Theory and modeling of flame acceleration and explosion triggering in tubes

V. Bychkov[1], V. Akkerman[1], A. Petchenko[1] and L.-E.. Eriksson[2],

[1]Dept. Physics, Umea University 90187 Umea, Sweden

[2]Dept. Applied Mechanics, Chalmers University of Technology
41296 Gothenburg, Sweden

1 Introduction

Acceleration of premixed flames and deflagration-to-detonation transition (DDT) is one of the most important and, probably, one of the least understood problems in combustion science [1]. Numerous experimental studies have demonstrated the following steps in the transition: a flame accelerates, pushes weak shocks, the shocks get stronger, compress and heat the fresh fuel mixture, which explodes ahead of the flame front and evolves into detonation. Until recently, there was very limited theoretical understanding of the flame acceleration, which is the reason and the most important part in DDT. The first explanation of the acceleration was suggested by Shelkin in 40-ies [1]; the explanation is related to the non-slip boundary conditions at the walls. Since the time of Shelkin, there was a common opinion that flame acceleration is impossible without external turbulent flow. That was a fatal trouble for constructing the acceleration theory, because turbulent burning is a key problem of combustion science, which has not been solved yet despite of almost a century of intensive research. Moreover, as the combustion science developed further, other explanations of DDT have been suggested. For example, a sequence of papers by Sivashinsky et al. discussed a 1D scenario of DDT due to hydraulic resistance, see [2] and references therein. Obviously, this scenario has little in common with the multidimansional Shelkin mechanism. By these reasons, Shelkin's explanation of the flame acceleration has not been transformed into a theory, which could describe the process and predict the acceleration parameters. However, recently a constructive idea was suggested [3] that turbulence plays a supplementary role in the Shelkin acceleration, which is possible even for laminar flames with non-slip at the tube walls. This idea allowed developing the analytical theory of laminar flame acceleration due to the Shelkin mechanism [4,5]. The theory was validated by extensive direct numerical simulations of accelerating flames. Success in the analytical theory of the first stage of Shelkin DDT mechanism inspired further work in that direction. Paper [6] presented an analytical theory of explosion triggering by accelerating flames. The theory demonstrated good agreement with previous numerical simulations [3].

Still, success of the Shelkin mechanism in describing DDT does not eliminate the possibility of alternative mechanisms like that dicsussed in [2]. As an option, these alternative mechanisms may play a supplementary role in DDT in addition to the Shelkin scenario. In the present paper we compare Shelkin mechanism of flame acceleration to another mechanism, which happens at the early stages of burning in tubes. This mechanism was suggested and studied experimentally in [7] in scope of the «tulip» flame phenomenon. We develop the analytical theory for this flame acceleration. We demonstrate that flame acceleration rate is quite strong in that case, but acceleration happens only during a rather short time. As a result of the acceleration, the flame surface area increases by a factor of 15 determined by thermal expansion of the burning matter. We also analyse the possibility of explosion triggering by such a flame and show that at normal conditions it does not lead to DDT. Still, it may work as a precursor for the Shelkin mechanism.

Correspondence to : vitaliy.bychkov@physics.umu.se

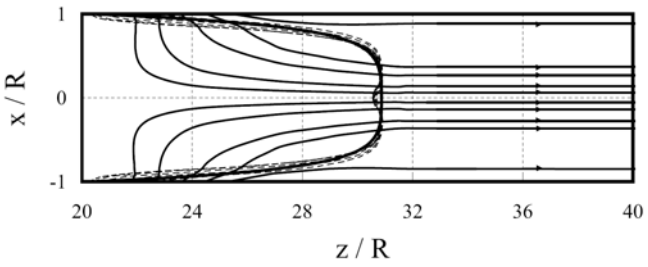

Fig. 1 Characteristic shape of an accelerating flame and streamlines of the flow. The dashed lines show the isotherms from 600K to 2100K. The solid line shows the theoretical prediction for the flame shape.

2 Acceleration because of non-slip walls (Shelkin mechanism)

Here we remind briefly the main analytical and numerical results on laminar Shelkin acceleration obtained in [4,5]. It was demonstrated that a flame propagating from the closed tube end generates a quasi plane-parallel flow, which in turn, distorts the flame shape. After a short transitional time, flame starts accelerating in a self-similar exponential regime with the burning rate U_w (proportional to the total flame surface) increasing as

$$U_w = U_f \exp(\sigma U_f t / R), \qquad (1)$$

where U_f is the planar flame velocity, R is the tube radius (channel half-width), and σ is the dimensionless acceleration rate. The self-similar shape of an accelerating flame is presented in Fig. 1. The acceleration rate was calculated in [4] in the case of a 2D channel as

$$\sigma = \frac{(\mathrm{Re}-1)^2}{4\,\mathrm{Re}}\left[\sqrt{1+\frac{4\,\mathrm{Re}\,\Theta}{(\mathrm{Re}-1)^2}}-1\right]^2, \qquad (2)$$

where $\mathrm{Re} = RU_f/\nu$ plays the role of the Reynolds number and the expansion factor Θ shows density ratio of the fuel mixture and the burnt matter. The analytical formula (2) is in a very good agreement with the results of numerical simulations [4]. In the case of large Reynolds number, Eq. (2) reduces to $\sigma = \Theta^2/\mathrm{Re}$. In the geometry of cylindrical tubes, a similar problem was solved in [5]. The acceleration rate was from 2 to 4 times larger in that case depending on the Reynolds number.

Second step in Shelkin DDT is explosion triggering by an accelerating flame. Paper [6] developed an analytical theory of explosion triggering within the approximation of a 1D isentropic compression wave pushed

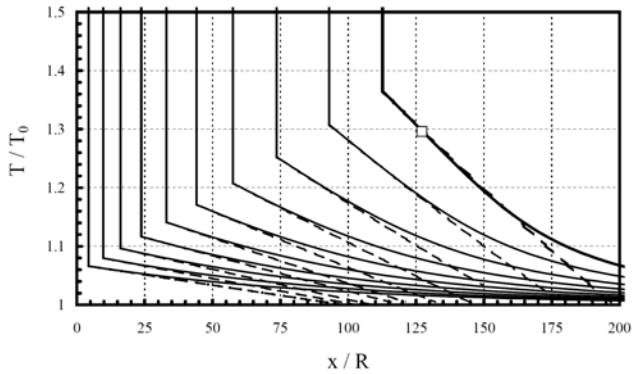

Fig. 2. Temperature profiles ahead of the flame front at $tU_f/R = 0.8-6.4$. Marker shows the gas element, which may explode ahead of the flame front (corresponding to $tU_f/R = 7.9$).

by the flame front. The condition of explosion in the gas mixture ahead of the flame front was derived; the instant of the explosion is determined provided that a mechanism of chemical kinetics for the low-temperature reactions is known. Paper [6] demonstrated how the problem is solved in the case of a single Arrhenius reaction controlling combustion both inside the flame and ahead of the flame. For example, Fig. 2 shows temperature profiles ahead of the flame front in a 2D channel of half-width $\mathrm{Re} = 50$ (other chemical parameters are as in [3]).

3 Flame acceleration at the early stages of burning in tubes

Another mechanism of flame acceleration was suggested and investigated experimentally in [7]. Here we present our recent theoretical and numerical results concerning the acceleration mechanism. The mechanism is related to the «tulip flame» phenomenon and does not require non-slip walls; it is illustrated in Fig. 3 (the simulations are performed for $\mathrm{Re} = 20$, $\Theta = 8$ in a cylindrical tube). Ignited at the tube axis at the closed end, flame expands first as a spherical front and generates an expanding «source»-flow (Fig. 3a, b). However, as the flame comes close to the walls, the flow in the radial direction is stopped, which makes the flow in the axial direction stronger and induces flame acceleration. Because of the acceleration a flame front acquires a «finger»-shape shown in Fig. 3c, d. The acceleration stops when the flame skirt touches the wall. Because of the strong slop of the flame front at that moment, the acceleration is followed by strong deceleration (Fig. 3 e,f) and by «tulip» flame (Fig. 3g), which also collapses (Fig. 3h). We have developed the theory of flame acceleration in this geometry (corresponding to Fig. 3 a-d) and validated it by direct numerical simulations. We have found positions of the flame skirt sweeping along the end wall and the flame tip moving along the axis as

$$r_f = \frac{\Theta R}{\alpha}\tanh\left(\alpha U_f t / R\right), \qquad z_f = \frac{\Theta R}{2\alpha}\sinh\left(2\alpha U_f t / R\right), \tag{3}$$

where $\alpha = \sqrt{\Theta(\Theta-1)}$, see [8] for calculation details. Acceleration starts at $t_{sph} \approx R/2\alpha U_f$, $r_f \approx 0.46\Theta R/\alpha$, when the flame front develops from the spherical shape to a «finger»-shape. Acceleration stops at

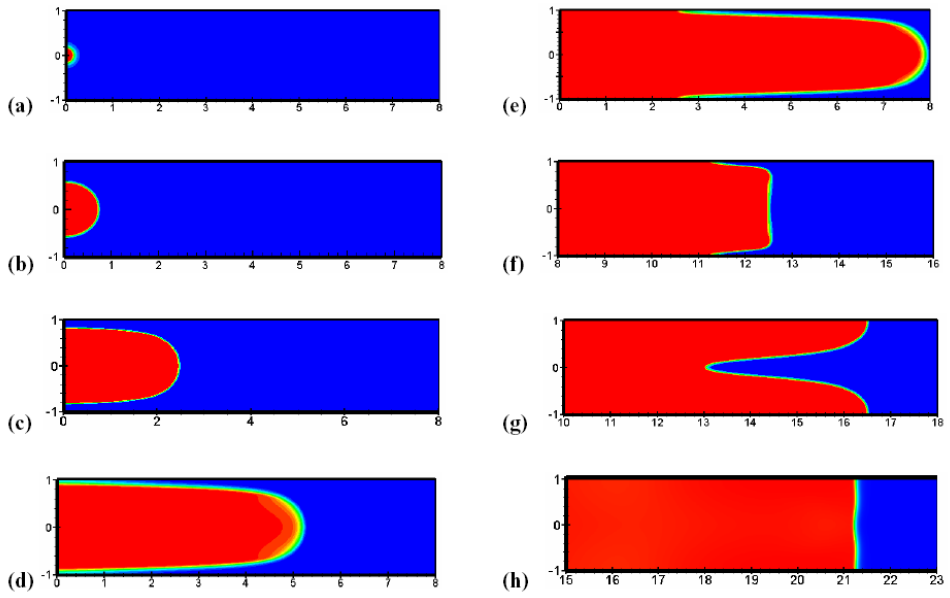

Fig. 3. Flame shape at the time instants $tU_f / R = 0; 0.12; 0.28; 0.32; 0.43; 0.64; 1.03$.

$$t_{wall} = \frac{R}{2\alpha U_f} \ln\left(\frac{\Theta+\alpha}{\Theta-\alpha}\right), \qquad (4)$$

when the flame skirt touches the wall $r_f = R$. During the interval $t_{sph} < t < t_{wall}$ (with $t_{sph} \approx 0.1R/U_f$ and $t_{wall} \approx 0.26R/U_f$ for flames with realistic expansion factors $\Theta = 6-8$) the flame tip accelerates in almost self-similar regime $z_{tip} \propto \exp(\sigma U_f t/R)$ with the acceleration rate $\sigma = 2\alpha = 2\sqrt{\Theta(\Theta-1)}$. At the end of acceleration, the flame tip is at $z_{tip}(t_{wall}) = \Theta$, and the total flame surface area (burning rate) increases as $S_w/\pi R^2 = 2\Theta^2/(\Theta+1)$, which implies a factor of 15 for flames with realistic expansion ratio. The theory is in a very good agreement with the experiments [7] and with our numerical simulations [8].

Finally, using the theory [6], we have checked if this mechanism of flame acceleration may trigger explosion in the fuel mixture. To be particular, we chose tube radius $R = 5\,cm$ typical in experiments, and the planar flame velocities $U_f = 40\,cm/s$ and $U_f = 10\,m/s$ corresponding to hydrocarbon-air flames and hydrogen-oxygen flames, respectively. Other flame parameters were chosen like in [3] including a single Arrhenius reaction with activation energy E both at high and low temperatures. We found that, in the case of hydrocarbon flames, explosion may be triggered only for $E/R_gT_0 < 15.5$, where R_g is the ideal gas constant and T_0 is initial temperature. Adopting $U_f = 10\,m/s$ like in hidrogen-oxygen mixtures, we obtained respectively $E/R_gT_0 < 30$. In both cases the scaled activation energies are not realistic; they become possible only for a noticeably preheated fuel mixture.

Thus, flame acceleration mechanism, considered in this section, is characterized by a rather high acceleration rate, and it acts during a short time. Burning rate increases by a factor of 15 because of the acceleration. Still, this increase is not sufficient to trigger explosion ahead of the flame front at normal conditions. As an option, the alternative acceleration mechanism may serve as a precursor to Shelkin acceleration in DDT.

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