A One-dimensional Model for Deflagration-to-detonation Transition of an Elongated Flame

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1 Introduction

Deflagration-to-detonation transition (DDT) remains one of the prominent unsolved problems in combustion theory. Since the pioneering experiments by Meyer et al. [1], it has been known that DDT can take place in different forms depending on experimental conditions, so that no single mechanism provides a complete explanation of the phenomenon. Reviews of such DDT mechanisms are presented in detonation textbooks [2, 3].

In this abstract, we present recent advances in the theoretical modeling of DDT for elongated flames in tubes [4]. A laminar flame starting from the closed end of a tube is considered, and a double-feedback mechanism for DDT of such a flame is proposed, in which compression heating by the lead shock is augmented by an effective piston acceleration due to the back-flow of burnt gas into the flame tip. After simplifying the problem into a one-dimensional flame supported by an accelerating piston, it is shown that a self-similar solution for the flow exhibits a turning point at which the flame acceleration diverges. Further analysis beyond self-similarity reveals the formation of a shockwave on the flame at the turning point. Such a shock formation is a good candidate to blow up the inner structure of the flame and produce the transition to a detonation.

2 Self-similar solution of flame acceleration

We consider a flame propagating from the closed end of a semi-open tube filled with a very energetic mixture, as shown in Figure 1a. The back flow of burnt gases towards the tip of the flame can be modeled by adding a source term to the one-dimensional equation of conservation of mass [5]. If the thermodynamic properties in the burnt gas are quasi-uniform and quasi-steady, the effect of this source term is equivalent to that of a piston pushing on the flame (Figure 1b), whose velocity is given by:

$$U_p = \overline{u}_{bf} = (\sigma - 1)\frac{\overline{\rho}_{uf}}{\overline{\rho}_{bf}}U_L, \tag{1}$$

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where the subscripts uf and bf denote the flow just upstream and downstream of the flame respectively, the overbar denotes quantities in the quasi-steady state, and U_L denotes the laminar flame velocity with respect to the upstream gas. The coefficient σ characterizes the flame elongation, and is related to the elongation length L and tube radius R by

$$\sigma \equiv 2\frac{L}{R} + 1. \tag{2}$$

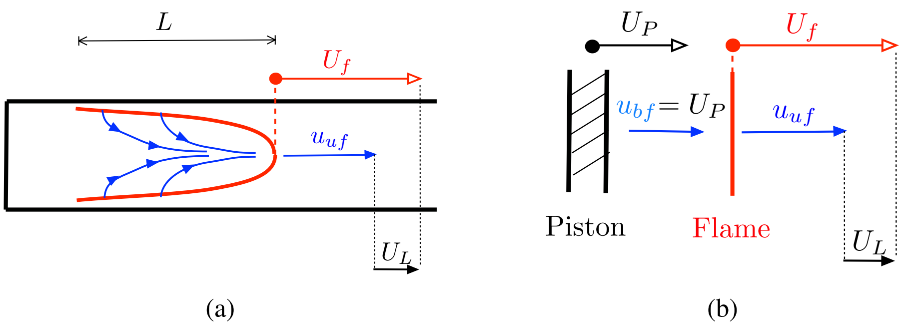


Figure 1: (a): Sketch of an elongated flame propagating from a closed end of a tube. Also sketched in (a) are the streamlines of burnt gas issued from the skirt of the elongated flame towards the tip (see Clanet and Searby [5]). (b): One-dimensional piston model, in which the back-flow of burnt gas is modeled by an accelerating piston behind the flame whose velocity is proportional to the flame elongation.

The flame propagation generates compression waves in the fresh gases which then coalesce into a lead shock. The flow velocity just ahead of the flame can be expressed as:

$$\overline{u}_{uf} = U_L \frac{\overline{\rho}_{uf}}{\overline{\rho}_{bf}} \sigma - U_L. \tag{3}$$

The laminar flame velocity U_L for a single-step Arrhenius kinetics can be computed using the solution obtained by Zel'dovich and Frank-Kamenetskii [6] as

$$\frac{U_L}{U_{Lo}} = \left(\frac{T_b}{T_{bo}}\right)^2 \left(\frac{T_u}{T_{uo}}\right)^{3/2} \exp\left[-\frac{E}{2k_B}\left(\frac{1}{T_b} - \frac{1}{T_{bo}}\right)\right] \tag{4}$$

where the subscripts u and b denote fresh and burnt gases respectively, and o denotes the reference state ahead of the lead shock.

When the flame acceleration is small enough that unsteady compressible effects in the flow between the flame and the precursor shock are negligible, a self-similar solution can be obtained for the shock-flame complex. The upstream condition for the flame will be the same as that given by Rankine-Hugoniot relations across the shock, so that we have

$$\frac{\overline{u}_{uf}}{a_o} = \frac{2}{\gamma+1}(M - 1/M) \tag{5}$$

$$\frac{\overline{T}_{uf}}{T_o} = \frac{2\gamma}{(\gamma+1)^2}\left(1 - \frac{\gamma-1}{2\gamma M^2}\right)\left[2 + (\gamma-1)M^2\right]. \tag{6}$$

Equation (6) along with the isobaric approximation of the flame

$$T_b = T_u + \frac{q_m}{c_p}, \tag{7}$$

where q_m is the total heat release per unit mass and c_p is the specific heat capacity at constant pressure, allow us to express U_L in equation (4) in terms of M only. Then, substituting the found expression for U_L in equation (3) along with the isobaric approximation

$$\frac{\overline{\rho}_{uf}}{\overline{\rho}_{bf}} = \frac{\overline{T}_{uf} + q_m/c_p}{\overline{T}_{uf}} \tag{8}$$

allow us to obtain an expression for $\overline{u}_{uf}$ in terms of M. Finally, substituting the found expression of $\overline{u}_{uf}$ into equation (5), results in a nonlinear equation for the Mach number M.

These substitutions can be difficult to work out explicitly for the general case. However, with the conditions of large heat release and $M \gtrsim 2$, a simplified equation for M can be written as

$$\Lambda^{-1}\mathcal{L}(M) = \mathcal{R}(M) \tag{9}$$

where

$$\mathcal{L}(M) \equiv \frac{M - 1/M}{1 + q/y} \tag{10}$$

$$\Lambda \equiv \frac{\gamma+1}{2}\frac{U_{Lo}}{a_o}\sigma \tag{11}$$

$$\mathcal{R}(M) \equiv \frac{U_L}{U_{Lo}} = \left(\frac{y+q}{1+q}\right)^2 y^{3/2} \exp\left[\frac{\beta_o(y-1)}{y+q}\right] \tag{12}$$

where

$$y \equiv \frac{\overline{T}_{uf}}{T_o}, \quad q \equiv \frac{q_m}{c_p T_o} \tag{13}$$

and

$$\beta_o \equiv \frac{E}{2k_B T_o} \tag{14}$$

is the reduced activation energy.

3 Finite-time singularity

According to equation (9), the self-similar solution does not exist above a threshold value of Λ denoted by Λ^*, as illustrated in Figure 2. Deriving equation (9) with respect to time, one obtains

$$\left[\Lambda^{-1}\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}M} - \frac{\mathrm{d}\mathcal{R}}{\mathrm{d}M}\right]\frac{\mathrm{d}M}{\mathrm{d}t} = \mathcal{R}(M)\frac{1}{\Lambda}\frac{\mathrm{d}\Lambda}{\mathrm{d}t}. \tag{15}$$

The tangency condition of the two curves $\mathcal{R}(M)$ and $\Lambda^{*-1}\mathcal{L}(M)$ in Figure 2 implies that, near the turning point, the factor in square brackets in equation (15) tends to zero, which means that $\frac{\mathrm{d}M}{\mathrm{d}t}$ has to diverge to infinity so that the right-hand side of equation (15) remains finite. Expanding the factor in brackets in powers of $M - M^*$, one obtains

$$\left(\frac{M - M^*}{M^{*2}}\right)\frac{\mathrm{d}M}{\mathrm{d}t} \propto \frac{1}{\Lambda^*}\frac{\mathrm{d}\Lambda}{\mathrm{d}t}\bigg|_{\Lambda=\Lambda^*}, \tag{16}$$

and a similar equation would apply to the flame velocity U_f

$$\left(\frac{U_f - U_f^*}{U_f^{*2}}\right)\frac{\mathrm{d}U_f}{\mathrm{d}t} \propto \frac{1}{\Lambda^*}\frac{\mathrm{d}\Lambda}{\mathrm{d}t}\bigg|_{\Lambda=\Lambda^*}. \tag{17}$$

Integrating equation (17), one obtains

$$\frac{U_f^* - U_f}{U_f^*} = \sqrt{\frac{t^* - t}{t_e^*}}, \qquad \frac{t_e^*}{U_f^*}\frac{\mathrm{d}U_f}{\mathrm{d}t} = \sqrt{\frac{t_e^*}{t^* - t}}, \tag{18}$$

where t_e^* is the time scale of flame elongation rate $\frac{\mathrm{d}\Lambda}{\mathrm{d}t}$ at the turning point. Therefore, at the turning point of the self-similar solution, a runaway of the flame's acceleration occurs systematically, with the acceleration diverging following a square-root law.

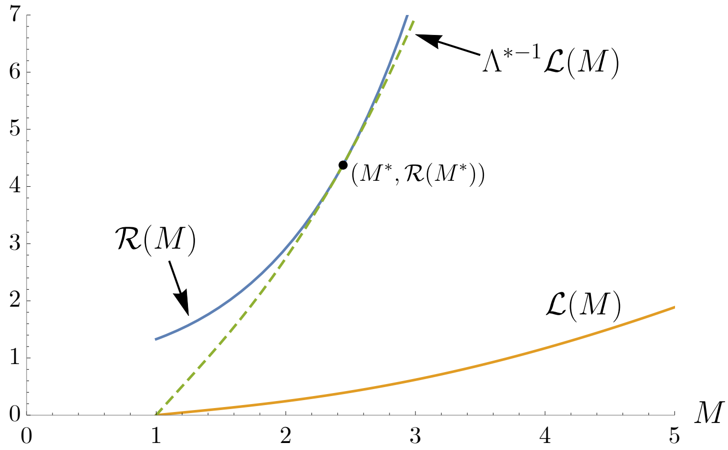


Figure 2: Plots of $\mathcal{L}(M)$ and $\mathcal{R}(M)$ for $\gamma = 1.4$, $q = 9$ and $\beta_o = 1.25$. These parameter values are chosen to be consistent with experimental studies on DDT of highly energetic mixtures [7, 8].

4 Shock formation on the flame front

The self-similar solution remains valid as long as the flame acceleration is small. More precisely, the time scale of flame acceleration should be larger than the transit time of acoustic waves in both directions between the flame and the lead shock. Clearly, in the neighborhood of the turning point, the acceleration of the flame diverges, and thus the self-similar solution is no longer valid.

Therefore, to study the flow behavior near the turning point, we consider an inert flow pushed by a piston whose velocity is the same as that in equation (18)[1]:

$$\frac{U_p^* - U_p}{U_p^*} = \sqrt{\frac{t^* - t}{t_e^*}} \tag{19}$$

starting from a steady state representing the self-similar solution, and we look for the formation of shockwaves using the characteristics method of Riemann [9].

Introducing the reduced variables

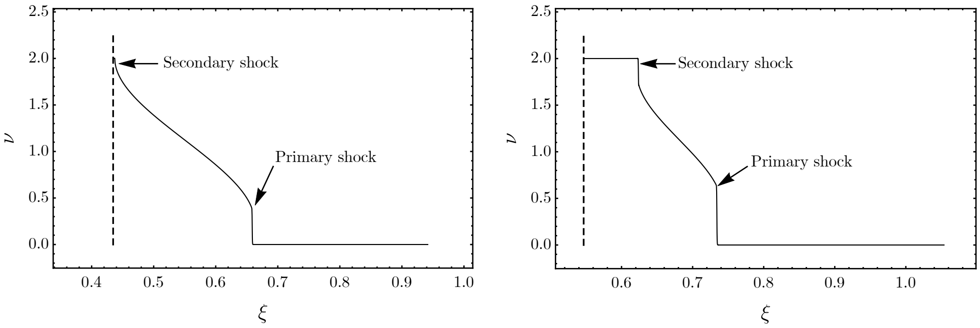
$$\tau \equiv \frac{t}{t_e^*}, \quad \xi \equiv \frac{x}{a_\infty t_e^*}, \quad m^* \equiv \frac{U_p^*}{a_\infty}, \quad \nu \equiv \frac{u - U_p(0)}{a_\infty}, \tag{20}$$

where a_∞ is the speed of sound in the initial state, it is found that shock-formation can occur in two different ways:

[1]It could seem questionable to use the scaling laws of the self-similar solutions in the unsteady flow near the critical condition. This is not the case since the feedback of the self-similar solution on the flame, namely the increase of the gas temperature, is similar to that of a compression wave.

- if $m^*\sqrt{\tau^*} < \frac{4}{\gamma+1}$, then a shock is formed on the piston at time $\tau_s = \tau^*$.
- else if $m^*\sqrt{\tau^*} > \frac{4}{\gamma+1}$, then a first shock is formed at the tip of the compression wave (Figure 3) at time $\tau_s = \frac{4}{\gamma+1}\frac{\sqrt{\tau^*}}{m^*}$.

These analytical solutions were verified to high accuracy with high-order numerical simulations using a spectral difference solver [10]. Furthermore, the simulations show that for the case $m^*\sqrt{\tau^*} > \frac{4}{\gamma+1}$, a second shock is always formed on the piston at $\tau = \tau^*$, as shown in Figure 3.



(a) $\tau = \tau^* = 0.64$ (b) $\tau = 0.7 > \tau^*$

Figure 3: Velocity profile for a flow pushed by an accelerating piston, with shock formation as obtained by a numerical simulation with $m^* = 2.5$ and $\tau^* = 0.64$, $\sqrt{\tau^*} = 0.8 > (1/m^*)4/(\gamma+1) = 0.666$. The dashed line represents the position of the piston, which is moving from left to right.

5 Conclusion and perspectives

The theoretical and numerical results presented above suggest that a shock can be formed in the inner flame structure on the tip of an elongated flame as soon as its velocity reaches the turning point of the self-similar solution. A detailed numerical analysis of DDT for a one-dimensional flame supported by a piston (Figure 1b) is under investigation and will be reported in the final paper.

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