Extinction of Premixed Flames by sudden Depressurization: Strain and Two-step Chemistry

K.R. Anil Kumar[1†], **A.C. McIntosh**[1], **J. Brindley**[2], **and X.S. Yang**[1]
[1]Energy and Resources Research Institute
[2]Department of Applied Mathematics
University of Leeds
Leeds LS2 9JT, United Kingdom
[†]Corresponding e-mail: fuerakk@leeds.ac.uk

Abstract

A numerical study of the response to a sudden drop in pressure of planar premixed flames modelled by the two-step Zel'dovich reaction scheme is presented. Critical minimum pressures are computed with different values of the ratio of pre-exponential factors of the constituent reactions. The computations show that the flame becomes more unstable as the temperature sensitivity of the rate of heat release increases. The increase in the activation energy of the first reaction is found to increase the critical minimum pressure significantly.

Keywords: Premixed flames, extinction, depressurization

Introduction

The bulk quenching of premixed flames is supposed to be one of the reasons for the emission of unburned hydrocarbons from internal combustion engines. Experimental observations [1], which showed the incomplete combustion of lean methane-air mixtures due to flame quenching in an expanding chamber, support this hypothesis. These results [1] also indicate that the point of flame quenching depends on the amount of volume expansion and is found to be nearly independent of the rate of chamber expansion. In this paper we consider one aspect of this process, namely, the response of a laminar premixed flame to sudden pressure drops.

The effect of a sudden pressure-drop on premixed flames has been studied extensively. Earlier modelling studies by Peters and Ludford [2] and Ledder and Kapila [3] found that, for a sufficiently rapid decrease in pressure, the solution for the flame speed did not exist. They suggested that indicated extinction. However, the extinction event itself was not modelled. Later Johnson *et al.* [4] solved the nonlinear governing equations numerically and showed that, for a sufficiently large decrease in pressure, extinction could occur. Most of the previous studies used single-step chemistry in their calculations, except the multi-step ozone flames used by Johnson *et al.* [4].

As discussed above the one-step global reaction model can predict extinction by depressurization. However, using a more realistic two-step scheme for hydrocarbon combustion, Hocks *et al.* [5] showed that the speed of quenching of a laminar flame at a cold wall depends on the concentration of the intermediate species or radicals. They also found that the high concentrations of radicals are realistic features of acetylene and methanol flames and the two-step process used is adequate to describe flame-quenching, whereas a one-step global mechanism is not. Hence, the objective of the present work is to study the response of a premixed flame to a sudden drop in pressure using a generic two-step reaction scheme, namely, the Zel'dovich mechanism [6]. The stability boundaries in terms of the critical minimum pressure have been computed.

The Physical Problem, Model and Solution Technique

We consider an unsteady, planar, one-dimensional premixed flame with the following assumptions: (1) pressure, p', is uniform in the flame; however, it can vary with time, (2) the thermal conductivity is proportional to temperature, and the specific heat is constant, (3) the diffusion coefficients of all species are equal, (4) molecular masses of all species are equal, and (5) Lewis number Le is constant.

The Chemical Reaction Scheme: The generic Zel'dovich two-step reaction mechanism was used in the present study.

$$\mathrm{A} + \mathrm{B} \xrightarrow{R_1} \mathrm{B} + \mathrm{B} \quad \text{and} \quad \mathrm{B} + \mathrm{B} + \mathrm{M} \xrightarrow{R_2} \mathrm{P} + \mathrm{M}, \tag{1}$$

where A is a reactant, B is an intermediate species, C is the final product, and M is a third body. The first step is a chain- branching reaction with a finite activation energy. The second step is a chain breaking recombination reaction with zero activation energy. The associated non-dimensional reaction rates [7] are given by

$$R_1 = \Lambda_1 p T^{-1} C_A C_B \exp[\theta_1(1 - 1/T)] \quad \text{and} \quad R_2 = \Lambda_3 p^2 T^{-2} C_B^2, \tag{2}$$

where R_1 is the rate of consumption of A in step 1, R_2 is the rate of production of P in step 2, Λ_1 and Λ_2 are the dimensionless pre-exponential factors of the first and second reactions respectively, θ_1 is the dimensionless activation energy of the first reaction, C_A and C_B are the dimensionless mass fractions of the species A and B, and T is the dimensionless temperature.

Governing Equations and Method of Solution: The non-dimensional governing equations for a 1-D laminar premixed flame, in a mass-weighted coordinate system as given by McIntosh *et al.* [7], are modified to include the two-step chemistry. First, these equations are solved numerically to obtain a steady-state solution ($T_s(x)$, $C_{A,s}(x)$, and $C_{B,s}(x)$) at $p = 1$ (for all values of Λ_2/Λ_1, Λ_1 is selected so that the nondimensional mass flux is unity at $p = 1$). The pressure is then instantaneously dropped to p_f. The temperature field immediately changes because of the expansion, assumed isentropic and adiabatic conditions. The new temperature is given by

$$T(x) = T_s(x) p_f^{1-\gamma^{-1}}, \tag{3}$$

which is now not consistent with steady flame propagation, so that there is a finite response time as the temperature and concentration fields adjust. The governing equations are then solved numerically, to obtain the evolution of temperature and mass fractions with time. We make the assumption that the gas expansion invoked by a planar pressure disturbance (through the momentum equation) takes place on a much shorter timescale than the combustion for the one-dimensional case and that the flow remains laminar [1, 8]. We also assume that the time scale associated with strained flow is larger than the diffusion-reaction time associated with the adjustment of the temperature and species fields.

Results and Discussion

Extinction of Unstrained Flames: In this section, the critical minimum pressures obtained with the Zel'dovich mechanism for different values of Λ_2/Λ_1 and Q_2 are presented. The critical minimum pressure, below which extinction occurs, is calculated as follows. First a steady state solution is obtained at $p = 1$. The pressure is then suddenly dropped to a lower value, p_f, and the evolution with time of the mass flux at the point of inflexion is computed. Note that for an adiabatic flame, where there is no heat loss, modelled by Arrhenius reaction so that there is always a small positive reaction rate, and the mass flux will eventually recover whatever the drop in pressure. However, for practical purposes, extinction is assumed to occur when the mass flux does not start recovering before some stipulated time, here taken to be $t = 50$ (for a methane-air flame at 1 MPa this corresponds approximately to 100 ms).

Figure 1 shows steady-state temperature and mass fraction profiles at $p = 1$ for different values Λ_2/Λ_1. In this case the entire heat release is assumed to take place during the second reaction ($Q_1 = 0$ and $Q_2 = 0.88$). As identified by Liñán [10], there are three regions: (1) $\Lambda_2/\Lambda_1 \gg 1$ where the recombination reaction is very fast compared to the chain branching reaction and the steady-state solution corresponds to that with an equivalent single step reaction, (2) $\Lambda_2/\Lambda_1 \sim 1$, and (3) $\Lambda_2/\Lambda_1 \ll 1$. In the latter two cases, the intermediate species concentrations are high and the chain branching reaction occurs in a thin reaction zone embedded in a relatively thick recombination reaction zone. As a result, for $\Lambda_2/\Lambda_1 \ll 1$ the heat release in the flame occurs in a relatively wider temperature range.

Figure 2 shows the evolution of the mass flux with time for different values of Λ_2/Λ_1 after the p is dropped suddenly to 0.4. It can be seen that the recovery time of the transient mass flux is the longest for $\Lambda_2/\Lambda_1 = 10^1$. However, as Λ_2/Λ_1 decreases the time for recovery of the mass flux after the initial drop decreases and hence the response becomes more stable. This could be attributed to a more distributed heat release associated with small values of Λ_2/Λ_1, and also the fact that the heat release due to the recombination reaction is not exponentially dependent on temperature ($\theta_2 = 0$). These two factors decrease the drop in the rate of heat release immediately after the drop in pressure. Consequently the critical minimum pressure decreases as Λ_2/Λ_1 decreases.

The steady-state solution and the transient mass flux after a sudden pressure drop is influenced also by the partition of heat release between the two constituent reactions. The mass flux recovery time decreases as Q_2 increases and consequently the critical minimum pressure decreases. So, the response becomes more stable as the larger portion of heat release takes place in the less temperature sensitive recombination reaction.

The critical minimum pressure was computed for different values of parameters Λ_2/Λ_1 and Q_2 and is shown in Fig. 3. It is found that in the present case the critical minimum pressure approaches 0.394 as Λ_2/Λ_1 increases. A decrease in Λ_2/Λ_1 or an increase in Q_2 stabilizes the burning by decreasing the critical minimum pressure. In the range of $0.01 < \Lambda_2/\Lambda_1 < 10^2$ the critical minimum pressure varies between 0.28 to 0.394. Experiments conducted with methane-air mixtures [1] in an expanding chamber found that for an equivalence ratio of 0.605 the volume expansion ratio (defined as the ratio of increase in volume to the initial volume) at quenching, is approximately 1.2. Assuming isentropic expansion, this corresponds to a critical minimum pressure of 0.33. Hence, the critical minimum pressures calculated in this work for the Zel'dovich mechanism compare well with the equivalent experimental values.

Effect of the Activation Energies: The activation energy is another important kinetic parameter which affects the temperature sensitivity of the reaction rates and the rate of heat release. Figure 4 shows the variation of the critical minimum pressure with θ_1. As θ_1 increases, the reaction zone thickness decreases and the heat release takes place more and more in the high temperature region. This makes the rate of heat release more temperature sensitive and hence the flame becomes easier to extinguish as θ_1 increases. The above results may also be interpreted to represent the variation of critical minimum pressure with the reactant mixture ratio. As the reactant mixture becomes leaner the flame temperature decreases. For the same dimensional activation energy, this increases the non-dimensional activation energy, θ. Therefore, it can be concluded that the critical minimum pressure increases, and hence the flame is destabilized, as the reactant mixture becomes leaner (effect of $T_{-\infty}$ and and the total non-dimensional heat release, $Q_1 + Q_2$, which are also varied with the flame temperature, on the critical minimum pressure is found to be very small). This behavior is in qualitative agreement with the experimental observations [1].

Extinction of Strained Flames: Similar calculations were also performed for a flame subjected to a positive strain. The mathematical model is similar to that used by McIntosh *et al.* [7]. As in the case of single step chemistry a positive strain decreased the steady-state burning rate with the Zel'dovich mechanism. Figure 5 shows the steady-state temperature and mass fraction profiles. The temperature profile became steeper and hence the reaction zone became thinner. Figure 6 shows the evolution of mass burning rate for $p_f = 0.4$. It is found that a positive strain of 0.5, with the Zel'dovich mechanism, delays the recovery of the mass flux, hence destabilizing the flame.

Conclusions

The critical minimum pressures for the Zel'dovich scheme depend on the ratio Λ_2/Λ_1 and the partition of heat release between the two constituent reactions. The critical minimum pressure asymptotically reaches its upper limit, in the present case 0.394, as Λ_2/Λ_1 increases. This upper limit is same for all values of Q_2. As expected, as fraction of the total heat released in the less temperature sensitive recombination reaction increases, the flame become more stable. Finally, an increase in activation energy is found to increase the critical minimum pressure significantly. This may also be considered to be a demonstration of the destabilizing effect of leaner mixtures because of the decreased reaction zone temperature.

Acknowledgment

The authors thank the U.K. EPSRC for their support for this work on Grant GR/M 18607.

References

[1] Smith O. I., Westbrook C. K., and Sawyer R. F., *Proceedings of the Combustion Institute* 17:1305 (1979).

[2] Peters, N., and Ludford, G. S. S., *Combust. Sci. and Technol.* 34:331 (1983).

[3] Ledder, G., and Kapila, A. K., *Combust. Sci. and Technol.* 76:21 (1991).

[4] Johnson, R. G., McIntosh, A. C., and Brindley, J., *Combust. Flame* 102:493 (1995).

[5] Hocks, W., Peters, N., and Adomeit, G., *Combust. Flame* 41:157 (1981).

[6] Zel'dovich, Y. B., *Theory of Flame Propagation*, NACA TM 1282 (1951).

[7] McIntosh, A. C., Brindley, J., and Yang, X. S., *Combust. and Flame* 125:1207 (2001).

[8] Batley, G. A., McIntosh, A. C., and Brindley, J., *Combust. Sci. and Technol.* 92:367 (1993).

[9] Johnson, R. G., McIntosh, A. C., Brindley, J., and Batley, G. A., *Combust. Sci. Technol.* 99:201 (1994).

[10] Liñán, A., *A Theoretical Analysis of Premixed Flame Propagation with an Isothermal Chain Reaction* Technical Report 1, Instituto Necional De Tecnica Aerospacial Esteban Terradas, Madrid (1971).

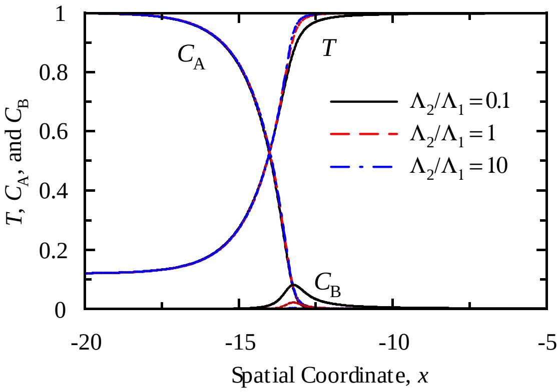

Figure 1: Temperature and mass fraction profiles with the Zel'dovich mechanism ($Q_1 = 0$ and $Q_2 = 0.88$).

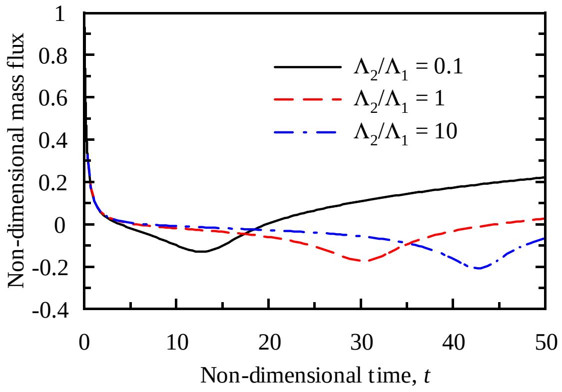

Figure 2: Evolution of mass flux after a sudden pressure drop for the Zel'dovich mechanism ($Q_1 = 0$ and $Q_2 = 0.88$).

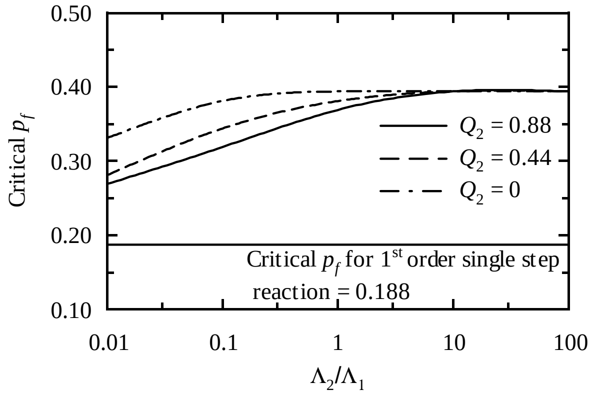

Figure 3: Effect of Λ_2/Λ_1 and Q_2 on the critical minimum pressure with the Zel'dovich mechanism

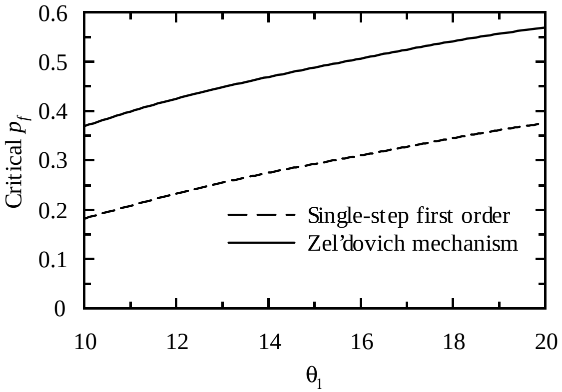

Figure 4: Effect of θ_1 on the critical minimum pressure with different reaction schemes ($Q_1 = 0$, $Q_2 = 0.88$, and $\Lambda_2 = \Lambda_1$)

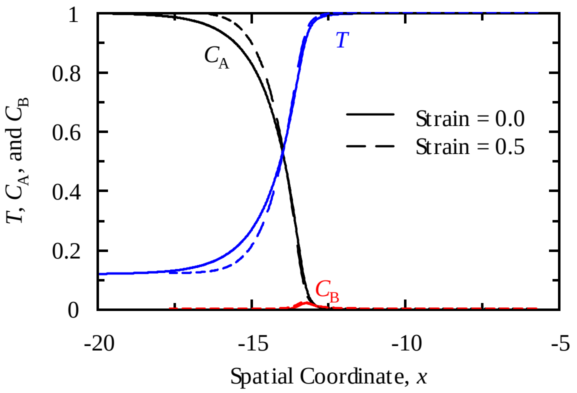

Figure 5: Temperature and mass fraction profiles with the Zel'dovich mechanism ($Q_1 = 0$ and $Q_3 = 0.88$).

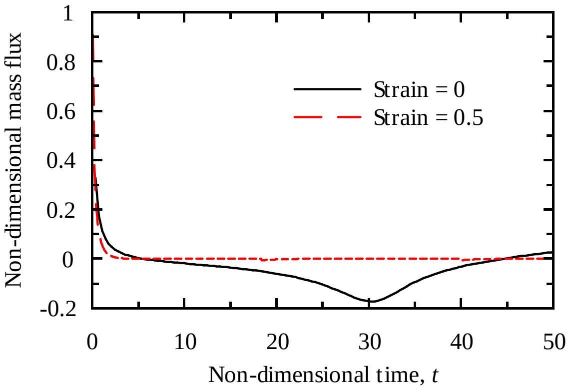

Figure 6: Evolution of mass flux after a sudden pressure drop for the Zel'dovich mechanism ($Q_1 = 0$ and $Q_3 = 0.88$).