Effects of Shock Waves, Boundary Layer and Turbulence on Flame Acceleration and DDT in Highly Reactive Mixtures

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1 Introduction

The problem of the deflagration-to-detonation transition (DDT) and a key role of shock waves, boundary layer and turbulence in the detonation preconditioning process is well known but still not resolved in the combustion theory. The ignition, flame propagation with a flow ahead of the flame, and shock waves generation with turbulent boundary layer behind the shock is the sequence of principal events leading to the deflagration-to-detonation transition in smooth channels [1-3]. As Ya. Zeldovich wrote [4], the turbulence is not only one and even not the major reason of the flame acceleration in smooth channels. Wrinkled flame stretch and non-uniformity of the flow across the channel can be the main reason of flame acceleration leading to DDT. Experimental schlieren photos indicated that location of the transition to detonation always originates somewhere within the shock-wave complex, sometimes near the wall in the boundary layer, sometimes in the center of a channel. One of the main peculiarities of the DDT process is that the detonation onset takes place in a preheat zone under conditions, which are very different from initial state of the mixture. We call such a state as the detonation preconditioning of the mixture with preheat zone formation. The mechanism of preheat zone formation due to the flame acceleration in presence of unsteady turbulent boundary layer and advancing shock amplification will be the main goal of this work.

2 Flame Acceleration and Boundary Layer Formation

The deflagration-to-detonation transition experiments with highly reactive hydrogen-oxygen mixtures at different initial pressures from 0.1 to 1 bar have been carried out in a channel geometry with respect to investigate effects of advancing shock waves, boundary layer and turbulence on flame acceleration and DDT. Linear rectangular channels of 50x50 mm^2 and 5x5 mm^2 with glass windows or transparent capillary tubes of 2-4 mm id were used for detonation experiments. In most experiments the channel was long enough (120-250 calibers) to exclude an effect of reflected shock on DDT. Three basic stages of DDT were observed experimentally: (1) the exponentially accelerated flame producing shock waves far ahead of the flame; (2) the second stage when the flame acceleration law changes so that the advancing shock waves are generated directly on the flame front, (3) the final stage is actual transition to a detonation. As a typical "finger" flame, the flame propagates initially due to the geometry factor with an exponential acceleration law against time [5]:

$$u = \frac{dx}{dt} = \Theta U_f \exp(kt) \qquad (1),$$

$$k \approx \frac{\Theta U_f}{R} \qquad (2)$$

where u is the visible flame speed; $\Theta = \frac{\rho_u}{\rho_b}$ is the expansion ratio; U_f is the laminar flame speed; R, x, t are the tube radius, distance and time. Exponential law of the primary flame acceleration (1)-(2) means that with a higher flame velocity and with a smaller tube radius the distance for the flame to be accelerated to sonic speed is decreased. Table 1 shows good consistency of experimental and theoretical characteristics of the flame acceleration law (1)-(2).

Table 1: Main characteristics of exponential flame acceleration

Pressure, bar	Initial flame speed ΘU_f, m/s		Flame acceleration increment k, s^{-1}	
	experimental	calculated (Lutz)	experimental	calculated (Lutz)
0.2	29	55	2500	2440
0.6	59	71	3270	3150
0.75	70	75	3750	3290

During the first stage, the flame velocity increases exponentially in time and at the end of the first stage the flame propagates in the laboratory coordinate system with the visible velocity, which is close to the speed of sound. It should be noted that influence of turbulence on flame velocity even in tubes with rough walls at this stage is negligible small and the upstream flow remains laminar in a bulk because the boundary layer is too thin, less than 1 mm (Fig. 1).

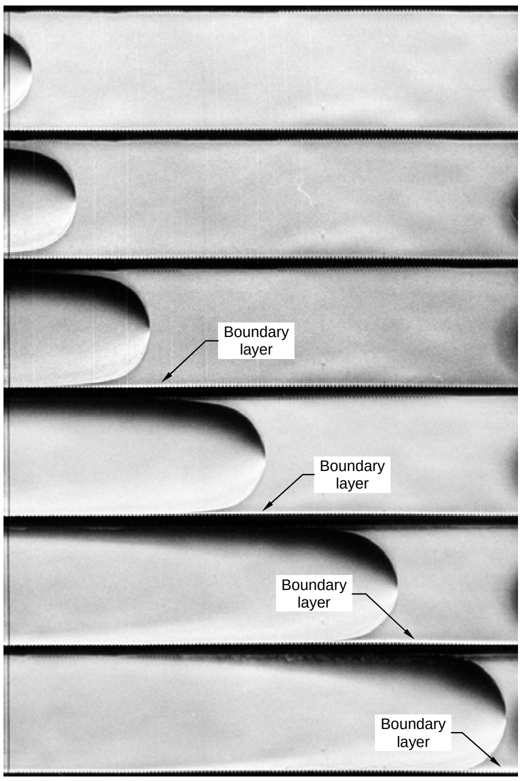

Figure 1. Flame structure and boundary layer during the first stage of flame acceleration.

The boundary layer thickness δ in an unstationary flow before the flame is proportional to the distance from flame to the precursor shock wave: $\delta = 0.01\cdot\Delta x$. The problem for highly reactive mixtures is that the distance between precursor shock and flame front is relatively small. This means that for highly reactive mixtures it will never be established a boundary layer as for stationary flow. Our experiments showed that real thickness of the boundary layer before the flame might be 2 to 10 times less as compared with the case of stationary flow (Fig. 2). Nevertheless, during the second stage the effects of turbulence and boundary layer on flame behavior become more important. As a result, the convex "finger" flame transforms into so called "tulip" flame due to Darrieus-Landau instability and boundary layer effect. This leads to significant changes of the flame acceleration law. After the flame reached the maximum velocity of 270–410 m/s, depending on the mixture reactivity, the flame propagates quasi-stationary in the pre-compressed and preheated mixture. Duration of the second stage is typically considerably longer than time of the first stage. It fits quite well with characteristic time of laminar flame $\tau_f = L_f / U_f$, where L_f is the laminar flame thickness. It was found [5] that the value of $t/\tau_f = 25$ is the characteristic dimensionless time of transition to detonation for wide range of mixture reactivity.

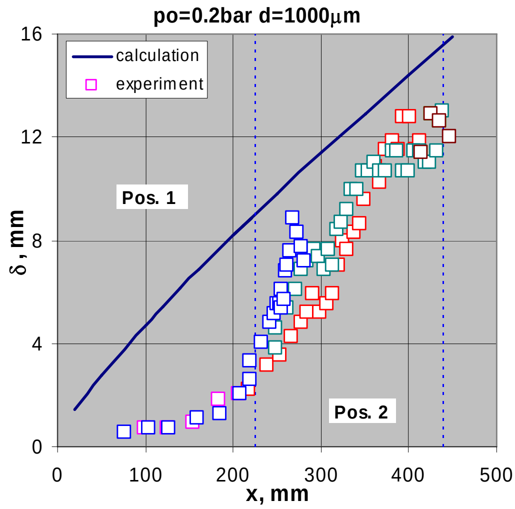

Figure 2. Turbulent boundary layer - comparison with prediction for hydrogen-air combustion at pressure 0.2 bar in a channel with 1 mm roughness: theory (line); experiments (points)

The detonation often starts near the wall likely due to viscous heating of the unburned mixture in the boundary layer. If T_0 is the temperature near the tube axis, and M_u is the flow Mach number ahead of the flame front, then the temperature excess in a stationary boundary layer [6] $\Delta T_{wall} = T_0\left(1 + \frac{1}{2}(\gamma - 1)\cdot M_u^2\right)$ becomes noticeable before the transition. For instance ΔT_{wall} = 527K if M_u = 3. This may considerably influence both extension and temperature of the preheating zone in the boundary layer, therefore favoring location of the transition somewhere near the wall. Some authors claim that the hydraulic resistance causes a gradual pre-compression and preheating of the unburned gas adjacent to the advancing deflagration which leads (after an extended induction period) to a localized thermal explosion triggering an abrupt transition from deflagration to detonation [7]. In our experience, the shock wave strength and flow velocity must be higher and the size of boundary layer must be larger than in reality to produce the near wall temperature sufficient for thermal explosion leading to DDT.

Since the location of transition to detonation sometimes originates in the boundary layer near the wall this was an idea that DDT occurs due to the flame thickening if turbulent boundary layer thickness is 10 times larger than detonation cell size [8]. The solution for a boundary layer in stationary flow showed that the turbulent velocity $v^*\sim 5U_f$ in boundary layer of the thickness δ = 100-200 L_f near the

DDT point is not enough to disturb the flame front strong enough in order to create pre-condition DDT zone inside the flame brush. Location of these points is inside the corrugated flame domain and quite far from distributed reaction zone in terms of Borghi diagram [9]. Perhaps beside the boundary layer we have to consider other factors in DDT process like flame generated shock waves which can be more significant for formation of the preheat zone prior to DDT.

3 Advanced Shock Wave Amplification and Preheat Zone Formation

Figure 3 shows shock waves structure and flame trajectory during DDT process obtained for our experiments with transparent micro-tubes of 2-5 mm id. The accelerating flame acting as a piston produces compression waves in the flow ahead (Part I, Fig. 3). The compression wave steepens to a shock wave at some distance from flame front (Point A, Fig. 3) according to Riemann solution [5]. The strength of precursor shock is M = 1.2 – 1.6 depending on mixture reactivity. This means that the flame propagates through preheated and pre-compressed mixture in presence of the boundary layer. Duration of this stage is order of $t \approx \tau_f \sqrt{D/\Theta L_f} \sim 5\tau_f$. The flame accelerates exponentially against time (see Equations (1)-(2).

During the second stage (Part II, Fig. 3) due to the "tulip" flame formation the flame velocity on the next stage can be approximated as $U_f \approx U_{eff}\left(1+\beta\left(t/\tau_f\right)^n\right)$, with n < 1 [10]. For a piston which moves with such velocity-time dependence, the function $u(x, t)$ is multi-valued for any n < 1. Therefore, during this stage shock waves are formed in the immediate proximity ahead of the flame front, formally on the flame surface (Point B, Fig. 3). These shocks coalesced and their intensity increases up to $M_{sh} \approx 2 \div 3$. During this stage the preheat zone adjusted ahead to the flame front is formed in the unburned chemically frozen material [11]. DDT occurs within the preheat zone if its temperature and size is high enough (Fig. 3). Using detailed chemistry for post-shock conditions it was shown that even without any turbulence the laminar flame speed increases 4-5 times for highly reactive mixtures for shock waves with M_{sh}=2.5-3.

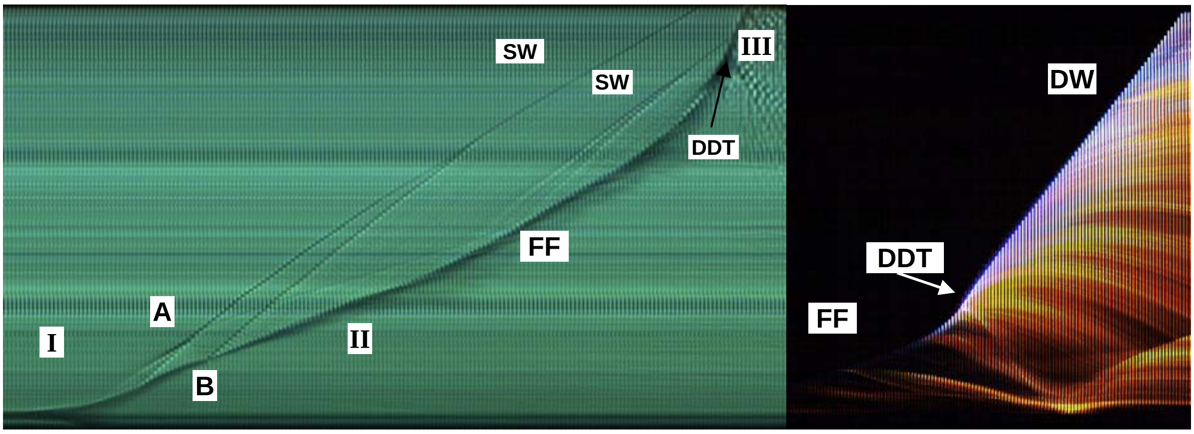

Figure 3. High-speed (250000fr.p.s.) shadow image of initial stage of flame acceleration and DDT process (left) and normal video of the detonation process (right) for H_2-O_2 mixture at 1 bar: FF=flame front; SW=shock wave; DW=detonation wave.

Another mechanism for flame acceleration, shock wave amplification and preheat zone formation prior to DDT was found in relatively short tubes when run-up-distance to DDT is comparable or larger than tube length. The detonation in such case was initiated after a collision of reflected precursor shock wave with flame front. It was experimentally found that due to the Richtmaier-Meshkov instability during the shock-flame interaction the flame velocity suddenly increases in 10 times. Such a shock-flame interaction might happen several times (up to 2-5, see Fig. 4). This results in an additional detonation preconditioning and leads to reduction of the run-up distance to DDT in several times compared to the long tubes (L/D >> 100). Detonation can also occur after 2-5 shock wave reverberations until pressure and temperature will reach conditions for the flame to be accelerated fast enough for DDT. For instance, in comparison with an initial state the pressure grows in 6 times, the temperature in 2 times and the laminar flame speed in 6 times after 5 reflections (Fig. 5). Effect of turbulence does not play a role in the case of DDT in relatively short tubes.

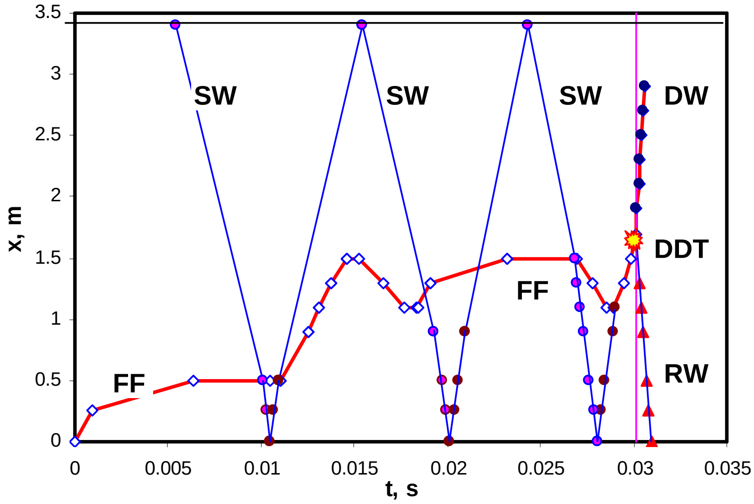

Figure 4. X-t diagram of DDT process in relatively short tube filled with H_2-O_2 mixture: FF=flame front (red line); SW=shock wave (blue lines); DW=detonation wave (red line); RW=retonation wave (blue line).

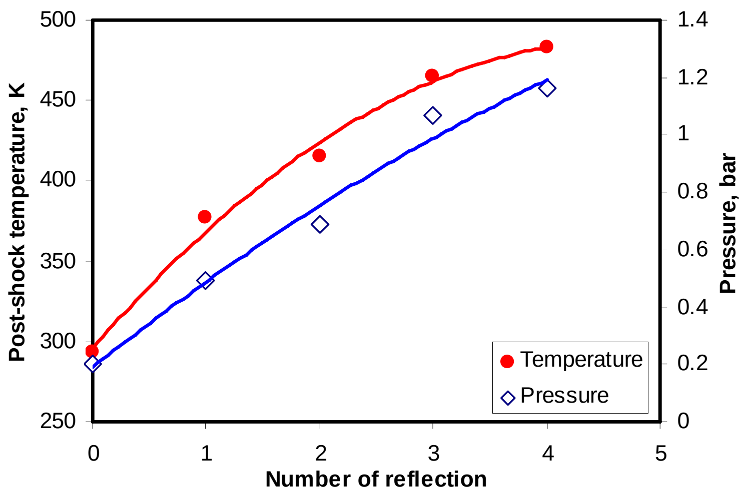

Figure 5. Actual post-shock pressure and temperature of unreacted material due multiple reflections.

4 Summary and Conclusions

The deflagration-to-detonation transition experiments with highly reactive hydrogen-oxygen mixtures have been carried out in a channel geometry with respect to investigate effects of advancing shock waves, boundary layer and turbulence on flame acceleration and DDT. Linear rectangular channels of 50x50 mm^2 and 5x5 mm^2 with glass windows or transparent capillary tubes of 2-4 mm id were used for detonation experiments. Three basic stages of DDT were observed experimentally: (1) the exponentially accelerated "finger" flame producing shock waves far ahead of the flame; (2) the second stage when the flame acceleration law changes so that the advancing shock waves are generated directly on the flame front, (3) the final stage is actual transition to a detonation.

- During the first stage the flame accelerates exponentially as "finger" flame due to geometry factor. Flame develops up to sonic speed in a laminar flow independent of tube roughness because boundary layer is too thin. It was shown that the smaller tube diameter the less distance is required for the flame to reach sonic speed.
- During the second stage due to the "tulip" flame formation the flame acceleration law changes in such way that shock waves are formed in the immediate proximity ahead of the flame front, formally on the flame surface. This provides the conditions for strong feedback between flame and advanced shock with formation of preheat zone. The preheat zone consisting of chemically frozen material adjusted ahead of the flame front. The role of turbulence again is not evident in smooth channels filled with highly reactive mixtures.
- For low pressures of p=0.1-0.2 bar the tube was not long enough and very intensive flame acceleration and DDT were initiated due to collision of reflected shock waves and flame.
- Detonation can also occur after 1-5 shock wave reverberations until pressure and temperature of unreacted material will reach conditions for the flame to be accelerated fast enough for DDT
- Shock-flame interaction and adiabatic compression of unreacted material play an important role for detonation preconditioning and DDT process. Boundary layer and turbulence do not play a role for DDT in relatively short smooth tubes filled with highly reactive mixtures.

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