Experimental Study of the Preheated Zone Formation and Deflagration-to-Detonation Transition

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1 Introduction

Zel'dovich was the first to introduce the idea of a reactivity gradient to explain acceleration and detonation ignition [1]. This idea was refined by Lee at al. [2] in a form of SWACER-mechanism which describes the mechanism of spontaneous detonation initiation as shock wave amplification by the coherent energy release. Nowadays it is generally accepted that a reactivity gradient must be involved in the DDT phenomena, but it remained unclear how it is formed in the course of transition. It was verified by means of 1D simulations (see e.g. [1, 3-4]) that a proper reactivity gradient, for example a gradient of temperature, might indeed initiate a detonation. The role of turbulence on detonation initiation in smooth channels is not significant, especially for high reactive mixtures. Moreover, detonation can occur in presence of laminar flow like in capillary [5] or in case of detonation of highly reactive mixtures in large-scale tubes or spherical bomb [6] when run-up-distance takes 5-7 cm and turbulent flow could not establish during so short path and time. It was shown [7] that the reactivity gradient initiating transition to detonation is created as the result of the flame restructuring caused by the preheated zone formed ahead of the accelerating flame. The present experimental study are focused on key characteristics of the DDT such as: flame acceleration and flame velocity, strength and location of shock waves produced by the accelerating flame, formation of the preheated zone, and critical parameters of the preheated zone capable to trigger transition to detonation.

2 Experimental details

Experimental investigation of DDT in stoichiometric hydrogen-oxygen and ethylene-oxygen mixtures at temperature 20°C and pressures 50÷750 mbar was used for variety of the experimental conditions with different sound speeds, overall reaction orders and different reactivity. Test mixtures were prepared by precise partial pressure method. Ignition of the test mixtures was provided by means of weak electric spark with energy about 20 mJ to prevent direct detonation initiation.

The experimental facilities are described in [8] involved a stainless steel detonation tube with rectangular cross-section of 50x50 mm and 3.4÷6.065 m length. Dynamics of the combustion was studied using light sensors, a high-speed optical schlieren system with stroboscopic pulse generator and high speed camera, germanium photodiodes and piezoelectric transducers were used to record flame evolution

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3 Experimental results and discussion

Fig. 1 shows x-t – diagram of stoichiometric hydro-oxygen combustion process in rough channel. Experimentally, three main phases of the flame development with following deflagration-to-detonation transition can be distinguished on this plot: (I) primary lame acceleration with leading shock wave formation (SW on Fig. 1); (II) flame velocity deceleration with following secondary flame acceleration and formation of the detonation preconditioning zone due to advancing shock waves (ACW) radiated with the origin located directly on the flame surface; (III) the DDT process itself.



Figure 1. X-t diagram of flame acceleration and DDT process: $2H_2+O_2$, P=0.6 bar, roughness 1000 µm. All experimentally obtained lines are: FF = flame front; DW = detonation wave; RW = retonation wave; SW = precursor shock wave; ASW = advancing shock waves; DDT = DDT point.

Fig. 2 shows an example of the flame dynamics during the first stage of the combustion process for stoichiometric hydrogen-oxygen mixture. First phase corresponds to the primary flame acceleration. Dynamics of such quasi-laminar flame is controlled by fundamental flame velocity, thermal expansion and the flame area. The cellularity of the flame increases with the initial pressure increase and becomes finer with time of combustions. It was found that the flame acceleration is the exponential function of time. The precursor shock wave is with M=1.2-1.6 depending on mixture reactivity is rather weak and formed relatively far from the flame front. Acceleration of the flame with transformation of convex flame to concave or "tulip" flame. As a result of such process visible flame velocity slows down because of flame area decrease. Deceleration of the flame prevents radiation of advancing shock waves by the flame front. This is the reason why we did not see any shocks after the leading one.



Figure 2. Visible flame velocity along the tube (left) and against time (right) during the first stage of the flame acceleration.

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Preheated zone formation

During the second phase, the developing boundary layer, elevated pressure and temperature behind the precursor shock wave promote the conditions for the secondary flame acceleration. Acceleration law changes in this case so that the advancing shock waves (ACW in Fig. 1) formed in the immediate proximity of the flame front and the preheated zone ahead of the flame is created. On the x-t-diagram obtained from schlieren photos and photodiodes and pressure records we can clearly see a sequence of strengthening advancing shock waves with Mach numbers M=(1.95; 2.16; 2.3; 2.65). After the last shock we could identify a preheated zone with temperature about 670K and pressure 4.4·P₀. The width of the preheated zone was measured to be $17 \cdot L_f$ or seventeen times larger than laminar flame thickness under initial state. After data processing of all hydrogen-oxygen experiments it was found that if temperature of preheated zone is less than 530K and the width is less than $16 \cdot L_f$ the detonation transition does not occur until the flame accelerates to required conditions of the preheated zone.

Almost the same flame behavior was obtained for ethylene-oxygen mixtures with lower reaction order (n=1.94-1.99<2). Fig. 3 shows schlieren photo of initial stage of the detonation onset which allows to define critical size of the preheated zone.



Figure 3. DDT formation into preheated zone (white stripes) in stoichiometric ethylene-oxygen mixture: $P_0 = 120$ mbar, $U_{f0} = 5.2$ m/s, $L_f = 0.61$ mm.

It was experimentally found that critical thickness of preheated zone $\Delta x = 17-21 \cdot L_f$ with the strength of advancing shock wave M=2.9-3.1 and temperature of preheated zone in the range 694-756K which is much higher than those for stoichiometric hydrogen-oxygen mixture with overall reaction order n=2.74. If preheated zone thickness at the same shock strength was less than 16·L_f the DDT did not originate in this part of the preconditioning zone.

Strength of advancing shock waves and preheated zone temperature defined as post-shock temperature have been calculated for fast flame as function of visual flame speed in laboratory coordinates. The calculations made for double discontinuity consisted of the flame, precursor shock wave and flow in between the flame and shock wave for the process shown if Fig. 1. Calculations of the preheated zone temperature give reliable results because calculated strength of advancing shock is in good consistency with experimental values. Fig. 4 demonstrates dynamics of preheated zone formation for hydrogen-oxygen combustion. It is seen that formation of preheated zone is mainly controlled by advancing shock interaction. Effect of turbulence might be insignificant here. For instance, calculated with Cantera code laminar flame velocity for stoichiometric hydrogen-oxygen mixture at the conditions of shock wave with Mach number M_{sh}=3 increases 4.75 times compared to initial state at pressure 0.6 bar. For ethylene-oxygen mixtures the laminar flame speed increases in 4.2 times for the advancing shock wave strength M_{sh}=3. Taking into account a geometrical factor, such a flame velocity increase can practically explain one of the reasons of the flame acceleration prior the DDT transition. It is also important in cases when the leading shock wave is not too far from the flame surface. How it was seen from schlieren pictures, the turbulent boundary layer in this case may occupy only 10% of flow cross-section and main part of the flow remained undisturbed.



Figure 4. Dependence of calculated advancing shock strength and preheated zone temperature against dimensionless time for the test in Fig. 1: dashed line corresponds to the DDT moment.

4 Summary

Experimental investigation of DDT in stoichiometric hydrogen-oxygen and ethylene-oxygen mixtures at temperature 20°C and pressures $50\div750$ mbar have been performed. Three main phases of the flame development which are responsible for formation of detonation preconditioning zone have been investigated. It was experimentally measured that characteristic critical width of preheated zone has to be 17 to 21 times larger than laminar flame thickness L_f with a temperature about 670 K for hydrogen-oxygen mixtures with reaction order n=2.74 and with temperature 700-750K for ethylene-oxygen mixtures with reaction order n=1.95. Preheated zone temperature corresponds to strength of advancing shock wave M_{sh} =2.65 for hydrogen-oxygen and M_{sh} =(2.9-3.1) for ethylene-oxygen mixtures. The data are in good consistency with results of numerical simulations created in [7].

References

[1] Zel'dovich, Ya. B., Librovich, V. B., Makhviladze, G. M, and Sivashinsky, G. I. (1970) On the development of detonation in a non-uniformly preheated gas, Astronautica Acta, 15: 313.

[2] Lee JHS. (1977) Initiation of gaseous detonation, Ann. Rev. Phys. Chem. 28: 75.

[3] Khokhlov, A. M., Oran, E. S., Wheeler, J.G. (1997) A Theory of Deflagration-to Detonation Transition in Unconfined Flames, Combust. Flame, 105: 503.

[4] Kapila, A.K., Schwendeman, D.W., Quirk, J.J., Hawa, T., Mechanisms of detonation formation due to a temperature gradient, Combust. Theory Modelling, 6, 553-594 (2003).

[5] Wu, M.-H., Burke, M.P., Son, S.F., Yetter R.A. (2007) Flame Acceleration and the Transition to Detonation of Stoichiometric Ethylene/Oxygen in Microscale Tubes, Proceedings of the Combustion Institute 31: 2429.

[6] Kuznetsov, M., Grune, J., Alekseev V., Breitung, W. (2007) Explosion Limits of Hydrogen-Oxygen-Steam Mixtures at Elevated Pressures and Temperatures, Proc. of the 21st ICDERS, 2007, Poitiers, France, 0290: 1-4.

[7] M. A. Liberman, M. Kuznetsov, I. Matsukov, A. Ivanov, Restructuring of a flame due to a preheated zone as a mechanism underlying the deflagration-to-detonation transition, submitted 22nd ICDERS. Formation of the preheated zone ahead of a propagating flame and the mechanism underlying the deflagration-to-detonation transition, Physics Letters A 373, 501–510 (2009).

[8] Kuznetsov, M., Alekseev, V., Matsukov, I., Dorofeev, S. (2005) DDT in a smooth tube filled with a hydrogen-oxygen mixture, Shock Waves 14, 205.