Restructuring of a flame due to a preheated zone as a mechanism underlying the deflagration-to-detonation transition

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1 Introduction

It is generally accepted due to Zeldovich [1] and Lee [2] that the mechanism of the detonation wave initiation, given the appropriate background conditions, involves reactivity gradients. There is substantial evidence that a detonation can indeed develop in a reactivity gradient [1, 3-5]. Nevertheless, the question of how exactly a reactivity gradient can originate in the DDT events remained open. There is a believe that formation of a reactivity gradient can occur in different ways in unreacted material associated with hot spots, turbulent mixing of the unburned and reacted gas, etc., and that the reactivity gradient in unreacted material ahead of the flame is required for propagation of spontaneous reaction waves that could undergo transition to a detonation.

Theoretical analysis, numerical simulations and experiments show that dynamics of the flame propagating in a tube with no-slip walls results in formation of the preheated zone ahead of the flame. In the present work we show that the presence of the preheated zone ahead of the flame, it does not matter there is or there is no a reactivity gradient within the zone, gives rise to the self-restructuring temperature profile within the flame such that a shallower temperature gradient, which can produce a detonation, arises from the initially steep temperature profile inherent to deflagration itself.

2 Flame acceleration and formation of the preheated zone

Usually the DDT phenomenon is exclusively associated with turbulent flames with velocities much larger than the laminar flame velocities. All the same, the DDT was observed in capillary tubes where both the flame and upstream flow are laminar. Our experimental studies of DDT in smooth tubes and in tubes with moderately rough walls show that the upstream flow ahead of the flame remains laminar in a bulk during the course of the event. We show in this case the deflagration-to-detonation transition exhibits three stages of evolution corroborating majority experimental observations: (1) flame accelerates producing weak shocks far ahead in the upstream flow, (2) acceleration of the flame slows down so that shocks are formed in the proximity of the flame creating preheated zone ahead of the

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flame front, (3) the third stage is self-restructuring of the initially steep temperature profile within the flame, formation of a reactivity gradient and the actual formation of the detonation wave itself. It should be noticed that the actual event of transition is distinct from the flame acceleration but inevitably connected to the sequence of particular flame accelerations.

During the first stage the upstream flow distorts the flame front so that it remains nearly flat in the bulk with the flame edges stretching backwards along the tube wall within turbulent boundary layer. So long thickness of the boundary layer is much less than the channel width D the flame velocity in the laboratory coordinate system during the first stage is

$$U_f = \Theta U_{eff} \cdot \exp\left\{\alpha\left(\frac{L_f}{D}\frac{t}{\tau_f}\right)\right\},$$

where U_{eff} and L_f are the effective velocity of the flame, which is, in general, larger than normal incipient velocity of a planar flame due to flame wrinkling caused by disturbances from turbulent boundary layer, $\Theta = \rho_u / \rho_b$ and $\alpha(\mathrm{Re})$ is a numerical factor, L_f is the thickness of a laminar flame.

The accelerating flame acts as permeable piston producing shock waves with intensity $M_{sh} = 1.5 \div 1.7$ far ahead in the upstream flow. Obviously, the deep and narrow fold formed between the flame edge and the wall can survive only for a short time. The tip of the fold runs forward and the flame surface diminishes considerably. This results in a drastic decrease of the flame acceleration. The flame acceleration reduces below a constant one and shocks will be formed in the immediate proximity ahead of the flame front. The shocks coalesced and intensified. The unburned mixture in the zone adjusted to the flame is compressed and heated by the shocks. This stage results in formation of the preheated zone of the unburned material adjusted to the flame front.

The analytical model describing the first and the second stages is well consistent with the experimental observations of the flame velocity evolution in stoichiometric H_2+O_2 and ethylene-oxygen mixtures shown on Fig. 1 and with 2D simulations shown on Fig. 2.

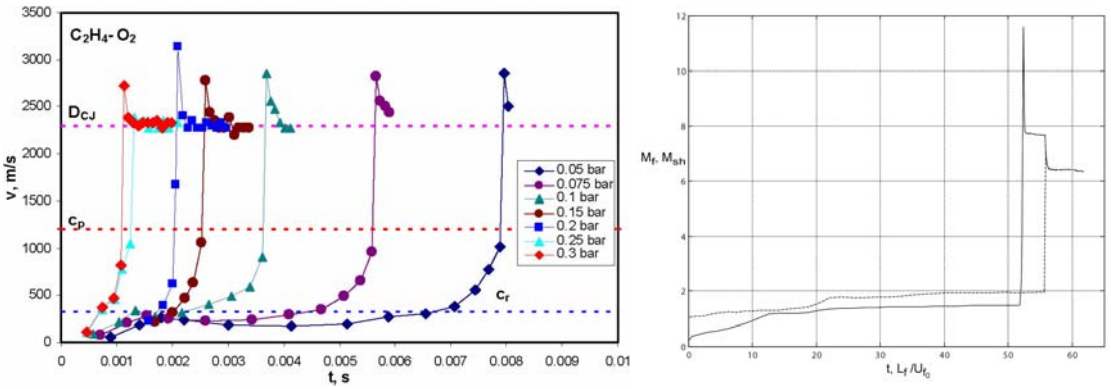


Fig. 1. Temporal evolution of the reaction wave velocities for DDT in stoichiometric ethylene-oxygen mixture.
Fig. 2: Calculated temporal evolution of the reaction wave (solid line) and shock (dashed line) velocities for $n = 2$, $D = 70L_f$, $M_{f0} = 0.05$, $\Theta = 8$, $\varepsilon = E / T_u = 32$.

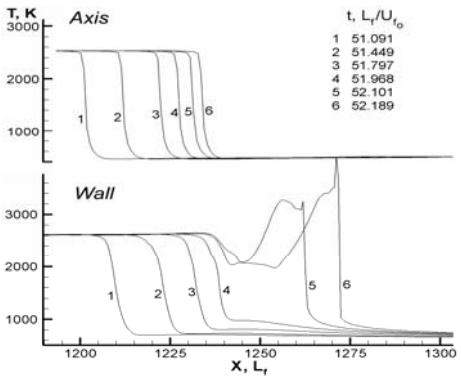
The computed at several consecutive instants temperature profiles for the conditions of Fig. 2 are shown in Fig. 3. It is seen that the temperature (curves 2-3-4) increases in the zone of unburned material adjusted to the flame just before the transition; corresponds to $t = 52.1\tau_f$. More intense preheated zone is often formed near the wall [6, 7]. Fig. 4 shows schlieren images of the experimentally observed preheated zone. On the first frame one can see well pronounced preheated zone which consists of spatially separated coalescing shock waves (white stripes). On the second frame the shocks are getting overlapped and amplified up to $M_{sh} \simeq 3$ and a uniform preheated zone of width of $\Delta x / L_f = 17 \div 20$ becomes ripe to trigger DDT ($L_f = 0.61mm$).

3 Formation of the temperature gradient and transition to detonation

The third stage of the formation of a temperature gradient and actual transition to detonation is very fast and calls for fine resolution, which is difficult for 2D or 3D simulations. For this purpose, we explore a more tractable one-dimensional model whose basic features are borrowed from the 2D simulations. Contrary to the studies of the detonation formation due to prescribed temperature gradient [1, 3-5] we considered situations when a temperature gradient expedient for the transition is born as the result of restructuring of the flame in the presence of the preheated zone.

In order to resolve accurately fine scales, the grid of appropriate density at each point was taken or the grid was refined recursively. The appropriate level of resolution was found 300 cells within the flame width. Convergence of the obtained solutions was tested by varying sizes of computational cells and time steps to the point where the solutions no longer change within accuracy of 2-3%. The initial spatial temperature distribution was specified in line with the temperature profile formed ahead of the flame in a channel with no-slip walls (Fig. 3). In numerous test calculations we found the whole scenario of the DDT much like the same independently on a particular profile of the temperature in the preheated zone. The picture is nearly the same for a stepwise temperature profile, or exponentially or linearly decreasing in the preheated zone from its maximum value T_m just ahead of the flame.

Because of higher temperature in the preheated zone, the flame accelerates, produces pressure pulses which rise temperature and compress matter in the preheated zone. The enhanced reaction in the preheated zone further heats the matter thereby further accelerating the reaction therein, so that accelerating flame produces stronger and stronger pressure pulses. As a result, the reaction zone extends towards the preheated zone. All these lead to the flame restructuring so that a shallower temperature gradient is formed from the initially steep temperature inherent to a deflagration. As the temperature gradient in the flame becomes gentler, velocity of the reaction wave increases and the course of events changes accordingly. Finally, the velocity of spontaneous wave defined by the temperature gradient becomes larger than the velocity defined by thermal diffusion and the speed of the reaction wave is now specified by the formed gradient of induction time rather than by thermal conduction. The detonation is settled when the velocity of the reaction wave becomes equal to the local sound speed. As faster a flame is, other parameters are identical to those of slower flame, as thinner can be the preheated zone or lower temperature in the preheated zone required for the flame restructuring and transition to detonation. The effect is more profound for the higher reaction order.



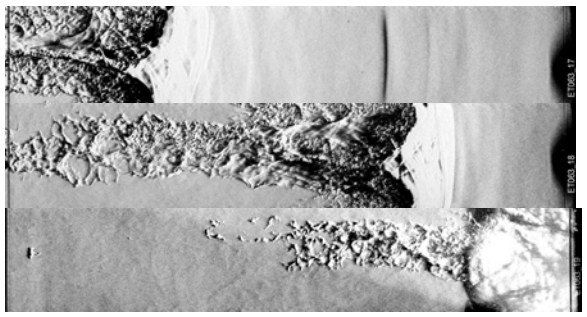


Fig. 3: Temperature profiles along the wall and axis at several consecutive instants for conditions of Fig. 2.Fig. Temporal evolution of the flame velocities and transition to detonation.

Fig. 4 Formation of a preheated zone adjusted to the flame and transition to detonation. Stoichiometric ethylene-oxygen flame, $P = 0.121\,\text{bar}$, $U_{f0} = 5.2\,\text{m/sec}$, $L_f = 0.61\,\text{mm}$

4 Experimental DDT studies

Experiments were performed at the Kurchatov Institute and Karlsruhe Research Center and focused on key characteristics responsible for the DDT: flame velocity, strength and location of the flame

generated shock waves, their effect on formation of the preheated zone, and minimal critical width of the preheated zone capable to trigger DDT. Experiments have been carried out in a rectangular channel with 50x50 mm cross-section and 3.4÷6.05 m long with 24 transparent ports for photo-gauges. The experimental facilities: a high-speed schlieren photo technique, germanium photodiodes, piezoelectric transducers, etc. are described in [8]. The effect of the boundary layer on the flame acceleration and pre-detonation-distance was investigated using variable smooth and rough walls of the channel. Table 1 summarizes selected experimentally measured data of the critical preheated zone thickness, for the advancing shock wave strength $M_{sh} \simeq 3$, and temperature in the preheated zone to be able ("GO") or not to be able to detonate ("NO GO") for ethylene-oxygen flames. The minimum width of the preheated zone, which is ripe to trigger DDT, is in the range 17÷25 of the laminar flame thicknesses, which is in a good agreement with the theoretical prediction.

Table 1: Critical thickness of characteristics of preheated zone for detonation initiation (P_0=0.12 bar)

Test	M	T, K	Δx, mm	$\Delta x/L_f$	Δx, mm	$\Delta x/L_f$
			GO		NO GO	
ET057	2.92	694	11	18	7	12
ET061	2.94	700	10.5	17	6	10
ET076	3.0	718	13	21	10	16
ET078	3.0	718	(*)	(*)	9.5	16
ET083	3.1	756	11	18	7	12

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