THE STRUCTURE OF PARTICLE CLOUD PREMIXED FLAMES

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1. Introduction.

The aim of this study is to provide a numerical and asymptotic description of the structure of planar laminar flames, propagating in a medium containing a uniform cloud of fuel-particles premixed with air. Attention is restricted here to systems where the fuel-particles first vaporize to form a known gaseous fuel, which is then oxidized in the gas-phase. This program is supported for the period September 14, 1991 to September 13, 1992. Some results of the study is shown in Ref. 1. The work summarized in Ref. 1 was initiated prior to September 14, 1991 and was completed on February 1992. Research performed in addition to that described in Ref. 1 in collaboration with Professor A. Linan, is summarized here.

The model developed here is built on previous asymptotic analysis structure of premixed particle-cloud flames [1]. In this previous analysis the vaporization rate of the fuel-particles was presumed to be proportional to $T_s^{1.33}$, where T_s is the temperature of the fuel-particles. Hence, the activation temperature in an Arrhenius-type rate law for the vaporization process is not large. For simplicity, the temperature of the fuel-particles was presumed to be equal to the gas temperature. The analysis was performed for values of $\phi_u > 1.0$, where ϕ_u is the equivalence ratio based on the gaseous fuel available in the particles. For given values of ϕ_u the analysis yields results for the burning velocity and ϕ_g, where ϕ_g is the effective equivalence ratio in the reaction zone [1]. The analysis shows that even though $\phi_u > 1.0$, for certain cases the calculated value of ϕ_g is less than unity.

A two-temperature model is described here, where the temperature of the fuel-particles is different from the temperature of the gas. However the size of the fuel-particle is assumed to be small enough so that its velocity is nearly equal to the gas velocity. A general treatment of flame propagation supported by volatile fuel-particles should consider both radiative and molecular transport mechanisms, the temperature difference and the differences in velocity between the gas and the particulates, the nonadiabaticity of combustible systems of finite size, as well as the detailed kinetics of oxidation and the kinetics of vaporization pyrolysis. This work has the somewhat limited aim of examining the interplay of vaporization kinetic and oxidative kinetic processes for cases where nonadiabatic and radiative transport mechanisms are not substantial.

2. Formulation.

A model is developed to describe steady, one-dimensional, planar flame propagation in a combustible mixture consisting of uniformly distributed fuel-particles in air. The initial number density of the particles, n_u (number of particles per unit volume) and the initial radius a_u are presumed to be known. All external forces including gravitational forces effects are assumed to be negligible. The kinetics of vaporization of a fuel-particle is represented by the expression

$$\dot{m} = 4\,\pi\, a^2\, A \exp\left(-\frac{T_{av}}{T_s}\right) = -\frac{4}{3}\,\pi\,\frac{d(a^3)}{dt}\,\rho_s, \tag{1}$$

where $\dot{m}$ represents the mass of gaseous fuel vaporized per unit time from the fuel-particle, a and ρ_s are the instantaneous radius and density respectively of a fuel- particle. The rate parameters A and T_{av} which respectively represent the frequency factor and the activation temperature of the vaporization process are presumed to be known. The ratio T_{av}/T_s is presumed to be a large quantity.

Consider a vaporizing fuel-particle in an ambient atmosphere. The balance equation for the mass fraction of the gaseous fuel vaporizing from the fuel-particle Y_F, and the energy balance equation can be written as,

$$\frac{\dot{m}}{4\,\pi\, r^2}\frac{\partial Y_F}{\partial r} - \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{k}{c_p L_F}\frac{\partial Y_F}{\partial r}\right) = 0, \tag{2}$$

$$\frac{\dot{m}}{4\,\pi\, r^2}\frac{\partial (c_p T)}{\partial r} - \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 k \frac{\partial T}{\partial r}\right) = 0, \tag{3}$$

where r is the radial coordinate. For the gas mixture k is the thermal conductivity, c_p the heat capacity, and T the temperature. The quantity $L_F = k/(\rho c_p D_F)$ is the Lewis number of the gaseous fuel which is presumed to be a constant and D_F is the diffusion coefficient of the gaseous fuel. Boundary conditions for Eqs. 2 and 3 far from the surface of the fuel-particle, and at the surface of the fuel-particle can be written as,

$$\begin{gathered} T = T_\infty,\ Y_F = Y_{F,\infty} \text{ as } r \to \infty, \\ T = T_s,\ \dot{m}\,(1 - Y_F) = -\frac{4\,\pi\, k\, r^2}{c_p L_F}\frac{\partial Y_F}{\partial r} \text{ at } r = a. \end{gathered} \tag{4}$$

The values of T_∞ and $Y_{F,\infty}$ will be determined from the solution of the equations governing the structure of the laminar flame. The temperature of the fuel-particle T_s can be calculated from the energy balance equation

$$q_g = \left(4\,\pi\, r^2\, k\,\frac{\partial T}{\partial r}\right)_{r=a} = \dot{m}\, L_v + \frac{4}{3}\,\pi\, a^3\, \rho_s\, c_s\,\frac{dT_s}{dt}, \tag{5}$$

where t represents the time, c_s represents the heat capacity of fuel-particle, and L_v represents the heat required to vaporize unit mass of vapor from a fuel-particle. The values of c_p and c_s are presumed to be constant. If the value of k is also presumed to be constant, then from integration of Eqs. 2 and 3, using Eq. 4 to determine the constants of integration, the profiles of Y_F and T can be expressed as

$$Y_F = 1 - \left(1 - Y_{F,\infty}\right)\exp\left(-\frac{\dot{m}\, c_p\, L_F}{4\,\pi\, k\, r}\right), \tag{6}$$

and

$$T = T_s - \frac{q_g}{c_p\,\dot{m}} + \left(T_\infty - T_s + \frac{q_g}{c_p\,\dot{m}}\right)\exp\left(-\frac{\dot{m}\, c_p}{4\,\pi\, k\, r}\right). \tag{7}$$

Introducing the definition,

$$\lambda = \left(\frac{\dot{m}\, c_p}{4\,\pi\, k\, r}\right)_{r=a}, \tag{8}$$

from Eqs. 5 and 7 it follows that

$$\frac{4\,\pi\, a\, k\,\lambda\left(T_\infty - T_s\right)}{\exp\left(\lambda\right) - 1} = \frac{4\,\pi\, a\, k\, L_v\,\lambda}{c_p} + \frac{4}{3}\,\pi\, a^3\,\rho_s\, c_s\,\frac{dT_s}{dT}. \tag{9}$$

The term on the left side of Eq. 9 denotes the rate of heat transfer from the gas to the fuel-particle, with the effective Nusselt's number denoted by $\lambda/[\exp(\lambda) - 1]$. The first term following the equality sign on the right side of Eq. 9 denotes the latent heat required to vaporize the fuel-particle, and the second term denotes the sensible heat required to raise the temperature of the fuel-particle. It follows from Eqs. 1, and 8 that

$$\lambda = \frac{a\, c_p}{k}\, A\,\exp\left(-\frac{T_{av}}{T_s}\right). \tag{10}$$

Let T_V denote a characteristic value of the temperature of the fuel-particle for which the value of λ evaluated from Eq. 10 is of order unity. For $T_S < T_V$, the vaporization rate and consequently the value of λ, is exponentially small. In the limit of small values of λ, $\lambda/[\exp(\lambda) - 1] = 1$. Hence the first term on the right side of Eq. 9 can be neglected in calculating the value of T_S. For $T_S = T_V$, λ is of order unity. If the value of T_S is allowed to increase beyond T_V, then the value of λ would become exponentially large and the term on the left side of Eq. 9 would become exponentially small, consequently the rate of heat transfer from the gas-phase to the solid, will be small. Therefore, for values of T_S beyond T_V, the value of the derivative dT_S/dt will be negligibly small, so that the value of λ remains of order unity. For simplicity, it is presumed that $\dot{m} = 0$

for $T_s < T_v$ and the value of T_s does not increase after it attains the value T_v.

The governing equations for the structure of the flame can be written as,

$$V = \rho_u u_u + \frac{4}{3}\pi \rho_s n_u u_u \left(a_u^3 - a^3\right), \tag{11}$$

$$\frac{d(V\,Y_F)}{dx} - \frac{k_u}{c_p L_F}\frac{d^2 Y_F}{dx^2} = \frac{n_u \rho_u u_u}{V}\dot{m} - w_F \frac{\rho_u}{\rho}, \tag{12}$$

$$\frac{d(V\,Y_{O_2})}{dx} - \frac{k_u}{c_p L_{O_2}}\frac{d^2 Y_{O_2}}{dx^2} = -\,w_{O_2}\frac{\rho_u}{\rho}, \tag{13}$$

$$\frac{d(V\,c_p\,T)}{dx} - k_u\frac{d^2 T}{dx^2} = \frac{n_u \rho_u u_u}{V} q_p + Q_R\, w_F \frac{\rho_u}{\rho}. \tag{14}$$

Here the subscript u denotes conditions in the ambient reactant stream. The subscript ∞ has been dropped from the quantities Y_F, Y_{O2} and T appearing in Eqs. 12-14. The quantities w_F and w_{O2} denote the rate of consumption of gaseous fuel and oxygen per unit volume, and Q_R is the heat released per unit mass of gaseous fuel consumed. The independent variable x is related to the spatial coordinate x' as,

$$x = \int_0^{x'} \left(\frac{\rho}{\rho_u}\right) dx'. \tag{15}$$

In the regions where $T_s < T_v$, the vaporization rates are assumed to be negligibly small hence the radius of the fuel-particle does not change and its temperature T_s and the quantity q_p can be calculated from the relations,

$$a_u^2 \frac{\rho_s c_s V}{\rho_u}\frac{dT_s}{dx} = \frac{3\,k_u}{2\,T_u}\left(T^2 - T_s^2\right), \tag{16}$$

and

$$q_p = -\frac{4}{3}\pi a_u^3 \rho_s c_s \frac{V}{\rho_u}\frac{dT_s}{dx}. \tag{17}$$

When the value of the temperature of the fuel-particle reaches T_v, they begin to vaporize and the increase in their temperature is negligibly small. The radius of the fuel-particle and the quantity q_p can be calculated from the expressions,

$$a\frac{da}{dx} = -\frac{k_u \rho_u}{T_u c_p \rho_s V}\left[T - T_v + \left(T_v - \frac{L_v}{c_p}\right)\ln\left(1 + \frac{c_p(T - T_v)}{L_v}\right)\right], \tag{18}$$

and,

$$q_p = \dot{m}\,(c_p - L_v),\ \dot{m} = -\rho_s \frac{4}{3}\pi \frac{V}{\rho_u}\frac{d(a^3)}{dx}. \tag{19}$$

In deducing the system of equations 12-19 the product ρk was presumed to be a constant. The chemical reaction between the gaseous fuel and the oxidizer is presumed to occur by a one-step process. The system of equations 12-19 were solved numerically.

3. Results

For purpose of illustration calculations were performed assuming that the gaseous fuel that evolves from the fuel-particle is methane. The chemical kinetic rate parameters characterizing the gas-phase oxidation were chosen such that the burning velocity for stoichiometric mixture of gaseous methane and air is 37 cm/s. The values of some of the parameters used in the calculations are k_u = 0.00035 cal/(cm s K), ρ_u = 0.001135 g/cm^3, ρ_s = 1.0 g/cm^3, T_u = 300 K, T_v = 600 K, L_v/Q_R = 0.01. Results of some of these calculations for values of a_u equal to 0.0007 cm, 0.0010 cm, and 0.0015 cm are shown in Figs. 1 and 2. Figure 1 shows the the burning velocity u_u, as a function of the equivalence ratio ϕ_u, calculated based on the gaseous fuel available in the fuel-particles. Figure 1 shows that steady flame propagation is possible in fuel-rich combustible mixtures. In Fig. 2 the structure of the flame is plotted at a value of ϕ_u = 1.89 and a_u = 0.0010 cm. The various non-dimensional quantities appearing in this figure are defined as,

$$z = \frac{\rho_u u_u c_p}{k_u} x, \ \theta = \frac{T - T_u}{T_b - T_u}, \ \theta_s = \frac{T_s - T_u}{T_b - T_u}, \qquad (20)$$
$$\alpha = \frac{a}{a_u}, \ y_F = \frac{4 Y_F}{Y_{O_2u}}, \ y_{O_2} = \frac{Y_{O_2}}{Y_{O_2u}}.$$

where T_b is the adiabatic flame temperature. Interpretations of results similar to those shown in Fig. 1 and 2 are currently in progress.

4. Future Research.

Future research is directed toward performing numerical calculations using the system of equations 12-18 over a wide parametric range. Asymptotic description of the flame structure will also be attempted.

5. References.

1). Seshadri, K., Berlad, A. L., and Tangirala, V., *The Structure of Particle-Cloud Flames*, Combustion and Flame **89**: 333-342 (1992)

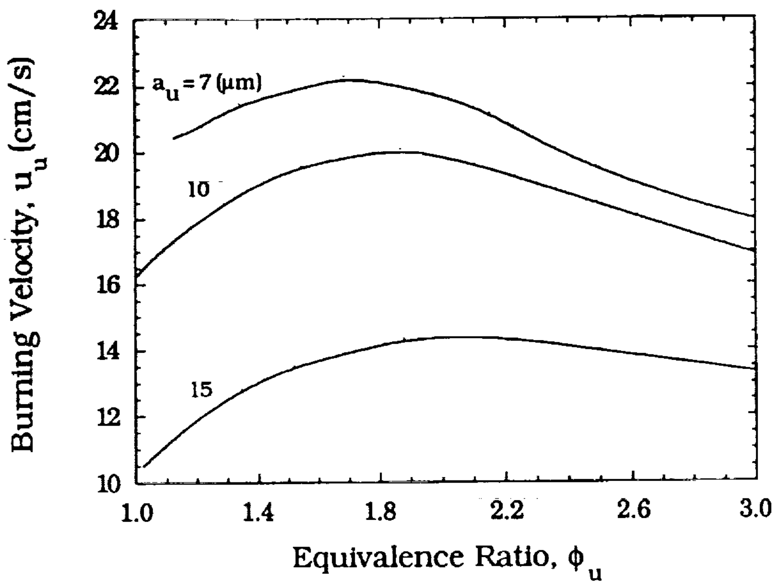

Figure 1. The burning velocity u_u (cm/s) as a function of the equivalence ratio ϕ_u, for various values for the initial radius of the fuel-partical a_u.

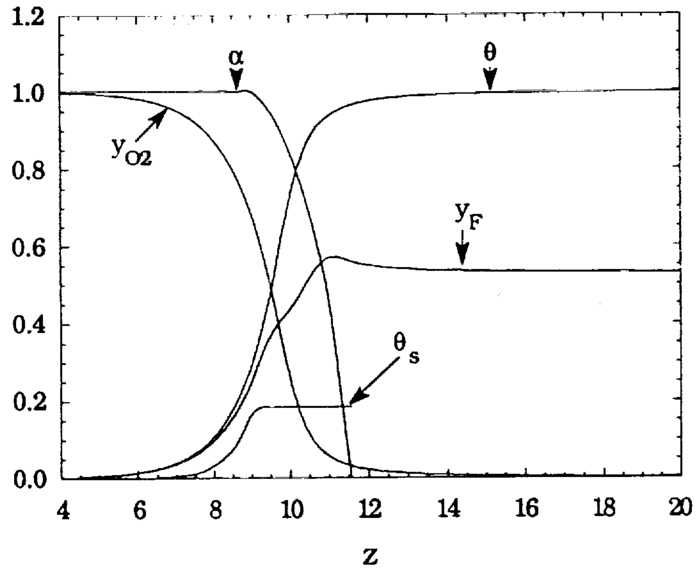

Figure 2. The structure of the flame for ϕ_u = 1.89 and a_u = 0.0010 cm.