Examination of the DDT Triggering in an Obstructed Tube

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Introduction

The phenomenon of deflagration-to-detonation transition (DDT) in gaseous mixtures was extensively studied especially during the last two decades. A tube filled by equidistantly placed circular orifice rings presents a typical instrument for DDT experiments. As it is known (Chan and Greig (1988), Teodorczyk et al. (1988) and others) the DDT process in an obstructed tube is featured by the formation of a flame-shock structure consisting of a leading shock wave followed by the reaction front (shock-flame packet). During the process of flame acceleration the velocity both of shock and combustion front increase, while the separation distance decreases. When propagation speed of the combustion front becomes roughly equal to the sound speed of combustion products the interaction of the shock-flame packet with the nearest obstacle can result into a violent local explosion and fast transformation to detonation.

The role of the flame following a leading shock in the DDT process is still an open question. Basing on experimental results and numerical simulations reported by Khokhlov and Oran (1999), Khokhlov et al. (1999), Brown and Thomas (2000), Thomas et al. (2002) one can suggest the following alternative approaches:

- 1) The accelerating flame plays an auxiliary role and it acts simply as a piston generating a sufficiently strong shock which reflection at the obstacle (ring) directly initiates detonation;
- 2) The shock reflected from an obstacle produces high instability of the flame front and detonation is initiated in a turbulent flame brush.

The present investigation considers what parameters of shock-flame packets are relevant to the conditions of detonation triggering. The analysis was performed on the basis of pressure and flame position measurements in the case of DDT in the obstacle-filled tube.

Materials and Method

The experimental setup is based on the shock/detonation tube TH-1 of the Shock Wave Laboratory of RWTH Aachen University. The inner diameter of the tube amounts to $D_0 = 141$ mm and the overall length of the tube is 7.2 m. The obstacle arrangement in the form of equidistantly placed orifice rings was chosen with the following parameters: distance between the adjacent rings $L \cong D_0$, blockage ratio BR = 0.59. The overall length of the obstacle arrangement is 2 m. An exploding wire at the closed end of the obstacle-filled section ignites the combustible mixture.

The basic idea of the tests is to realize transition to detonation at the last orifice ring of the obstacle arrangement. In this case detonation wave starts to propagate into the obstacles-free section and therefore no additional pressure disturbances influence on the flow pattern of the DDT event. Another advantage of this technique is a possibility to group recording devices immediately in the location of detonation onset. It should be noted that for a single fuel composition (e.g. hydrogen in air mixture) and for the fixed initial pressure the condition of detonation onset at the last obstacle can be attained by selection of at most two values of fueloxidizer percentage (i.e. lean and rich limits of DDT). To extend the spectrum of combustibles under investigation along with hydrogen-air mixtures we use triple compositions consisting of methane(or propane)+hydrogen+air. The initial pressure p_0 is 1 bar. The pressure measurements are performed by Kistler 603B pressure gauges. The ionization probes are used to determine the arrival time of the detonation/combustion products.

Results and Discussion

The main attention of the present investigation was focused on the measurements of parameters of the shockflame packets immediately before detonation onset. These parameters are intensity (Mach number) of the leading shock, the velocity of the combustion front and the separation distance between the shock and the combustion front. The use of pressure gauges and ionization probes located in the same cross-sections of the tube enables to evaluate the amplitude (overpressure) $p_{\rm S}$ of the leading shock and the time lag of the flame front $t_{\rm F}$. An example considered in Fig. 1 reflects peculiarities of two outcomes, namely DDT and no DDT (deflagration), which can be realized when a shock-flame packet arrives at the last orifice ring. In the DDT case (Fig. 1*a*) the leading shock overpressure is larger than that in the deflagration case (Fig. 1*b*). Simultaneously the value of the time lag is found to be larger for the deflagration case.



Figure1. Shock overpressure p_S and time lag of a flame front t_F measured by a pressure gauge (PG) and an ionization probe (IP) at the distance 25 mm from the upstream face of the last orifice ring. *a*) DDT; *b*) no DDT (deflagration)

A summary of the available experimental results for different hydrogen-air and hydrocarbon-hydrogenair mixtures is presented in Fig. 2. In spite of some scattering of the data points one can recognize a proper boundary between DDT and no DDT events. This opens a way to elucidate critical conditions of transition to detonation in terms of the structure of the shock-flame packets.



Figure 2. Measured values of the leading shock overpressure and time lag of the flame front corresponding to DDT and deflagration regimes. (DDT is due to the interaction of shock-flame packets with the last orifice ring of the obstacle arrangement).

The parameters of a leading shock can be expressed in terms of the shock Mach number $M_{\rm S}$, calculated by the formula: $M_{\rm S}^2 = (\gamma + 1)p_{\rm S}/(2\gamma) + 1$, where γ is the ratio of the specific heat capacities of the mixture. Thus one can calculate the shock velocity $v_{\rm S}$, which is defined by the relation $v_{\rm S} = M_{\rm S}a_0$ (a_0 is speed of sound in the undisturbed combustible mixture). It was found that the shock velocities corresponding to detonation initiation are equal or slightly higher than the sound speed of the combustion products $c_{\rm SP}$. Taking into account that transition to detonation is possible if the flame speed approaches a value close to $c_{\rm SP}$ one can conclude that immediately before the DDT event takes place the velocity of the flame front roughly equals the velocity of the leading shock. This result is in agreement with the observations of Chan and Greig (1988). Therefore, the measured values of $t_{\rm F}$ can be used for the evaluation of the local shock-flame separation distance $L_{\rm SF}$ by means of the simple relation $L_{\rm SF} = v_{\rm S}t_{\rm F}$.

To elucidate the conditions of the detonation triggering one can analyze characteristics of self-ignition due to the reflection of leading shock at the obstacle. Thomas et al. (2002) introduced the parameter η to describe the influence of the expansion process due to the finite size of the obstacle (partially obstructing obstacle or bulge) on the self-ignition process behind a reflected shock wave: $\eta = h/(a_S \tau_{ind})$, where τ_{ind} is the chemical induction time for the reflection of a planar shock wave at a flat surface, *h* is the height of the obstacle and a_S is the sound speed in the undisturbed reflected shock region (i.e. sound speed behind the incident shock). It was supposed in Thomas et al. (2002) that a critical condition, below which direct initiation of detonation might not occur, could be expressed as $\eta < 1$. We found that the San Diego chemical-kinetic mechanism (San Diego (2003)) is suitable for the calculations of induction time both in methane-hydrogen-air and propanehydrogen-air mixtures and in hydrogen-air mixtures as well. The calculations were made by the via Internet freely distributed program CV (2004) for the conditions of the performed experiments.

Figure 3 presents a correlation between the parameter η and the shock-flame separation distance L_{SF} . The domain marked with (I) corresponds to the DDT events at which the condition $\eta > 1$ is satisfied. Remind that this criterion was suggested by Thomas et al. (2002) based on the experiments with non-reactive incident shock waves produced by conventional shock tube procedure rather than by an accelerating flame. Thus, in the performed experiments the domain (I) in Fig. 3 corresponds likely to the case of direct initiation of detonation immediately downstream the obstacle when accelerating flame generates a sufficiently intensive shock wave that supply the condition $\eta > 1$.



Figure 3. Correlation between parameter η and shock-flame separation distance. (*I*) – DDT due to the direct initiation of detonation at the reflection of a leading shock wave at the ring obstacle; (*II*) – DDT due to the interaction between reflected shock and flame.

Another domain of the observed DDT events in Fig. 3 is marked with (II). In this case the parameter η falls in the range $0.03 < \eta < 1$, i.e. detonation cannot be initiated in the same way as above since the intensity of the leading shock is insufficient to fulfill the condition $\eta > 1$. However, as it is easy to see the DDT events correspond to the relatively small values of $L_{SF} < 80$ mm. Hence, a leading shock wave reflected at the obstacle can immediately interact with the approaching flame surface. According to Khokhlov and Oran (1999), Khokhlov et al. (1999) this interaction leads to a rapid creation of a turbulent flame brush and, for sufficiently high shock intensity, to the subsequent transition to detonation. Thus for weaker leading shocks (at which $\eta < 1$) initiation of detonation is still possible but by another mechanism than direct initiation. For the realization of the mechanism described by Khokhlov and Oran (1999), Khokhlov et al. (1999) an additional necessary condition is the presence of a flame front at a sufficiently short distance behind the leading shock. Thus based on the data presented in Fig. 3 on can evaluate the conditions for detonation initiation via reflected shock – flame interaction as $0.03 < \eta < 1$ and $L_{SF} < 80$ mm. It should be noted that a successful detonation initiation via shock – flame interaction depends on many local factors and exhibits stochastic features. This is reflected in the performed experiments since some "no – DDT" outcomes meet the conditions of domain (II) in Fig. 3.

Conclusion

The parameters of shock-flame packets which are necessary for transition to detonation in the obstacle-filled tube were evaluated. The conditions of self-ignition due to the reflection of a leading shock wave at the orifice ring obstacle were investigated on the basis of calculations of the induction time. Representation of the DDT/no DDT boundary in terms of the criterion of Thomas et al. (2002) and shock-flame separation distance allows to draw a line between two different modes of detonation onset. Direct initiation of detonation is associated with the reflection of a sufficiently intensive leading shock. In this case the accelerating flame plays an auxiliary role and it simply acts as a piston supporting a shock wave. Another mode of detonation onset is observed for a weaker shock that is not capable to initiate detonation directly. In this case DDT is caused by the reflected shock - flame interaction that produces a high distortion of the flame front and detonation is initiated in a turbulent flame brush by the mechanism of Khokhlov et al. (1999).

Acknowledgements

This research was supported by the Fifth Framework programme of the European Commission under the Energy, Environment and Sustainable Development, Contract No EVG1-CT-2001-00042 EXPRO. Theoretical part of this study was partially supported by the Russian Foundation for Basic Research (project No 05-03-32931-a).

References

Brown CJ, Thomas GO (2000) Experimental studies of ignition and transition to detonation induced by the reflection and diffraction of shock waves. Shock Waves 10: 23-32

Chan CK, Greig DR (1988) The structures of fast deflagrations and quasi-detonations. In: Proc 22th Symp (Intern) on Combustion, The Combustion Institute, pp 1733-1739

CV (2004) Explosion Dynamics Laboratory. CV - Constant volume explosion simulation program. http://www.galcit.caltech.edu/EDL/public/tools.html

Khokhlov AM, Oran ES (1999) Numerical simulation of detonation initiation in a flame brush: the role of hot spots. Combustion and Flame, **119**: 400-416

Khokhlov AM, Oran ES, Thomas GO (1999) Numerical simulation of deflagration-to-detonation transition: the role of shock–flame interactions in turbulent flames. Combustion and Flame, **117**: 323-339

San Diego (2003) Chemical-Kinetic Mechanisms for Combustion Applications 20030830. http://maemail.ucsd.edu/~combustion/cermech/

Teodorczyk A., Lee JHS, Knystautas R (1988) Propagation mechanism of quasi-detonations. In: Proc 22th Symp (Intern) on Combustion, The Combustion Institute, pp 1723-1731

Thomas GO, Ward SM, Williams RL, Bambrey RJ (2002) On critical conditions for detonation initiation by shock reflection from obstacles. Shock Waves **12**: 111–119