Reignition of Methanol Droplet Flames under Acoustic-Pressure Oscillation

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Abstract

Reignition as a special case of acoustic pressure response of a flame is numerically studied by employing a methanol droplet flame as a laminar flamelet model. Quasi-steady flame responses occur in the range of small amplitude, low frequency oscillation. Reignition phenomenon occurs when, by increasing the frequency of large amplitude acoustic oscillation, the magnitude of characteristic acoustic time becomes the same order of characteristic reaction time. Excessive increase in the amplitude of acoustic pressure induces direct extinction of flame. Flame can sustain its own intensity even below the steady extinction temperature in case of high frequency acoustic oscillation, and this tendency becomes pronounced with increasing frequency.

Introduction

The laminar flamelet model has been widely adopted to simulate turbulent flames, where the characteristics of flamelets as functions of flame stretch or pressure are important issues. Especially, steady-state extinction characteristics need to be incorporated in the model.

When a flame is under external perturbation such as pressure or strain rate, unsteady interaction of a flame with the external perturbation could maintain the flame to be sustained even though the flame already encounters a steady-state extinction criterion. Such unsteady behavior should be accounted for accurate simulation of turbulent flames. In this regard, Mauss et al. [1] performed a stochastic simulation of flamelet extinction and reignition in a counterflow by applying sudden increase and subsequent decrease in strain rates. Ezekoye and Zhang [2] studied the effects of time scale of unsteady fuel flux into flame sheets for a diffusion flame with fuel supplied through a porous sphere, and extinction-reignition processes were observed in the quasi-periodic burning mode. These studies on reignition phenomena are restricted to either temporary perturbation in strain rate or qualitative nature.

Recently, the response of flamelets under acoustic-pressure oscillation has been investigated to elucidate acoustic instability mechanism in turbulent flames [3, 4, 5]. It has been demonstrated that nonlinear responses have been observed for flames near extinction and such flames have an amplification contribution to acoustic instability. When pressure oscillation is imposed on a flamelet, the flame could encounter a pressure condition which is beyond the quasi-steady extinction criteria. The present study is intended to address the quantitative response under such situation. A methanol(CH_3OH) droplet flame under acoustic-pressure oscillation is adopted as a model problem.

Formulation

In order to formulate the problem in a more tractable form without sacrificing the essentials of droplet combustion, a number of approximations and assumptions are introduced. Since the characteristic time of droplet surface regression is longer than that of the molecular diffusion of reactants and thermal energy [6] by an order of ρ_{ℓ}/ρ_g , where ρ is the density and the subscripts ℓ and g indicate liquid and gaseous states, respectively, the effect of surface regression can be neglected. Consequently, droplet diameter can be considered to be instantaneously constant in the numerical realizations carried out in the framework of diffusion-time scale. Although the quasisteadiness prevails, the resulting governing equations are unsteady due to the unsteady pressure oscillation imposed on droplet flames. The unsteadiness in the present problem is related only to pressure oscillations. In addition, a spherical symmetry by neglecting natural and forced convections reduces the analysis into a one-dimensional problem. Since droplet flames are burning at sufficiently subcritical pressures, the gas phase is assumed to be ideal and the liquid phase is in equilibrium evaporation. Finally, the effect of viscous dissipation is neglected because the Mach number of flow in droplet flames is much smaller than unity.

Under the aforementioned assumptions, the conservation equations for the mass, momentum, energy and species, and the equation of state are as follows [5]:

$$\frac{\partial\rho}{\partial t} + \frac{1}{r^2}\frac{\partial m}{\partial r} = 0 \tag{1}$$

$$p = p(t) = p_m + p_a \sin(2\pi\omega t) \tag{2}$$

$$\frac{\partial(\rho h)}{\partial t} + \frac{1}{r^2} \frac{\partial(mh)}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \lambda \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \rho \sum_{j=1}^{n_s} h_j Y_j V_j \right) - \frac{\partial p}{\partial t} = 0$$
(3)

$$\frac{\partial(\rho Y_j)}{\partial t} + \frac{1}{r^2} \frac{\partial(mY_j)}{\partial r} + \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \rho Y_j V_j \right) = w_j M_j \tag{4}$$

$$p = \rho \bar{R} T / \bar{M} \tag{5}$$

where t is the time, r is the radial coordinate, T is the temperature, p is the pressure. The radial mass flux m is defined as $m \equiv \rho u r^2$, ω and subscripts m and a are frequency, the mean and amplitude of pressure oscillations, respectively. And h and \overline{M} are the specific enthalpy and the average molecular weight of mixture.

The diffusion velocity V_j is given by $V_j = -(D_j/X_j)(\partial X_j/\partial r) + (D_j\Theta_j/X_j)\{\partial(\ln T)/\partial r\} + V_c$ where the correction velocity V_c is included to insure $\sum_{j=1}^{n_s} Y_j V_j = 0$. The applicable boundary conditions are

$$r = r_s : \lambda r^2 \frac{\partial T}{\partial r} = mL, \quad T = T_{B,CH_3OH}, \quad mY_j + \rho r^2 Y_j V_j = m\delta(j - CH_3OH)$$

$$r \to \infty : T \to T_\infty : \text{steady}, \quad \frac{\partial(\rho h)}{\partial t} = \frac{\partial p}{\partial t} : \text{oscillation}, \quad Y_j \to Y_{j,\infty} = \delta(j - \text{air})$$
(6)

where L is the latent heat of liquid methanol. A detailed reaction mechanism including 28 species and 92 elementary reaction steps is adopted [7].

Results and Discussions

To obtain information on basic flame behaviors, steady-state characteristics of methanol droplet flames as a function of pressure are investigated numerically by employing the detailed kinetic mechanism. An inverse numerical method is used, in which the flame structures are calculated as a function of maximum temperature instead of pressure. Figure 1 shows the steady-state behavior of maximum temperature, T_{max} , with pressure represented by a dotted line, demonstrating the upper branch of a typical characteristic S-curve.



Figure 1: Typical flame responses with pressure oscillation for $\omega = 10^2$ Hz and $r_s = 70 \mu m$ demonstrating quasi-steady, reignition, and extinction behaviors.

The response of a flame to the imposed acoustic pressure oscillation $p' = p_a \sin(2\pi\omega t)$ with $\omega = 10^2$ Hz is then analyzed for a methanol droplet flame with 70 μm radius at the mean pressure of $p_m = 1$ atm. When a small amplitude of pressure oscillation is imposed, the response does not show significant deviation from the steady S-curve (Fig. 1 inset), thus demonstrating a quasi-steady response. As the amplitude of pressure oscillation increases, the locus of maximum temperature begins to deviate significantly from the steady-state S-curve. At a certain amplitude, the minimum temperature during the pressure oscillation becomes even smaller than the steady extinction temperature, T_{ext} corresponding to the temperature at the turning point of the steady state S-curve. Then, the flame response passes through an unstable region, that is, the middle branch of S-curve. In this unstable, middle branch of the characteristic S-curve, the response shows two different modes depending on the amplitude of pressure oscillation. The flame can be either extinguished and has transition to lower branch, or reignited and has transition to upper branch. An excessive amplitude leads to direct extinction of flame due to low pressure which reduces chemical reaction rate. The reignition can be defined as the condition when a flame response passes through middle branch and having transition to upper branch again.

The relation between acoustic amplitude and temporal minimum temperature during one cycle of pressure oscillation, T_{min} , is shown in Fig. 2 for various oscillation frequencies. When a small amplitude of pressure oscillation is imposed, T_{min} is nearly the same temperature corresponding to the minimum pressure during one cycle, $(p_m - p_a)$, on the characteristic S-curve. As amplitude increases, flame temperature decreases significantly and becomes even lower than T_{ext} , such that there exists a regime where flames can sustain and recover their intensity even after the temporal state passes the steady-state extinction criterion. This is because the characteristic acoustic time is short, that is, the residence time of passing temporal minimum pressure is short especially when the oscillation frequency becomes large. In such cases, the flame passes through the steady extinction point, *i.e.*, the temporal minimum temperature can be lower than T_{ext} . The reignition regime can be defined when $T_{min} < T_{ext}$ and the flame could recover to the upper branch.



Figure 2: Variations of minimum temperature during one cycle at several acoustic frequencies.

The boundaries among quasi-steady response regime, reignition regime, and extinction regime vary in the parameter space of acoustic amplitude and frequency. Figure 3 shows these acoustic response characteristics. Here, the steady critical amplitude is defined as the percentage difference between mean pressure (1 atm) and steady extinction pressure (0.88 atm), which is 12 % in this calculation. If the acoustic frequency is lower than 10^2 Hz, reignition of flame does not occur, while the reignition regime broadens with acoustic frequency. The reason is that the characteristic acoustic time becomes the same order of characteristic reaction time, as the acoustic frequency increases. This effect becomes more pronounced with the increase in frequency and simultaneously, the possibility of occurring direct extinction decreases.



Figure 3: Quasi-steady response, reignition and extinction regime with respect to acoustic amplitude and frequency.

Concluding Remarks

Reignition phenomenon has been investigated when an acoustic pressure oscillation was imposed on the steady methanol droplet flame near extinction. The trend of reignition was analyzed by fixing frequency of acoustic pressure oscillation. The reignition regime was obtained with respect to acoustic amplitude and frequency as an overall characteristic response. Reignition phenomena can occur under the condition that the characteristic acoustic time becomes the same order of characteristic reaction time. Reignition does not occur if the frequency of acoustic pressure oscillation is small, and the possibility of occurring reignition increases with acoustic frequency.

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