Preheating within the flame fold and hydraulic resistance as mechanisms of Deflagration-to-Detonation Transition

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1 Introduction

Although significant insights have been obtained through many experimental as well as theoretical and numerical studies, a comprehensive first-principle understanding of the phenomenon is still far from complete. As has recently been realized [1], the hydraulic resistance alone is capable of triggering the transition even if the multi-dimensional effects, such as the flame acceleration due to folding, are completely suppressed and the system is regarded as effectively one-dimensional with the confinement being accounted for through the velocity-dependent drag-force term added to the momentum equation. The basic predictions of the one-dimensional model were recently corroborated in direct numerical simulations of premixed gas combustion in thin channels, where the hydraulic resistance is incorporated through the no-slip boundary condition [2,3]. Deflagration-to-detonation transition in unconfined systems is more problematic. In this case the transition is commonly attributed to the flame acceleration induced by spontaneous flame wrinkling due to the Darrieus-Landau (DL) instability. Yet, the acceleration resulting from the wrinkling seems to be rather a weak effect, whose ability to cause the transition is not at all obvious.

One of the purposes of the present work is to gain a better insight into this question. As is well known, in wide channels the DL instability results in the formation of wrinkled flames and the flame speed enhancement due to the increase of the flame area. The wrinkled flame generates a shock with a Mach number of about 1.2 – 1.5, which is too low to trigger detonation. Yet, as shown below, there is another previously overlooked aspect of the DL instability. The folded reaction zone creates a preheating of the fresh mixture trapped within the fold interior. This, under favorable conditions, may invoke autoignition triggering the transition. The formation of a suitable for DDT fold in the flame brush would require high compressibility and accordingly high speed of a laminar flame. The effect is found to be sensitive to the flame's normal speed and the reaction rate pressure-dependency, favoring fast flames and high-order reactions. Apart from discussing the impact of the DL instability on the transition, the present paper reports new results on the influence of adhesive and rough walls.

2 Flame folding and DDT due to the Darrieus-Landau instability

To visualize the spatial picture of the transition, a wave of premixed gas combustion spreading from the closed to the open end of a rectangular channel is studied by direct numerical simulation of the two-dimensional Navier-Stokes equations for a compressible reactive flow. The energy release rate for is modeled by a one-step Arrhenius kinetics, which is assumed to be of the first order with respect to the deficient reactant and of the 2nd order with respect to the density. The adopted parameters approximately correspond to the stoichiometric acetylene-oxygen mixture at $P_u = 1\,\mathrm{atm}$ and $T_u = 393\,\mathrm{K}$ with laminar flame speed about (12-15) m/sec. Other

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parameters are specified as, $C_p = 10^3 m^2/s^2/K$, $\rho_u = 1.16 kg/m^3$, $\mu_u = 1.7 \times 10^{-5} kg/s/m$, $Le = 1$, $Pr = 0.75$, $\gamma = 1.4$, $\Theta = T_b/T_u = 8 \div 10$. The incipient velocity of the initially planar flame is specified by the Mach number, $M_{f0} = U_f/a_u$, where $a_s = 346 m/s$ is the sound speed. The computations were made for the widths of the rectangular channel, $D = (70-200)L_f$, where $L_f = \mu_u/Pr\rho_u U_f$ is the characteristic flame width. An adaptive numerical code is employed to ensure high resolution of the flame front, pressure waves and shocks; its validation is described in [4,5].

To single out the impact of the DL instability, the gas flow is subjected to the free-slip and adiabatic boundary conditions, thereby eliminating possible influence of the momentum and heat losses. The effect is found to be sensitive to the flame's normal speed, the reaction rate temperature and pressure-dependences, favoring fast flames, and high order reactions. One of the typical scenario of the transition is shown in Figures 1-4: evolution of the flame front; the flame and the advancing shock velocities; evolution of the fold near the transition point; and the temperature, pressure and velocity profiles along the fold axis, where detonation first develops, and thereupon spreads over the channel's interior. Here one readily observes formation of the large-scale preheat zone in the unburned mixture trapped within the fold interior, very fast acceleration of the fold-tip reaction zone, and formation of the high-pressure peaks. The transition occurs when the pressure peak becomes high enough to produce shock wave capable of supporting detonation.

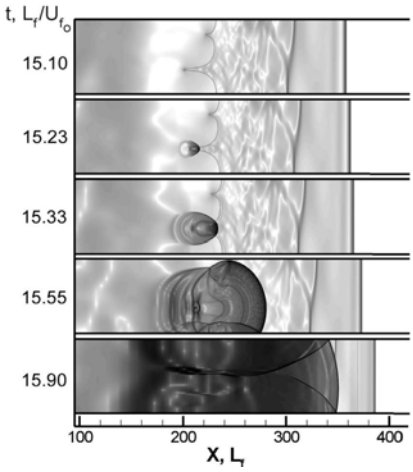


Fig.1

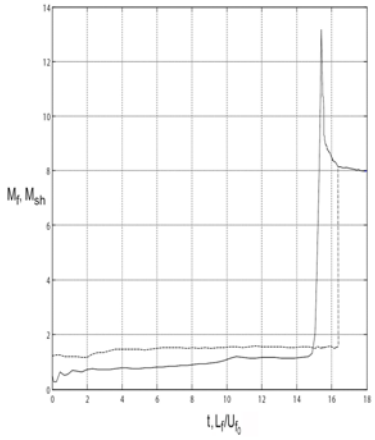
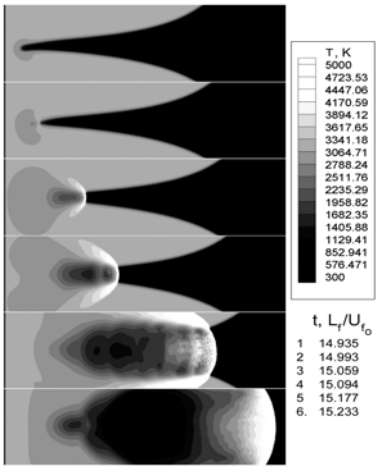


Fig.2

Fig. 1: Time sequence of images for the flame/shock dynamics near the transition point for $D=70L_f$, $M_{f0}=0.05$, $\varepsilon=8$, $\Theta=10$. Stronger shading corresponds to higher-pressure gradient.

Fig. 2: Temporal evolution of the reaction wave (solid line) and shock (dashed line) velocities for Fig. 1.



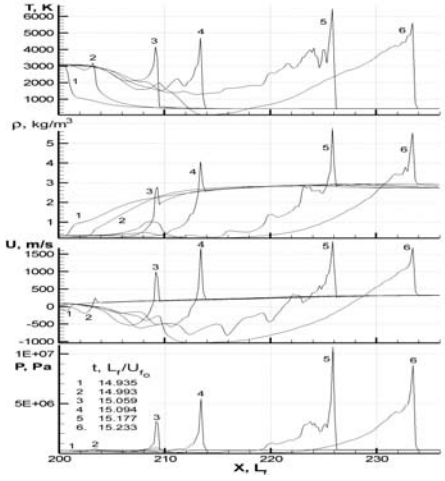
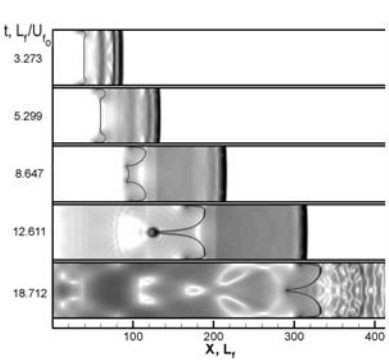


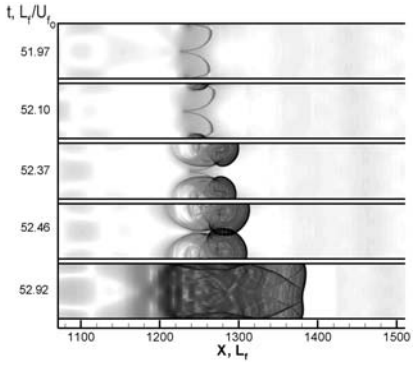
Fig.3 Fig.4

Fig. 3: Time sequence of zoomed images of the flame fold evolution near the transition point, where DDT starts, corresponding to conditions of Fig. 1.
Fig. 4: Temporal evolution of the temperature, density, velocity and pressure profiles along the fold axis in Fig.3.

3 Transition to detonation in a channel with adhesive and rough walls

It was recently shown that the hydraulic resistance alone, incorporated through the no-slip boundary condition, is capable of triggering the transition even if the multi-dimensional effects, such as the flame acceleration due to folding, are completely suppressed and the system is regarded as effectively one-dimensional [1,2]. A similar effect was observed in wide channels and is even more pronounced in the case of rough walls [5]. In the case of the no-slip or rough walls the transition is triggered predominantly by hydraulic resistance inducing formation of an extended preheat zone at the boundary layer near the wall, ahead of the advancing flame, and thereby creating conditions pertinent to the flame acceleration. Typical flame dynamics is shown in figures 5,6. Here, soon after the ignition the flame front develops bulges near the channel's walls (Fig. 5), which grow and merge forming the tulip shaped flame. The transition occurs as soon as the fresh near-wall mixture adjacent to the flame becomes appropriately preconditioned. The temporal evolution of the flame and shock velocities is similar to that of Fig.2 and is quite typical for DDT. The calculated profiles of the temperature along the channel wall and the axis are plotted on Fig.7, showing clearly the formation of an extended preheat zone at the wall, prior to the transition.





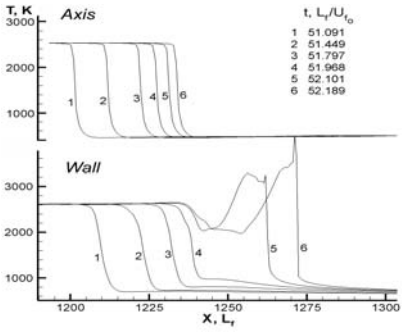


Fig.5 Fig.6 Fig.7

Fig. 5: The incipient flame dynamics: formation of the flame bulges and emergence of the tulip flame.
Fig. 6: Temporal evolution of the flame and transition to detonation for no-slip boundary conditions; $D=70L_f$, $M_{f0}=0.05$, $\varepsilon=4$, $\Theta=8$.
Fig. 7: Temperature profiles along the wall and axis at several consecutive instants of time for conditions of Fig. 6.

Since the classical experiments of Schelkin and co-workers [6], it is known that the wall roughness may significantly facilitate the transition to detonation. The dynamical picture of the transition in the channels with rough walls shown in Fig.8 is basically similar to that of smooth channels with adhesive walls: the transition is conceived near the wall where the hydraulic resistance leads to the precompression and preheating ahead of the advancing flame. In the case of a rough wall, the wakes of the pressure waves-flow interaction is responsible for formation of a preheat zone in the unburned gas. The transition to detonation occurs in the near-wall mixture adjacent to the edge of the tulip's petals where the fresh mixture develops an appropriately extended preheat zone shown in Fig. 9.

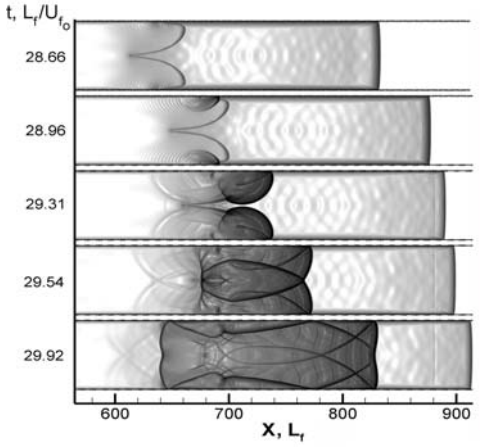


Fig.8

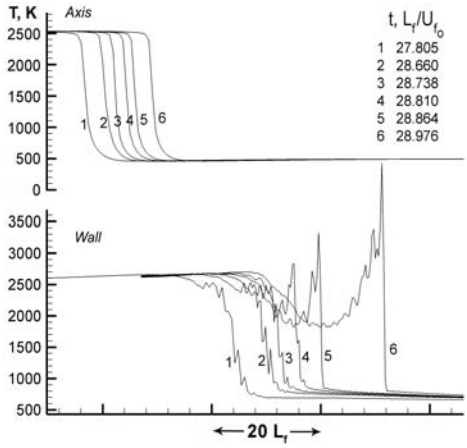


Fig.9

Fig. 8: Sequence of images for the flame-flow evolution and transition to detonation for the rough wall boundary conditions; $D=70L_f$, $M_{f0}=0.05$, $\varepsilon=4$, $\Theta=8$, wall roughness $\Delta= L_f$.
Fig.9: Evolution of temperature profiles along the channel wall and axis at several consecutive instants for Fig. 8

4 Concluding remarks

The numerical simulations described in Sec. 3 were conducted under the condition of thermally isulated walls, so that the detonation first develops in the boundary layer, where the impact of hydraulic resistance is stronger. The subsequent study of the impact of heat losses to the walls [7] and its extension for wider channels [8], have shown that the transition does not occur if the reaction kinetics is assumed monomolecular. However, for the bimolecular kinetics (other conditions being the same) the transition is feasible. For the isothermal instead of adiabatic walls, the flame accelerates less then it does in case of adiabatic wall, or even it may decelerate. Higher molecularity implies a higher sensitivity of the explosive mixture to the pressure change, which in these problems is quite substantial.

A more tractable one-dimensional model was explored for better insight into the transition and flame acceleration depending on the shape and extension of a preheat zone [5]. Due to the preheat zone the incipient flame speed markedly exceeds the normal flame speed associated with the uniform initial state and in the course of the subsequent evolution the process settles either into the deflagrative or detonative combustion, depending on details of the initial data – maximum temperature and extension of the preheated mixture. It was found that the critical length of the preheat zone is sensitive to the reaction order and the incipient flame speed. It becomes unrealistically large for the monomolecular kinetics, and it drastically decreases for flames with bimolecular or higher order kinetics. The critical length of the preheat zone required for transition to detonation considerably decreases with the increase of the normal flame speed.

Under normal conditions the incipient laminar flame speed used in the present simulations are of the order of 10-15 m/sec. Yet, in the case of the 3D problem one can expect that transition can be feasible for slower flames due to higher rate of the DL instability. While the laminar flame speed in hydrogen/oxygen or ethylene/oxygen mixtures are of the order of 10-14 m/sec, the turbulent flame speed in these mixtures can be as high as 20-40 m/sec. These speeds are fast enough to build up preheat and pre-compression in the unburned gas. An analogous effect of the formation of an extended preheat zone in the folding flame may apparently be induced also by the flow turbulence developing in wide channels, or by the wake behind the flow produced by obstacles. Apart from deepening the folds/tulips brought on by the DL instability and the flame-boundary layer interaction, the turbulence will result in an additional flame convolution and hence acceleration and effectively higher compressibility favoring the transition. Thus, for both the DL fold formed in the flame brush or in case of no-slip or rough walls, the transition to detonation is associated with the formation of a preheat zone ahead of the advancing flame. It should be noticed that the necessary geometry of the narrow fold providing preheat and

acceleration of the reaction zone required for DDT may be achieved by other means, for example, by initiating a flame by the hot wall in the form of a funnel with a small enough tip angle [9].

Acknowledgments

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