \theta^0}{dz^2} + \omega \frac{\rho_u}{\rho} \quad (12)$$

$$\frac{dy_F}{dz} = \frac{d^2 y_F}{dz^2} - \omega \frac{\rho_u}{\rho} + \gamma_s \frac{2}{3} \theta^n \quad (13)$$

$$\frac{dy_s}{dz} = -\gamma_s \frac{2}{3} (\theta^0)^n \quad (14)$$

$$\frac{d\theta_s^0}{dz} = \xi (\theta^0 - \theta_s^0) \quad (15)$$

The above nondimensional parameters are gained from following Equations:

$$\omega = \frac{\lambda_u w_F}{(\rho_u v_u)^2 C Y_{FC}} \quad (16)$$

$$\gamma = \frac{4.836 A n_u^{1/3} \lambda_u (T_f - T_u)^n}{v_u^2 \rho_u^{4/3} C Y_{FC}^{1/3} \rho_s^{2/3}} \quad (17)$$

$$q = \frac{Q_v}{Q} \quad (18)$$

5.1 Preheat Zone

In this zone, as said, the Zeldovich number is considered too large so chemical reaction between the gaseous fuel and oxidizer is negligible and due to the different temperature between gas and particle, the heat exchanger between them is considered. Nondimensional Equations in this zone are as:

$$\frac{d\theta^0}{dz} = \frac{d^2 \theta^0}{dz^2} \quad (19)$$

$$\frac{dy_F}{dz} = \frac{d^2 y_F}{dz^2} - \omega \frac{\rho_u}{\rho} + \gamma_s \frac{2}{3} \theta^n \quad (20)$$

$$\frac{dy_s}{dz} = -\gamma_s \frac{2}{3} (\theta^0)^n \quad (21)$$

$$\frac{d\theta_s^0}{dz} = \xi (\theta^0 - \theta_s^0) \quad (22)$$

Boundary conditions for above Equations are:

$$\begin{aligned} \text{at } z = -\infty \quad \theta^\circ = 0, \quad \theta_s^\circ = 0, \\ \text{at } z = -\infty \quad y_s = \frac{Y_{FU}}{Y_{FC}} = \alpha, \quad y_F = y_{Ff} = 0 \end{aligned} \quad (23)$$

$$\text{at } z = 0 \quad \theta^\circ = 1$$

The above Equations and boundary conditions are solved simultaneously and results for gas are obtained as:

$$\theta^0 = e^\varepsilon \quad (24)$$

$$-\left[\frac{dy_F}{dz}\right]_{0^-} = (3a\alpha^{2/3} - 3a^2\alpha^{1/3} + a^3 - y_{Ff}) \quad (25)$$

$$a = \frac{\gamma}{3n} \quad (26)$$

$$y_s = [\alpha^{1/3} - ae^{nz}]^3 \quad (27)$$

The obtained results for particle are:

$$\theta_s^0 = \frac{\xi}{1+\xi} \theta^0 \quad (28)$$

$$-\left[\frac{dy_F}{dz}\right]_{0^-} = (3a\alpha^{2/3} - 3a^2\alpha^{1/3} + a^3 - y_{Ff}) \quad (29)$$

$$a = \frac{\gamma\xi}{3n(\xi+1)} \quad (30)$$

$$y_s = [\alpha^{1/3} - ae^{nz}]^3 \quad (31)$$

5.2 Reaction Zone

In order to analyze the structure of this zone the expansions:

$$z = \varepsilon\eta \quad y_F = \varepsilon(b+y) \quad \theta^0 = 1 - \varepsilon t \quad (32)$$

are introduced, where $b = y_{Ff}/\varepsilon$, $\varepsilon = 1/Ze$ is the expansion parameter, which is presumed to be small. The quantities b and t are assumed to be of order unity. Introducing these parameters in the conservation Equations yields the following Equations:

$$\frac{d^2t}{d\eta^2} = \Lambda(b+y)e^{-t} \quad (33)$$

$$\frac{d^2(t+y)}{d\eta^2} = 0 \quad (34)$$

$$\Lambda = \frac{v_F \lambda_u B \varepsilon^2}{\rho_u v_u^2 C} \exp\left(-\frac{E}{RT_f}\right) \quad (35)$$

For gas phase:

$$\frac{dt}{d\eta} = -1 \quad \eta \rightarrow -\infty \quad (36)$$

For particles:

$$\frac{dt}{d\eta} = -\frac{\xi}{\xi+1} \quad \eta \rightarrow -\infty \quad (37)$$

Equation (33) can be integrated and by using boundary conditions, Equation (38) and (39) for gas and particles can be extracted respectively.

$$2(1+b)\Lambda = 1 \quad (38)$$

$$2(1+b)\Lambda = \left(\frac{\xi}{\xi+1}\right)^2 \quad (39)$$

6 BURNING VELOCITY

Introducing Equation (38) and (39) into (34) yields the burning velocity for gas and particle in Equations (40) and (41) respectively:

$$v_u^2 = \frac{2(1+b)v_F \lambda_u B \varepsilon^2}{\rho_u C} e^{-\frac{E}{RT_f}} \quad (40)$$

$$v_u^2 = \frac{2(1+b)v_F \lambda_u B \varepsilon^2}{\left(\frac{\xi}{\xi+1}\right)^2 \rho_u C} e^{-\frac{E}{RT_f}} \quad (41)$$

Equations (40) and (41) can be used to calculate the burning velocity if b and T_f are known. In order to determine these quantities, it is necessary to analyze the structure of the convection zone.

For sufficiently high values of T_f , it is reasonable to set $y_{Ff} = 0$ which implies that $b = 0$. The value of T_f can be determined by solving the following Equation means:

$$\left[\frac{d\theta^0}{dz}\right]_{0^+} + \left[\frac{dy_F}{dz}\right]_{0^+} = \left[\frac{d\theta^0}{dz}\right]_{0^-} + \left[\frac{dy_F}{dz}\right]_{0^-} \quad (42)$$

By substituting the parameters in Equation (42), the flame temperature can be derived for gas and particle using Equations (43) and (44) respectively.

$$3a\alpha^{2/3} - 3a^2\alpha^{1/3} + a^3 - 1 = 0 \quad (43)$$

$$3a\alpha^{2/3} - 3a^2\alpha^{1/3} + a^3 - \frac{\xi}{1+\xi} = 0 \quad (44)$$

If the heat of vaporization is considered, then the Equation of burning velocity can be written:

$$v_u = v_u e^{(-qz_e/2)} \quad (45)$$

Where Ze is assumed to be large and can be calculated by:

$$Z_e = \frac{E_a(T_f - T_u)}{RT_f^2} \quad (46)$$

The final adiabatic temperature attained in the convection zone after all the oxygen is consumed, neglecting the heat of vaporization of the particle, from the expression:

$$C(T_b - T_u) = \frac{v_F W_F Q}{v_{O_2} W_{O_2}} Y_{O_2u} \quad (47)$$

Numerical calculations were performed for $\phi_u \geq 1$.

Thus, for combustible mixtures of fuel particles and air, the equivalence ratio correlations are measured by:

$$\phi_u = 17.18Y_{FU} / (1 - Y_{FU}) \quad (48)$$

$$\phi_g = 17.18Y_{FC} / (1 - Y_{FC}) \quad (49)$$

7. RESULTS

The variation of dimensionless temperature for gas and particle with Z is plotted in Figure 1 for a given value of $r=20 \mu\text{m}$. Figure 2 shows the mass fraction of the particles as a function of Z for different equivalence ratios and for a given value of $r=20 \mu\text{m}$. As seen, it is illustrated that for given value of equivalence ratios the amount of mass fraction decreases with increasing the distance Z . Also a considerable rise in the mass fraction can be observed when the equivalence ratio increases.

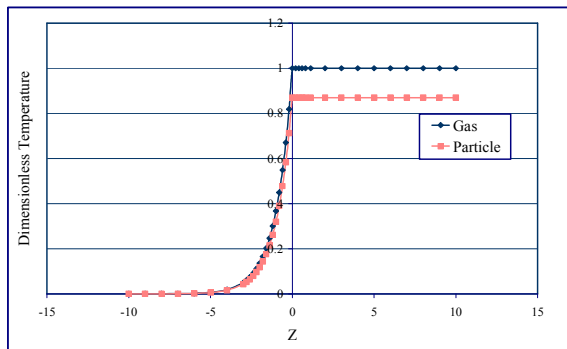


Figure 1. Variation of dimensionless temperature with Z

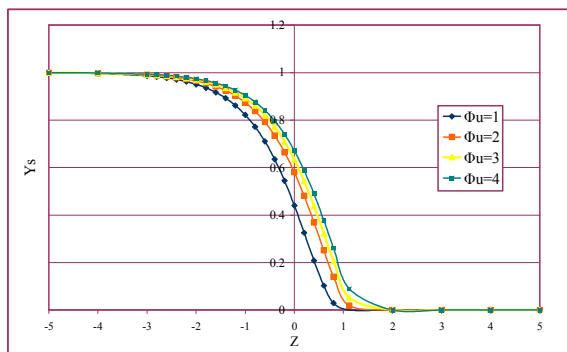


Figure 2. The mass fraction of the particles for different equivalence ratios

In Figures 3 and 4 the flame temperature and adiabatic temperature are shown as a function of Φ for gas and particle respectively. As seen in these figures, the flame temperature can't exceed the adiabatic temperature and it means that for each radius, there is an acceptable equivalence ratio and this amount of equivalence ratio changes for different radius.

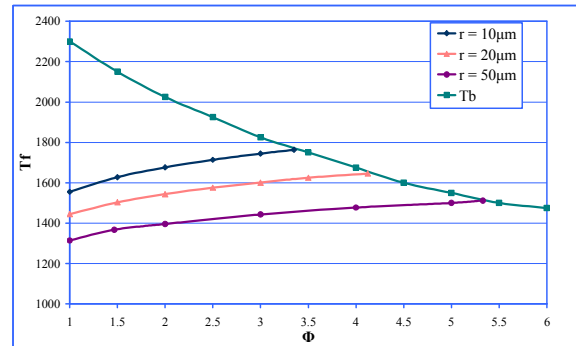


Figure 3. The variation of gas flame temperature and adiabatic temperature for different radius with equivalence ratio

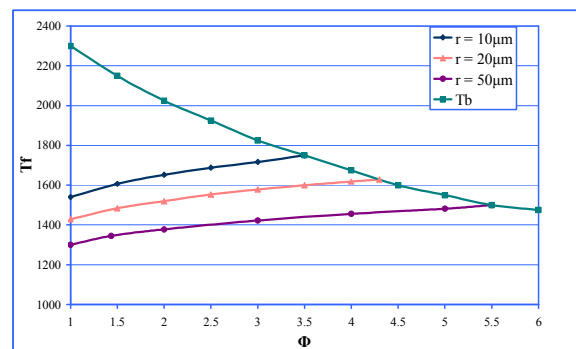


Figure 4. The variation of particle flame temperature and adiabatic temperature for different radius with equivalence ratio

Figures 5 and 6 manifest the variation of burning velocity with equivalence ratio for gas and particle respectively. As perceived in both figures, the trend is upward and shooting up the radius causes to plunge the burning velocity due to the fact that surface area increases. While in the gaseous fuel, it is expected that the burning velocity reaches to its maximum at the stoichiometric condition, the burning velocity variation for the combustion of particles is totally upward and its variation has a great compatibility with the published experimental data and this model acceptably predicts this trend.

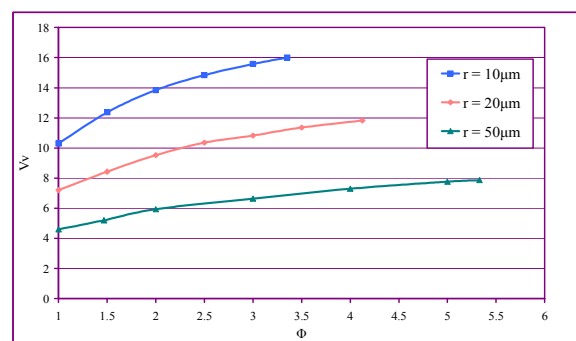


Figure 5. The variation of burning velocity with equivalence ratio for gas

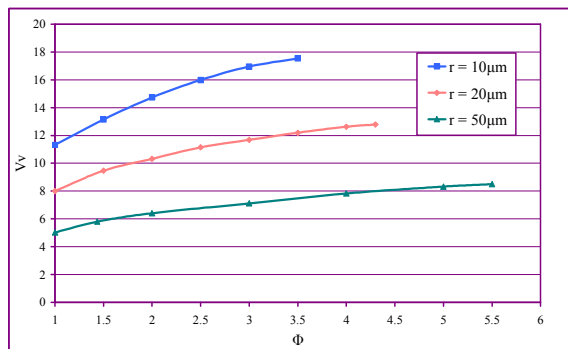


Figure 6. The variation of burning velocity with equivalence ratio for particle

It must be considered that with declining values of radius to zero, the value of burning velocity can be determined for a purely gaseous combustible mixture.

8. DISCUSSION

In this article, effect of temperature difference between gas and particle in the structure of premixed flames propagation in combustible system, containing uniformly distributed volatile fuel particle, in an oxidizing gas mixture, is analyzed. It must be said that the structure of the flame consists of a preheat zone, a reaction zone and a convection zone and in each zone, Equations based on the premixed flames of organic dust are used and then required relations for gas and particle are derived. Consequently, governing Equations and needed boundary conditions are applied and an analytical method is used for solving these Equations. From the above analysis, following conclusions are derived:

1. The dimensionless temperature for gas and particle is plotted.
2. The mass fraction of particle increases with raising the equivalence ratio.
3. The flame temperature and adiabatic temperature are plotted as a function of equivalence ratio for different radius.
4. The burning velocity for gas and particle goes up and down when equivalence ratio and radius increase respectively.
5. In spite of the fact that in the gaseous fuel, burning velocity has the maximum quantity at the stoichiometric condition, the quantity of burning velocity in the dust explosion increases when the equivalence ratio goes up.

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