

# Investigation on effect of flame instability on flame acceleration mechanism

Wang Cheng, Wenhui Han, Jianguo Ning

State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology  
Beijing, China, 100081

## 1 Introduction

The mechanism of flame acceleration and deflagration to detonation transition (DDT) remains one of the most interesting unsolved problems of combustion theory. Flame acceleration in channels has been attributed qualitatively by Shelkin to wall friction [1]. It was Shelkin who explained the flame acceleration by flame instability caused by flow interaction with the nonslip tube walls. Due to the thermal expansion of the burning material a flame front pushes a flow of the fuel mixture, which becomes non-uniform because of friction at the walls. The nonuniform flow makes the flame shape curved, which leads to the flame instability and acceleration. According to Shelkin's idea, flame with realistic thermal expansion has to accelerate in a tube with one end closed and with nonslip at the walls. The numerical simulations [2] demonstrated the possibility of laminar flame acceleration and the DDT in channels with adiabatic walls. The process from acceleration of laminar flame to DDT is also observed in the experiments for flames in tubes. It contains the different stages of the evolution of a chemically reactive flow: ignition by a small spark, rapid flame acceleration, development of shocks, shock-flame interactions, and detonation. This requires final model having the ability to simulate these stages. Kessler and Oran et al. [3] built a composite model and used the model to simulate the different stages of DDT well. Furthermore, the interaction of leading shock waves with the flame fronts results in distortion of the flame, the increase in the energy release rate, and further can lead to considerable flame acceleration [4]. However, the detailed mechanism of flame acceleration and DDT, which results from the flame instability and interaction of the boundary layer with shock wave, and the effect of duct width on flame acceleration remain unclear. In this paper, we study flame acceleration in different width channels (channel width is the order of the flame thickness) with adiabatic walls by using Oran's reaction model [3] to describe the chemical-energy release. And we present the results of numerical simulations of flame acceleration in tubes of different width and show how an accelerating flame can lead to a detonation. We also investigate the effect of obstacles on flame acceleration and reveal the mechanism of flame acceleration in order to display effect of obstacles on flame instability and the interaction between reflection wave and flame front.

## 2 Governing equation and numerical methods

The reactants are assumed to be fully premixed and behave as an ideal gas, so that the flow is governed by the compressible reactive Navier-Stokes equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0 \quad (1)$$

$$\begin{aligned} \frac{\partial \rho u}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} + \frac{\partial \rho uv}{\partial y} = \frac{\partial}{\partial x} \left[ \rho \mu \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \right] \\ + \frac{\partial}{\partial y} \left[ \rho \mu \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \right] \end{aligned} \quad (2)$$

$$\begin{aligned} \frac{\partial \rho v}{\partial t} + \frac{\partial(\rho vu)}{\partial x} + \frac{\partial(\rho v^2 + p)}{\partial y} = \frac{\partial}{\partial x} \left[ \rho \mu \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \right] \\ + \frac{\partial}{\partial y} \left[ \rho \mu \left( \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right) \right] \end{aligned} \quad (3)$$

$$\begin{aligned} \frac{\partial \rho e}{\partial t} + \frac{\partial(\rho e + p)u}{\partial x} + \frac{\partial(\rho e + p)v}{\partial y} = \frac{\partial}{\partial x} \left[ K \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[ K \frac{\partial T}{\partial y} \right] \\ + \frac{\partial}{\partial x} \left[ u \rho \mu \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) + v \rho \mu \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \right] \\ + \frac{\partial}{\partial x} \left[ u \rho \mu \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) + v \rho \mu \left( \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right) \right] \end{aligned} \quad (4)$$

$$\frac{\partial \rho Y}{\partial t} + \frac{\partial \rho Yu}{\partial x} + \frac{\partial \rho Yv}{\partial y} = \frac{\partial}{\partial y} \left[ \rho D \frac{\partial Y}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \rho D \frac{\partial Y}{\partial y} \right] - \Omega \quad (5)$$

$$\rho e = \frac{p}{\gamma - 1} + \frac{1}{2} \rho (u^2 + v^2) + q \Omega \quad (6)$$

$$\Omega = A \rho Y \exp(-E_a / RT) \quad (7)$$

where  $\rho$ ,  $T$ ,  $u$ ,  $v$ ,  $p$ ,  $e$ ,  $q$ , and  $Y$  are the density, temperature, streamwise velocity, transverse velocity, pressure, specific energy, heat release, and fuel mass fraction of the gas mixture, respectively. The viscosity coefficients  $\mu$ , mass diffusivity  $D$ , and thermal diffusivity  $k = K/qc_p$ , where  $K$  is the thermal conductivity, can be obtained according to

$$\mu = \mu_0 T^{0.7} / \rho, D = D_0 T^{0.7} / \rho, k = k_0 T^{0.7} / \rho$$

The parameters  $\mu_0$ ,  $D_0$ , and  $k_0$  are assumed to be constant.

In this paper, the composite model [3] is employed to describe the chemical-energy release. We use 9th order WENO scheme to discrete convection term, 10th order central difference scheme to discrete diffusion term, and the third-order TVD Runge-Kutta scheme for temporal discretization. Based on this, a parallel code is developed to simulate effect of the flame instability caused by boundary layer on flame acceleration in the ducts of different width and with obstacles.

### 3 Effect of flame instability on flame acceleration at different duct width

The flame front is driven by thermal expansion of the combustion products and its velocity increases with the amount of heat released by the flame front, which is related to the surface area of the flame. And flame instability has influence on the area of flame front. Therefore, we simulate modeling a flame ignited at the left and then propagating to the right of the two-dimensional rectangular channel with no-slip walls and investigate the effect of the flame instability on flame acceleration at different duct width. The width  $D$  of duct is 1.0cm, 2.0cm and 4.0cm, respectively. The viscosity, thermal diffusivity coefficients and other parameters of methane-air mixture can be seen in [3]. An initially planar flame is set at the left of the tube and propagates from the closed end of tube. We give 50 points per flame length to divide the computational domain. By mesh resolution verification, 50 points per flame length can resolve flow structure of turbulent boundary layers.

Fig. 1 presents temporal evolution of pressure contours under the duct width of  $D=1.0$ cm. At  $t=6.86$ ms, pressure is low and leading compression wave is weak. With the flame constantly accelerating, leading

compression wave in the front of flame becomes strong and superimposes into shock wave. At  $t=29.12\text{ms}$ , the flame front catches up with the leading shock wave, and couples with the shock wave. Thus DDT occurs at position of  $x=147.5\text{cm}$  ( $x$  is the position of flame propagation direction) and detonation is formed. Triple points appear at detonation front.

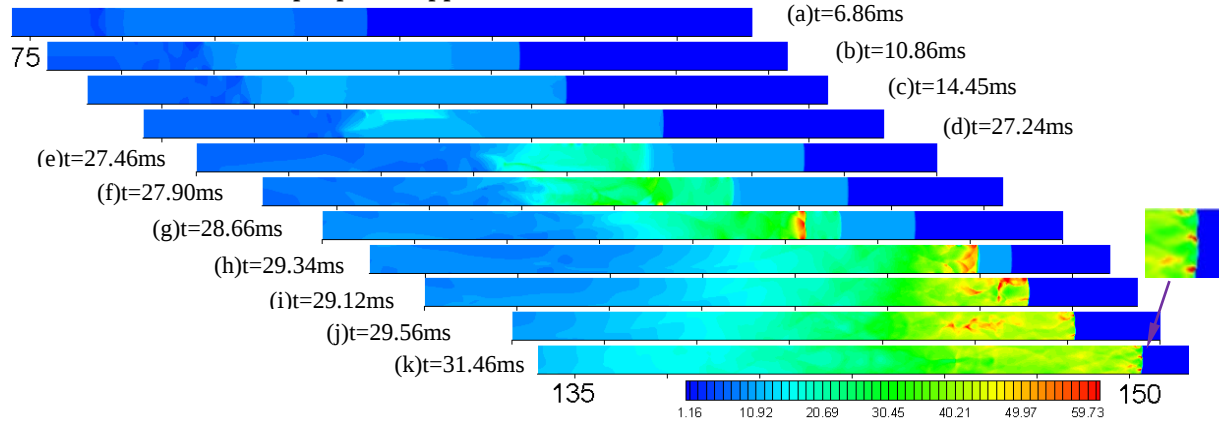


Fig.1 Temporal evolution of pressure contours under the duct width of  $D=1.0\text{cm}$

Fig. 2 presents the typical evolution of flame front propagating. The velocity of the flame near boundary layer is low, but one in the middle of channel is high. So the flame front is curved and takes on lordosis at  $t=8.573\text{ms}$ . The boundary layer is formed between the leading shocks and the flame front. At  $t=27.06\text{ms}$ , the flame near the top wall propagates forward quickly along the top boundary layer, and a narrow band of flame is formed nearby the top wall, which result in the flame stretch and increase of flame front area. At  $t=27.46\text{ms}$ , the flame band near top wall spreads forward, simultaneously extends toward the bottom wall. This makes the area of flame front increase and leads to increasing of flame velocity. At  $t=27.68\text{ms}$ , the flame propagates quickly along lower wall, and long and narrow flame band is formed in the lower boundary layer. The flame front contains a narrow band of un-reacted gas, and the stronger compression wave appears in front of flame. When the upper flame and lower flame collide, un-reacted gas in the band is ignited and lots of energy released pushes the local flame to catch up with the head flame, as shown in Fig. 2(e). As the flame accelerates constantly, a strong shock wave formed by superposition of compression wave ignites gas in the boundary layer and the flame propagates along the top and bottom wall. At  $t=29.78\text{ms}$ , the flame in boundary layer couples with leading shock wave and DDT appears and an un-reacted gas pocket appears behind the detonation front, as shown in Fig. 2(g, h). Hence, for the duct width of  $D=1.0\text{cm}$ , the interaction of compression waves with the lead part of the flame near the boundary layer is responsible for the final triggering of the onset of detonation [5].

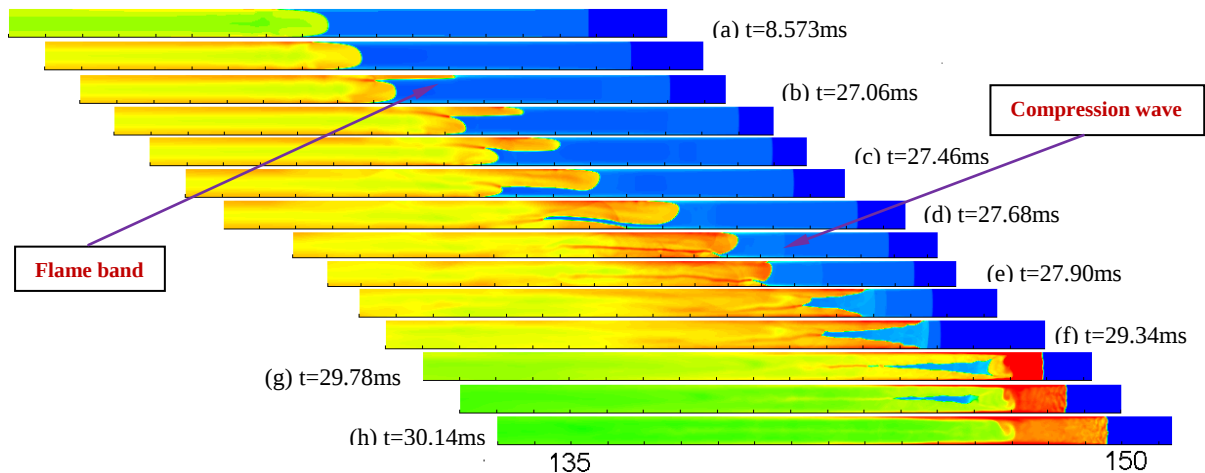


Fig. 2 Temporal evolution of flame front under the duct width of  $D=1.0\text{cm}$ 

Fig. 3 shows the typical evolution of flame front propagating when duct width is  $2.0\text{cm}$ . The results of Fig. 3(a) resemble the analytical curves in [5] except for the cusp at the axis. Similar cusps were also observed in the previous numerical studies of the flame acceleration [2]. The cusps are related to the intrinsic instability of the flame front: the Darrieus–Landau and the Rayleigh–Taylor instabilities[6, 7]. At the position of the cusps, thermal diffusion dominates relative to material diffusion, and the cusps moves constantly at the top wall. The cusp disappears eventually and flame front becomes smooth. The area of flame front increases and then the flame is further accelerated.

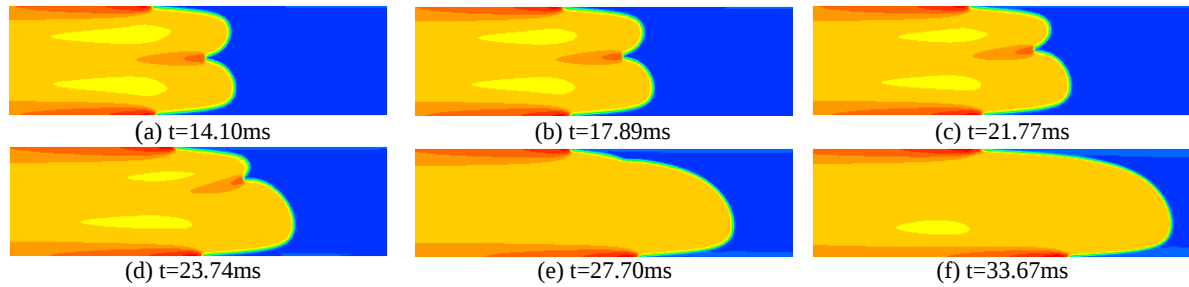
Fig. 3 Temporal evolution of flame front under the duct width of  $D=2.0\text{cm}$ 

Fig. 4 presents temporal evolution of the flame front in ducts of different width. It can be seen that when duct width is  $1.0\text{cm}$ , flame front is stretched and becomes curved due to flame instability. Eventually, DDT occurs at site of  $x=147.5\text{cm}$ . For the duct width of  $D=2.0\text{cm}$  and  $4.0\text{cm}$ , the cusp moving toward the top wall leads to the difference in velocity of flame near the top and the bottom wall, which makes the flame front extruded and long. The influence of energy released by boundary layer on flame acceleration is small. This results in slow flame acceleration. Therefore, DDT still do not occur when the flame spreads to the position of  $x=160.0\text{cm}$ . Compared Fig. 4(b, c), it can be observed that the larger the duct width is, the longer the time from the flame instability to flame stretching.

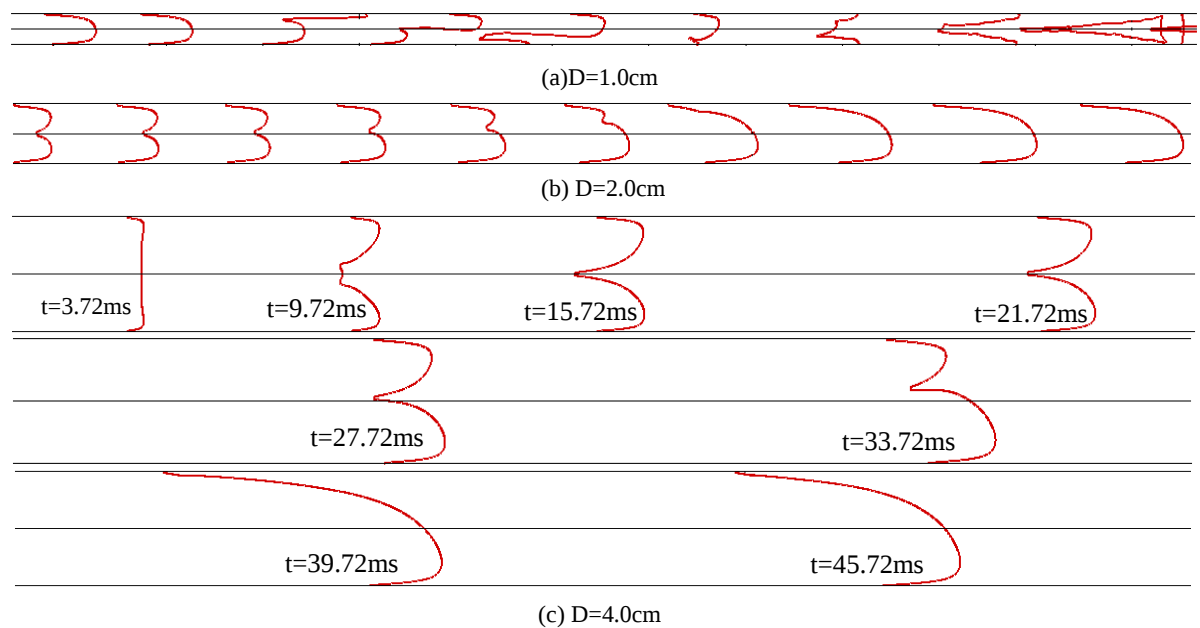


Fig. 4 Temporal evolution of the flame front under different duct width

Fig. 5 shows that position of the flame tip versus time in ducts of different width. It can be seen that for the duct width of  $D=0.5\text{cm}$  the flame is accelerated quickly, and soon its velocity reaches to deflagration velocity. Then DDT comes into being. For the duct width of  $D=1.0\text{cm}$ , flame acceleration begins until the flame propagates to the location of  $x=80\text{cm}$ . When duct width is  $4.0\text{cm}$ , the flame acceleration don't begin at the location of  $x=100.0\text{cm}$ . So, we can know that the larger the duct width is, the slower the flame acceleration is.

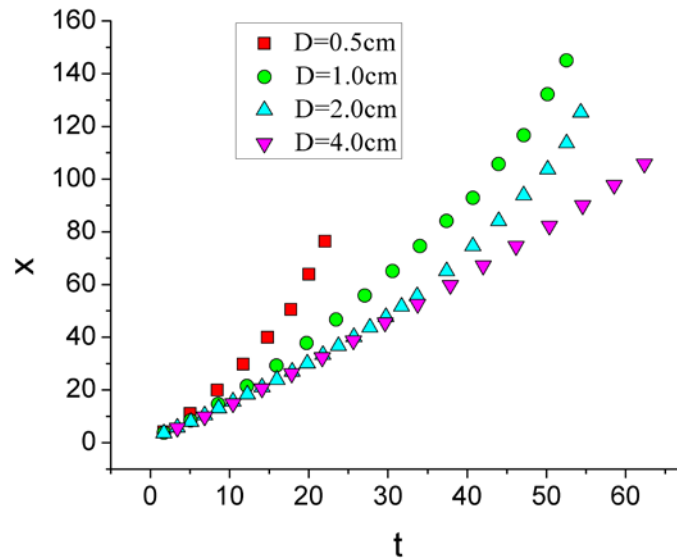


Fig. 5 Position of the flame tip versus time under different duct width

#### 4 Effect of obstacles on flame front instability

It is simulated that a flame propagates in two-dimensional rectangular channel with obstacles. The width of the channel is  $18.0\text{cm}$ , and height and width of obstacles is  $6.0\text{cm}$  and  $2.0\text{cm}$ , respectively. The space between obstacles is  $18.0\text{cm}$ . An ignition zone is set at the left and upper corner, and its energy is less than detonated energy.

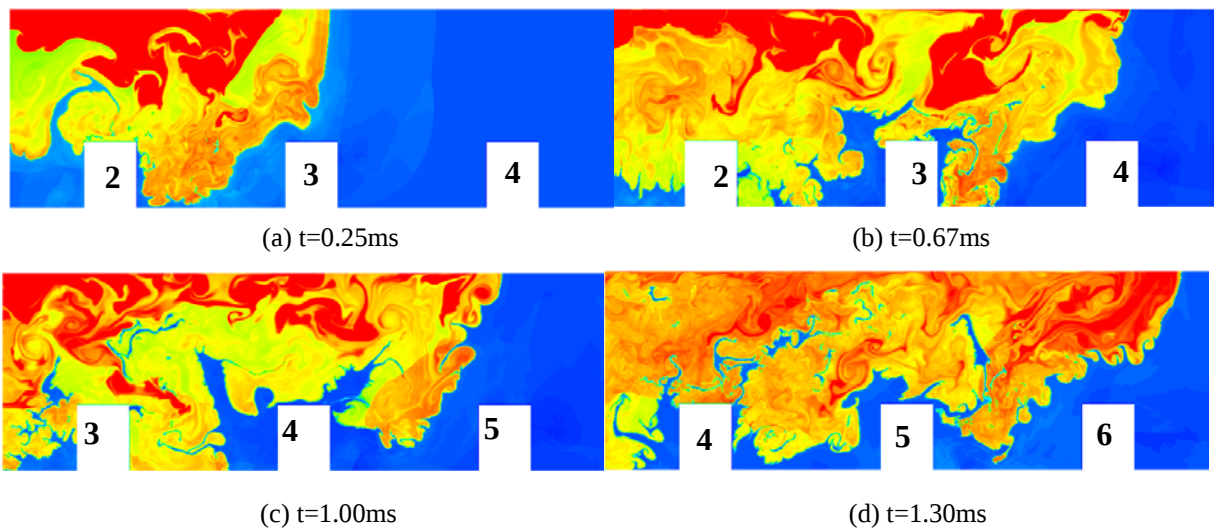


Fig. 6 Interaction of obstacles with flame front

Fig. 6 shows the instability of flame front after flame passes through obstacles. At  $t=0.248\text{ms}$ , the flame front is not very distorted, shown in Fig. 7(a). When flame passes obstacle 6, leading compression wave is reflected by the obstacles and reflection wave is formed. Then the reflected wave interacts with flame front and smashes the flame front. Therefore, it can be seen that lots of flamelets appear at the flame front, the flame front becomes highly distorted and surface area of flame front increase, as shown in Fig. 6(d). Eventually, the flame can be accelerated quickly.

## 5 Conclusions

In this paper, the effect of flame instability on flame acceleration mechanism is investigated in the ducts of different width and with obstacles. Some conclusions are obtained:

- 1) For the duct width of  $D=1.0\text{cm}$ , energy released from boundary layers and increasing of flame front area lead to the flame acceleration. The interaction between compression waves and the lead part of the flame near the boundary layer is responsible for the final triggering DDT.
- 2) With the duct width increasing, influence of energy released by boundary layer on flame acceleration is small. This results in slow flame acceleration. Therefore, DDT still do not occur when the flame spreads to the position of  $x=160.0\text{cm}$  and may require longer DDT distance.
- 3) In the wide duct with obstacles, reflection wave by obstacles makes the flame front break, and even smaller flamelets form. This increases surface area of flame front and eventually results in flame acceleration.

## Acknowledgments

This research is supported by the National Natural Science Foundation of China under grants 11221202 and 11272056, National Basic Research Program of China (Grant Nos. 2010CB832706 and 2011CB706904), and the Foundation of State Key Laboratory of Explosion Science and Technology (Grant No. ZDKT11-01).

## References

- [1] Shchelkin KI. (1940). Influence of tube roughness on the formation and detonation propagation in gas. *J. Exp. Theor. Phys.* 10: 823,
- [2] Kagan L, Sivashinsky G. (2003). The transition from deflagration to detonation in thin channels. *Combust. Flame.* 134:389.
- [3] Uchida M, Kessler DA, Gamezo VN, Oran ES. (2010). Simulation of flame acceleration and deflagration to detonation transitions in methane-air systems. *Combust. Flame.* 157:2063.
- [4] Liberman MA, Ivanov MF, Kiverin AD, Kuznetsov MS, Chukalovsky AA, Rakhimovab TV. (2010). Deflagration-to-detonation transition in highly reactive combustible mixtures. *Acta Astronautica.* 67:688.
- [5] Akkerman V, Bychkov V, Petchenko A, Eriksson LE. (2006). Accelerating flames in cylindrical tubes with nonslip at the walls. *Combust. Flame.* 145: 206.
- [6] Landau LD, Lifshitz EM. (1989). *Fluid Mechanics*, Pergamon Press. Oxford.
- [7] Bychkov V, Liberman M. (2000). Dynamics and stability of premixed flame. *Phys. Rep.* 325:115.