Acceleration and Extinction of Flames In Channels With Cold Walls

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1 Introduction

Deflagration-to-detonation transition (DDT) is one of the most important and fascinating combustion phenomena with wide range of applications from pulse-detonation engines to safety issues such as the prevention of mining accidents [1-3]. The reason and the key element of DDT is spontaneous flame acceleration in tubes and channels from a low laminar flame speed to nearly sonic values, which implies ultra-sonic propagation in the reference frame of the tubes walls by the end of the process [4-6]. Two major mechanisms of flame acceleration in channels have been elucidated: the Shelkin mechanism in the case of smooth walls [7,8] and the mechanism of ultra-fast flame acceleration in channels with obstacles [9]; the present work focuses on a geometry with smooth walls.

The most typical geometry of DDT in experiments and energy-production devices corresponds to a relatively long channel, with the flame propagating from the closed channel end to the open one. According to the Shelkin mechanism, a flame front in channels with smooth walls accelerates because of the thermal expansion of the burning gas and the non-slip boundary conditions at the walls. Expansion of the burning gas produces a flow of the fuel mixture, which becomes non-uniform due to the non-slip boundary conditions. The non-uniform flow makes the flame front curved, which increases the burning rate and creates a positive feedback between the flame and the flow, hence leading to the flame acceleration. Although the qualitative idea of flame acceleration was suggested by Shelkin already in the 1940’s [7,8], the quantitative theory of the process has been developed and supported by extensive numerical simulations only recently, by Bychkov et al. [10]. Among other results, the theory [10] predicted powerful exponential flame acceleration in micro-channels (at least at the initial, almost isobaric stage of the process), and a decrease of the scaled acceleration rate with the channel width characterized by the Reynolds number $\mathrm{Re} \equiv S_L R / \nu$, where S_L is the laminar flame speed, R is the channel half-width (radius), and ν is the kinematic viscosity. The theoretical predictions [10] have been supported by later experiments on DDT in micro-channels with diameters about 1 mm and below [11,12]. At the same time, the experiments [11,12] have demonstrated some features of flame dynamics different from the theoretical predictions [10], such as a linear regime of flame acceleration instead of the exponential one. Reference [5] has explained the difference by the influence of gas compression effects ignored in [10], which moderate the acceleration process and make it linear for sufficiently large values of the flow Mach number, see also Ref. [13] for the theoretical explanation of this effect. By the end of the acceleration process, the flame propagation speed saturates to the Chapman-Jouguet deflagration speed [14-16], unless an explosion of the fuel mixture happens earlier.

Thermal losses to the walls, which are inevitably present in any experiment on DDT, is another effect expected to work against the flame acceleration mechanism. For example, in channels with isothermal cold walls, the thermal losses eventually cool the burnt gas down to the wall temperature, thus reducing effectively the effect of thermal expansion as the key element of the flame acceleration

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mechanism. In spite of the obvious importance of the thermal losses, quite surprisingly, not a single theoretical work on DDT has yet considered the influence of this effect on flame acceleration. At the same time, in the presence of strong thermal losses, one may question the very possibility of flame acceleration and DDT in channels with cold walls. Indeed, one should naturally expect a dominating role for thermal losses in sufficiently narrow channels, which may not only stop flame acceleration, but even lead to complete extinction of the burning process; the problem is of special importance for micro-combustion applications [17,18]. In wide channels the role of thermal losses decreases, but the flame acceleration mechanism becomes weaker too with the increase of the Reynolds number [10], and it remained unclear which of these two effects prevails.

2 Problem formulation

We consider a flame front propagating in a long 2D channel from the closed end to the open. The problem formulation is quite similar to that of Ref. [10], with one important difference that here we study flame dynamics in channels with cold isothermal walls instead of the adiabatic ones investigated in Ref. [10], thus focusing on the influence of thermal losses to the walls on flame acceleration. The case of adiabatic walls will be also considered for the sake of comparison. We study the flame dynamics by using numerical simulations of the Navier-Stokes combustion equations. We consider a flame propagating in a two-dimensional tube of half-width R with non-slip boundary conditions at the walls. Both isothermal ($T = T_f$) and adiabatic walls are considered and compared. We take the initial pressure and temperature of the fuel mixture $P_f = 10^5\,\mathrm{Pa}$ and $T_f = 300\,\mathrm{K}$, respectively. The thermal and chemical parameters of the fuel mixture were chosen to reproduce the most important properties of methane and propane laboratory flames. We use the dynamic viscosity $\zeta = 1.7\times10^{-5}\,\mathrm{N\,s/m^2}$ and the Prandtl number $\mathrm{Pr} = 1$. To avoid the thermal-diffusion instability we take unit Lewis number $\mathrm{Le} \equiv \mathrm{Pr}/\mathrm{Sc} = 1$. The activation energy was $E_a = 32 R_p T_f$. We take the planar laminar flame speed $S_L = 34.7\,\mathrm{cm/s}$ corresponding to the initial Mach number 10^{-3}. The flame thickness in our calculations is defined conventionally as $L_f \equiv \nu / \mathrm{Pr}\, S_L$, then the Reynolds number associated with the flame speed $\mathrm{Re} \equiv S_L R/\nu$ indicates the channel half-width scaled by the flame thickness $\mathrm{Re} = R/\mathrm{Pr}\, L_f$. Thermal expansion in the burning process is determined by the energy release in the reaction and characterizes the density ratio of the fuel mixture to the burnt gas $\Theta \equiv \rho_f / \rho_b$; we took $\Theta = 8$, typical for methane and propane burning.

We use a two-dimensional Eulerian code. The numerical scheme of the code and the computational methods were described in details in our previous papers, see, *e.g.*, [5,6,9,10]. In the present simulations, we considered different channel half-widths $5L_f < R < 25L_f$, and took the tube length much bigger than the tube width, $\sim(100-1000)R$, dynamically changing as the flame propagates.

3 Simulation results

For the fixed density ratio $\Theta = 8$ used in the present work, the main simulation parameter is the Reynolds number Re, which indicates the scaled half-width of the channel. Depending on the Reynolds number, we obtain qualitatively different flame behavior: extinction for narrow channels or acceleration for sufficiently wide channels. For too narrow channels the flame is not ignited and the initially heated region by the tube end gets eventually cooled down by the walls. This result agrees well with the commonly accepted knowledge that a propagating flame stands away from a cold wall with the quenching region about six times the laminar flame thickness [19]. Taking a wider tube $R = 10L_f$ with $\mathrm{Re} = 10$, we manage in igniting a self-sustained flame, which starts propagating for a

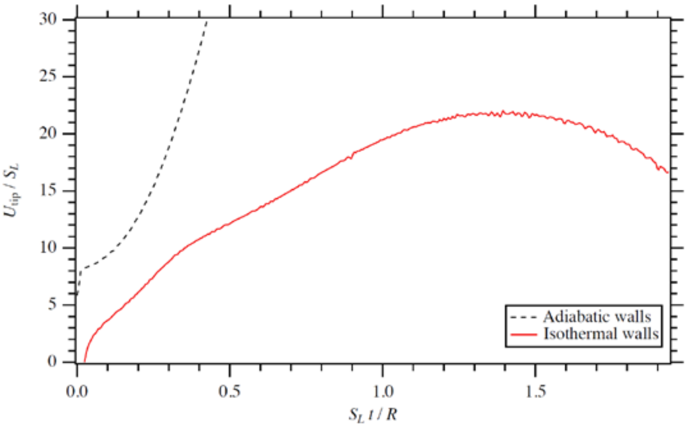

Figure 1. Propagation speed of the flame tip versus the scaled time $S_L t / R$ for $\mathrm{Re} = 10$ for isothermal and adiabatic walls.

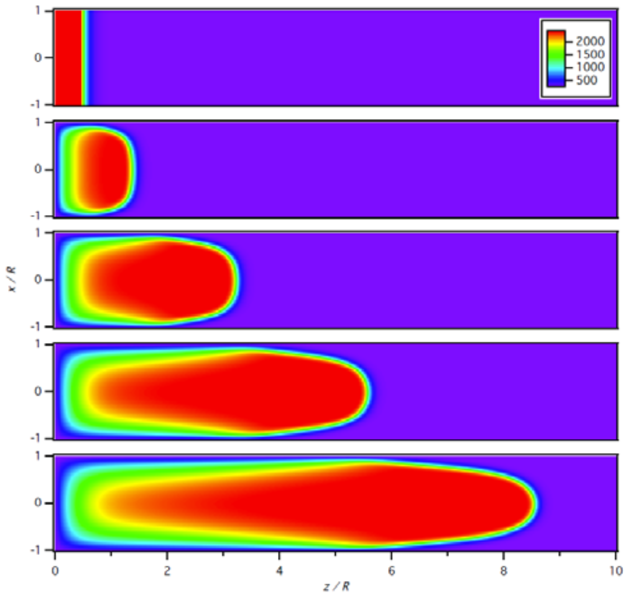

Figure 2. Temperature distribution (in K) for the flame acceleration in the channel with isothermal walls for $\mathrm{Re} = 15$ at the time instants $S_L t / R = 0;0.2;0.4;0.6;0.8$.

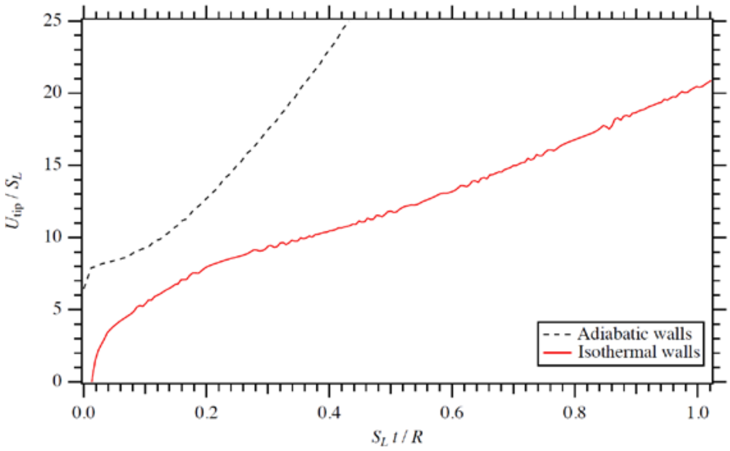

Figure 3. Propagation speed of the flame tip versus the scaled time $S_L t / R$ for $\mathrm{Re} = 15$ for isothermal and adiabatic walls.

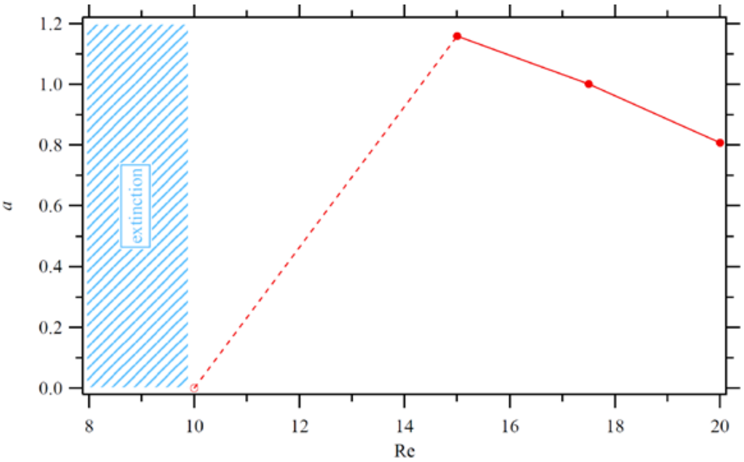

Figure 4. Scaled flame acceleration versus the Reynolds number for channels with isothermal walls.

while. Still, in contrast to the adiabatic case we observe relaxation of the burnt gas temperature down to the wall temperature because of the heat losses. The relaxation process is especially strong by the tube end, although we observe similar effects by the side walls too with the quenching distance between flame "skirt" and the walls about $\sim 4L_f$, in reasonable agreement with [19]. In the case of $\mathrm{Re} = 10$, the losses to the cold walls eventually prevail over the flame propagation and, after an initial short acceleration, we find a slowing down of the flame front, as shown in Fig. 1, with subsequent flame quenching. For comparison, Figure 1 presents also the propagation speed of the flame tip for the case of adiabatic walls with the same Reynolds number, $\mathrm{Re} = 10$, which exhibits powerful acceleration in agreement with the previous works [5,10].

By increasing the tube width further, with $\mathrm{Re} > 10$, we finally obtain flame acceleration in channels with cold isothermal walls too; the snapshots of the characteristic temperature patterns are presented in Fig. 2 for $\mathrm{Re} = 15$ at the time instants $S_L t / R = 0;0.2;0.4;0.6;0.8$. In Fig. 2 we also observe temperature relaxation by the tube end and the side walls; however this time the heat loss is not strong enough to stop the self-sustained flame acceleration - the curved flame front produces more gas volume per unit time than the losses can "remove" by relaxation of the burnt gas temperature. The propagation speed of the flame tip for $\mathrm{Re} = 15$ and isothermal channel walls is shown in Fig. 3 versus the scaled time $S_L t / R$; the associated adiabatic case is also presented on the figure for comparison. According to Fig. 3, after some initial transitional time, the flame front accelerates in approximately linear regime in the channel with isothermal walls, which may be described roughly as

$$U_{tip} / S_L = a(S_L t / R) + const \,, \qquad (1)$$

where a is the scaled flame acceleration. This linear acceleration regime differs considerably from the powerful exponential acceleration $U_{tip} / S_L \propto \exp(\sigma S_L t / R)$ predicted theoretically and validated numerically in Ref. [5] for channels with adiabatic walls. At the same time, we point out that the experiments on flame acceleration in ethylene-oxygen fuel mixtures in micro-channels have reported a linear acceleration law rather than the exponential one [11,12]. Although efficiency of heat losses to the walls has not been directly investigated in the experiments [11,12], still, in the realistic combustion process in channels some losses are inevitable. It would be natural to assume that the experimental situation of Ref. [11,12] corresponds to something intermediate in-between the asymptotic cases of isothermal cold walls and adiabatic ones. The linear regime has been also observed at the developed stages of flame acceleration in adiabatic channels when the gas compressibility effects become important and the Mach number of the flow approaches unity [5]. Besides, linear flame acceleration has been encountered in numerical modelling even at the initial stages of DDT in adiabatic channels provided for a sufficiently small density ratio or sufficiently large Reynolds number [20]. By comparing all these cases, one can presumably discuss a common tendency of the linear flame acceleration regime replacing the adiabatic one as soon as the acceleration mechanism gets moderated and weakens by some reason. One is also tempted to treat the linear regime of flame acceleration, Eq. (1), as the first term in the Taylor expansion for the weak exponential acceleration $U_{tip} / S_L \propto \exp(\sigma S_L t / R) \approx 1 + \sigma S_L t / R$ with a small acceleration rate $\sigma << 1$. One has to be cautious as the linear acceleration regime has been observed up to the instants with noticeable increase of the flame propagation speed, when the term $\sigma S_L t / R$ is not small any more.

By investigating the flame acceleration process in channels of different width, we have obtained that acceleration goes slower for wider tubes. The scaled acceleration a extracted from the velocity plots according to Eq. (1) is presented in Fig. 4 versus the Reynolds number; the decrease of the scaled flame acceleration with Re may be observed for $\mathrm{Re} \geq 15$ (filled markers). This tendency agrees qualitatively with the results obtained for the channels with adiabatic walls [10]; we remind that the theory of Ref. [10] predicted asymptotic decrease of the acceleration rate σ with the Reynolds number as $\sigma = \Theta^2 / \mathrm{Re}$ in wide tubes with $\mathrm{Re} >> 4\Theta$. The scaled flame acceleration at the developed stages of the process decreases with the Reynolds number too, as found in Ref. [5]. Thus, all these cases demonstrate the same qualitative tendency of the flame acceleration mechanism becoming weaker for wider tubes with smooth walls.

The domain of narrow tubes $\mathrm{Re} < 10$ in Fig. 4 corresponds to flame quenching and extinction. The border case of $\mathrm{Re} = 10$ is indicated by the empty marker with some minor acceleration extracted for the initial stage of the flame propagation. So, unlike the adiabatic case, the flame acceleration in channels with cold isothermal walls depends on the Reynolds number in some non-monotonic way with the maximal acceleration attained for $10 < \mathrm{Re} < 15$.

4 Summary

In the present work we have investigated the problem of flame dynamics – extinction versus acceleration – in narrow long channels with cold isothermal walls with flame propagating from the closed channel end to the open one. The problem is very important in the context of the DDT studies; in particular, it is needed to reduce the gaps between the theoretical models and simulations for the flame acceleration in channels with adiabatic walls presented so far [5,10] and the experimental results on DDT in micro-channels [11,12]. The problem is solved by means of numerical simulations of the complete set of hydrodynamic equations including transport properties and Arrhenius chemical kinetics. We have obtained qualitatively different flame behavior in sufficiently narrow and wide channels. For the channel half-width smaller than about ten flame thicknesses heat losses to the cold walls prevail and burning is eventually quenched. In wider channels flame acceleration is found even for the conditions of cold walls in spite of the heat loss. In that case flame accelerates in the linear regime, which differs considerably from the powerful exponential acceleration predicted theoretically and obtained computationally for the adiabatic channels in Ref. [10]. At the same time the linear regime is consistent with the previous experimental observations [11,12], which inevitably involve thermal losses to the walls. We also find that the scaled flame acceleration decreases with the Reynolds number of the flow for channels with cold isothermal walls; this tendency is qualitatively similar to the case of adiabatic channel walls studied previously.

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