Steep Pressure Interactions With a Methane-Air Flame: The Inclusion of Multi-step Chemistry

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1 Introduction

Sharp pressure changes interacting with flat premixed flames have been investigated in earlier works both for a single-step reaction scheme, and for multistep ozone flames (Johnson et al, 1995). The intention of this work is now to consider realistic hydrocarbon flames such as methane.

The numerical computation of structures of one-dimensional methane-air flames over a wide range of conditions has been made (Westbrook and Dryer, 1984; Peters and Williams, 1987) and some reaction schemes involve 18 species and 40 reactions (Maass and Peters, 1993) or even nearly 200 elementary steps. Several reduced schemes have been proposed (Peters and Williams, 1987; Griffiths, 1995) and reproduce most of the chemistry from the earlier work (Westbrook and Dryer, 1984). Peters and Williams (1987) developed a three-step scheme, which is a simplied version of the four-step scheme proposed by Reitz and Bracco (1983) and more recently by Peters (1993). This reaction scheme was effectively used by Bradley et al (1996) to study the burning velocities for spherical methane-air flames. Therefore, the three or four-step reaction scheme is naturally a good starting point for these studies.

Most of the work on multi-step chemistry has focused on the computational simulations at steady-state or on using the partial-equilibirum approximations (Peters and Williams, 1987), for modelling the multi-layer structure of methane-air flames. In this paper, we intend to study sharp pressure disturbances and their interactions with premixed flames characterised by three or four step chemistry, in a similar way to our work on ozone decomposition flame (Johnson et al, 1995). We focus on the effect of a sharp pressure drop on the time response of the flame and the influence of the three activation energies and Lewis numbers defining the reaction.

2 Governing Equations

Based on the work on methane-air flames (Peters and Williams, 1987; Bradley et al, 1996), we use the simplified three-step reaction mechanism

$$\begin{array}{ll} \mathrm{I} & CH_4+O_2 \xrightarrow{\mathcal{R}_1} CO + H_2 + H_2O, \\ \mathrm{II} & CO + H_2O \overset{\mathcal{R}_2}{\rightleftharpoons} CO_2+H_2, \\ \mathrm{III} & O_2+2H_2 \xrightarrow{\mathcal{R}_3} 2H_2O, \end{array}$$

Here we assume that the concentration of [H] is in a pseudo-steady state. This multistep scheme leads to the following equations in nondimensional form

$$\frac{\partial T}{\partial t} + m_0 \frac{\partial T}{\partial x} - \frac{\partial^2 T}{\partial x^2} = (1-\gamma^{-1}) \frac{T}{p} \frac{dp}{dt} + Q \sum_{j=I}^{IV} \mu_j \mathcal{R}_j, \tag{1}$$

$$\frac{\partial Y_i}{\partial t} + m_0 \frac{\partial Y_i}{\partial x} - Le_i \frac{\partial^2 Y_i}{\partial x^2} = \sum_{j=I}^{IV} \nu_{ij} \mathcal{R}_j, \quad j = 1, 2, ..., N-1, \tag{2}$$

with

$$\mu_j = \frac{Q_j}{(T_b - T_u) W_F}, \tag{3}$$

where we have rescaled the space and time with respect to thermal diffusion. W_F is the molecular weight of the fuel (CH_4), Q_j is the heat release from reaction step $j = I, II, III$ and the overall reaction heat release is $Q = T_b - T_u = \sum_{j=I}^{IV} Q_j$. Le_i is the Lewis number of species i defined as

$$Le_i = \frac{D'_0(\text{premixed})}{\lambda' / \rho'_0 c'_p}, \tag{4}$$

and D'_0 is the diffusion coefficient. The reaction rates are given by

$$\mathcal{R}_j = \Lambda_j k_j G_j(Y_i), \quad \Lambda_j = \frac{A'_j D'_{0j} e^{-\theta_j}}{u'_{0j}}, \quad k_j = T^{n_j} e^{\theta_j (1 - 1/T)}, \tag{5}$$

where $G_j (j = I, II, III)$ are the function of the related species concentrations Y_i $(i = 1, 2, ..., N-1)$. For example,

$$G_I = [\mathrm{CH_4}][H], \quad G_{II} = \frac{[H]}{[\mathrm{H_2}]}([\mathrm{CO}][\mathrm{H_2O}] - \frac{[\mathrm{CO_2}][\mathrm{H_2}]}{K_{II}}), \tag{6}$$

$$G_{III} = [H]([\mathrm{O_2}] - \frac{[H]^2[\mathrm{H_2O}]^2}{[\mathrm{H_2}]^3 K_{IV}}). \tag{7}$$

where the H-atom concentration is given by

$$[H] = (1 - \frac{k_3}{k_4} - \frac{k_1[CH_4]}{k_4[O_2]})^{1/2} K_{IV}^{1/2} [O_2]^{1/2} [H_2]^{3/2} / [H_2O]. \tag{8}$$

The nonlinear features of these coupled partial differential equations, make mathematical analysis intractible so we use the full numerical simulation to study the response of the premixed flame to sharp pressure drops where a new temperature environment is suddenly experienced due to the small (but significant) cooling effect. Thus the new temperature field is given by

$$T(x) = T_s(x) p_0^{(1-1/\gamma)}, \tag{9}$$

and equation (1) is solved with this new temperature as a starting condition (Figure 1). At this time scale, the pressure transient is no longer felt so that $dp/dt = 0$. The The full unsteady equations are solved by first considering the steady state equations using a Runge-Kutta technique, followed by a shooting method in order to obtain the initial temperature and species concentration profiles. These are then input into the unsteady program which solves the full equations using a finite difference scheme with higher resolution near the reaction zone. This involves an adaptive grid scheme with a denser grid near the reaction zone. At each time step, the mass burning rate is calculated and the profiles of temperature and species concentration are also updated. The adaptive grid scheme near the reaction ensures high accuracy in order to follow the evolving temperature profile.

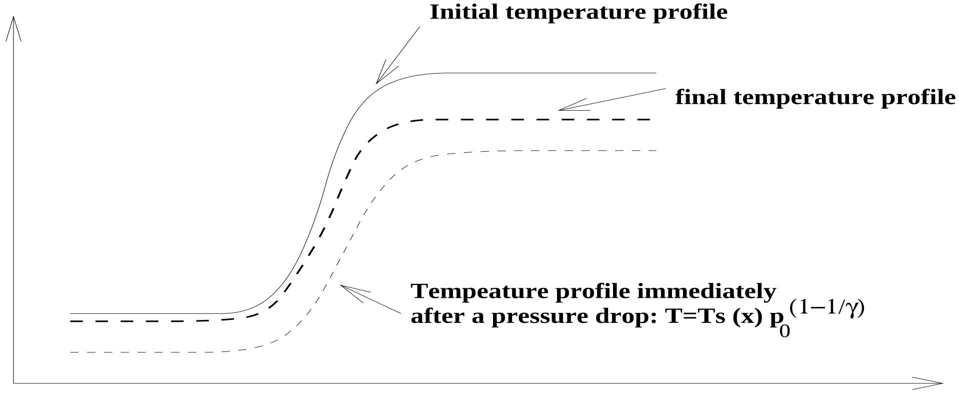

Figure 1 Temperature profiles before and after the pressure drop.

3 Numerical Simulations

By using the direct numerical method described in the above section, we can study many different features of the premixed flame, and how pressure changes affect the flame behaviour in different regions of parameter space arising from the multi-step chemistry. In a similar approach, as with the earlier work on interactions of pressure changes and premixed flames with single step chemistry, we focus here on the critical pressure leading to the boundary of extinction and recovery.

Sharp Pressure Change: Extinction and Recovery

For a given sharp pressure drop, earlier work (Johnson et al, 1995) suggests a critical value (p_{min}) of pressure drop where extinction just happens. This critical value depends on activation energy, Lewis number and details of flame chemistry. For a three or four step reaction scheme, the activation energy (θ_1) of the chain-branching step is relatively large compared to that of the recombination steps (θ_2 and θ_3). Figure 2 shows how the critical pressure varies with these different activation energies. We can see that the activation energy has a very strong influence on the extinction behaviour of the premixed flame. Compared with the one-step flame where $\theta_1 = \theta_2 = \theta_3 = 10$, the flame with the multistep reaction scheme is relatively thicker, and thus more stable.

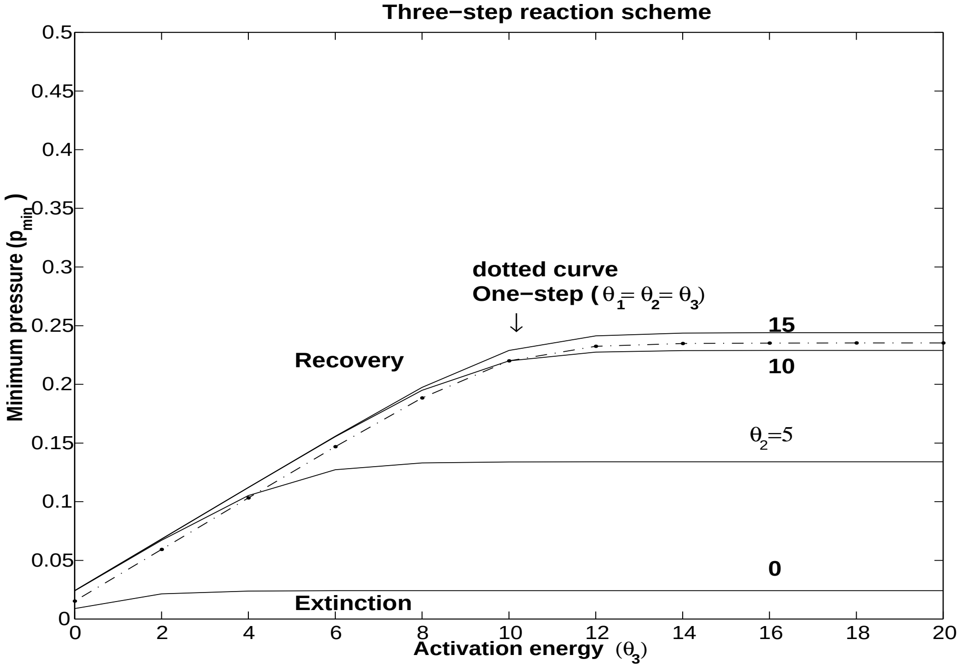

Figure 2 Effect of the activation energies of three-step reactions on the critical extinction pressure drop ($\theta_1 = 10$ for three-step reaction).

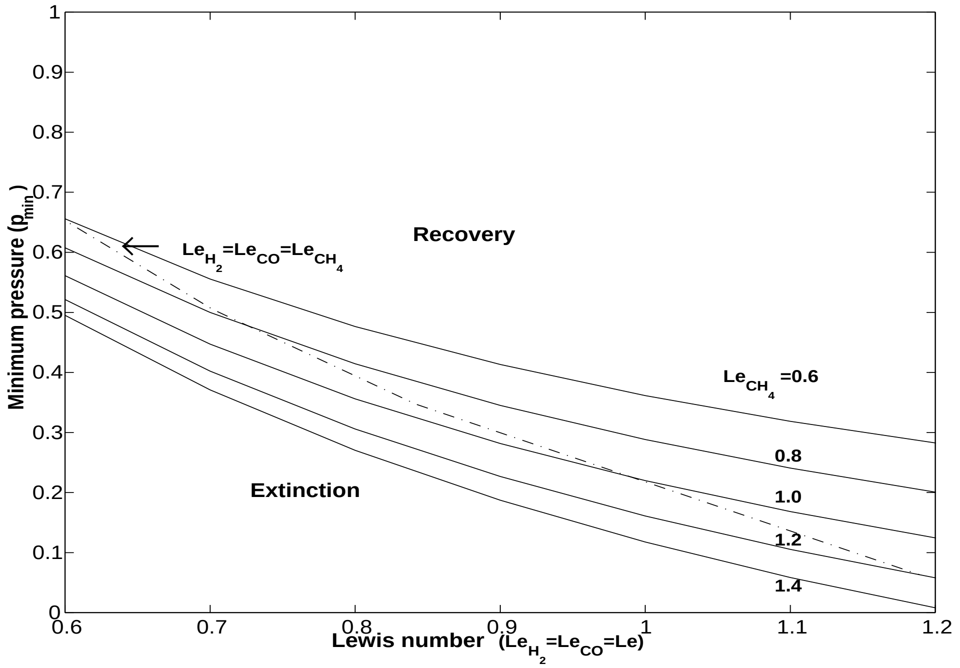

Figure 3 Effect of Lewis number on the critical extinction pressure drop. The values of activation energies used in this figure are $\theta_1 = 20, \theta_2 = \theta_3 = 15$.

Effect of Lewis number

It is well-known that Lewis number can affect the flame properties significantly. Our numerical simulations shown in Figure 3 support this result. For fixed Lewis numbers of the intermediate species such as H_2 and CO, we can see how the change of Lewis number of methane affects the critical extinction value of pressure drop.

4 Conclusions

A numerical investigation has been carried out into the effect of sharp pressure drops on methane-air premixed flames with multi-step chemistry. The time response of the mass burning rate of the flame for different values of pressure drop has also been calculated. A critical minimum pressure drop is found such that drops below this value, lead to extinction of the premixed flame. The extinction pressure drop depends on the three activation energies and Lewis number.

For sudden pressure drops, the flame is extinguished, if the pressure drop is sufficiently large. For large activation energies and low Lewis number, the flame is very susceptible to pressure changes.

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