Transition to Quasi-Detonation via Shock – Obstacle Interaction

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1 Introduction

The mechanism of transition from fast supersonic flame to detonation in obstacle-filled tubes is a subject of numerous investigations during the last two decades. The key event of the deflagration-to-detonation transition (DDT) is a violent local explosion behind a leading shock wave supported by the accelerating flame. The photographic studies of the DDT have revealed complicated wave pattern ahead of the combustion front. An interpretation of the visualizations is hampered by the multiple interactions of shock with repeated obstacles (e.g. orifice rings), and usually the results of a limited set of experiments give no way of deducing general DDT laws.

Nevertheless in some cases the employment of simple criteria enables to gain insight into the DDT mechanism. In the previous work [1] we used a criterion suggested by Thomas et al. [2] (condition of detonation initiation by shock reflection from an obstacle) for description of different DDT modes observed in hydrogen-hydrocarbon-air mixtures. The goal of the current investigation is further development of the parameters suited for examination of hydrogen-air DDT experiments.

2 Thomas' Criterion and Associated Relationships

The explosion, which triggers a detonation, is generally associated with a strong mode of auto-ignition due to the interaction of a leading shock with the obstacle. According to Thomas et al. [2] if the reflection of a planar shock wave at a local obstacle is considered then a necessary condition for the consequent development of a detonation is that the induction time τ_i in the gas heated by a reflected shock will be less than the characteristic time of lateral expansion which necessarily occurs due to the finite size of the obstacle. In a circular tube the rarefaction wave (RW) propagates along upstream surface of the obstacle from the edge (orifice) towards sidewall. The RW starts to propagate immediately after shock reflection and temperature fall in the RW prevents combustible mixture from an auto-ignition. The velocity of the head of rarefaction wave is equal to the sound speed a_R behind the non-reactive reflected shock and the characteristic cooling time is defined as h/a_R, where h is obstacle height. Thomas' parameter is as follows:

$$\eta = \frac{h}{a_R \tau_i}, \qquad (1)$$

In accordance with [2], a critical condition, below which direct initiation of detonation might not occur, could be expressed as $\eta < 1$.

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Note that an orifice ring with a blockage ratio of BR mounted inside a tube of D_0 in diameter represents an obstacle of the following height: $h = D_0 \dfrac{1-\sqrt{1-BR}}{2}$. Thus, the η parameter is strongly scale-dependent.

The program for simulation of constant volume explosion developed by group of Prof. J. Shepherd (http://www.galcit.caltech.edu/EDL/public/tools.html) was used for the induction time calculations. The Konnov chemical-kinetic mechanism (Release 0.5, http://homepages.vub.ac.be/~akonnov/) was found suitable for the evaluation of induction time both in hydrogen-air and hydrocarbon-air mixtures. It should be emphasized that the initial conditions for calculations of τ_i are restricted to the parameters behind the reflected shock wave, namely pressure p_R and temperature T_R. Particularly, it is convenient to express both pressure and temperature in terms of Mach number M of an incident shock wave. The pairs of $p_R(M)$ and $T_R(M)$ values constitute limited field of initial conditions and it offers scope for building reliable analytical expressions for calculation of induction time. We obtained the following relationship for practically important case of (7–70%) hydrogen in air mixtures at initial pressure of 1 bar:

$$\tau_i = \frac{200}{[H_2]^{0.7} T_R^3} \exp\left(\frac{23000}{T_R}\right), \tag{2}$$

where τ_i – in μs, T_R – in K, $[H_2]$ – mole fraction of hydrogen in air. The expression (2) is recommended for the Mach numbers ranged between 2.2 and 3.2.

The above relations can be added by correlation between sound speed a_R and Mach number M:

$$a_R \approx a_0 \left[1 + 0.6(M-1)\right] \tag{3}$$

Here a_0 is sound speed in an undisturbed mixture, the ratio of specific heats is assumed to be constant ($\gamma = 1.4$). A simplified expression for T_R is as follows:

$$T_R = T_0 \left(\frac{a_R}{a_0}\right)^2 = T_0 \left[1 + 0.6(M-1)\right]^2 \tag{4}$$

Thus, the relationships (1)-(4) represent implicit analytical dependence of parameter η on Mach number of a leading shock in the case of different hydrogen – air mixtures at initial pressure of 1 bar and initial temperature of T_0. Mach number of M_c corresponding to the condition $\eta = 1$ will be referred as a critical intensity of shock at which rarefaction wave starts to prevent ignition behind the reflected shock.

3 Analysis of Hydrogen - Air DDT Experiments

The experiments [3-5] in the obstacle-filled tubes revealed distinct modes of explosion process in combustible gaseous mixtures. Different propagation velocities feature these modes. The attention of the present research is focused on the transition from a choked regime (where the flame speed is comparable with the sound speed of the combustion products c_{SP}) to a quasi-detonation regime (with a velocity between c_{SP} and Chapman-Jouguet detonation velocity D_{CJ}).

Figure 1 represents the results of experiments [3-5] on measurements of terminal flame velocities W in a wide spectrum of hydrogen-air mixtures in tubes equipped by the equidistantly placed circular orifice rings. Solid symbols denote quasi-detonation regimes in accordance with an interpretation given by the authors of [3-5]. Full curves in Fig.1 represent c_{SP} and D_{CJ} values.

The dashed and dotted lines in Fig.1 represent the calculated values of critical shock velocity $W_c = M_c\, a_0$. Calculations were performed for different h values taken from [3-5]. As it is seen from Fig.1 the calculated curves describe satisfactorily the lower limit of the quasi-detonation velocity. The W_c – $[H_2]$ dependences exhibit progressive rising in contrast to the sound speed in combustion products. As it could be expected a minimum absolute difference between W_c and c_{SP} parameters is observed in the vicinity of stoichiometric mixture that is

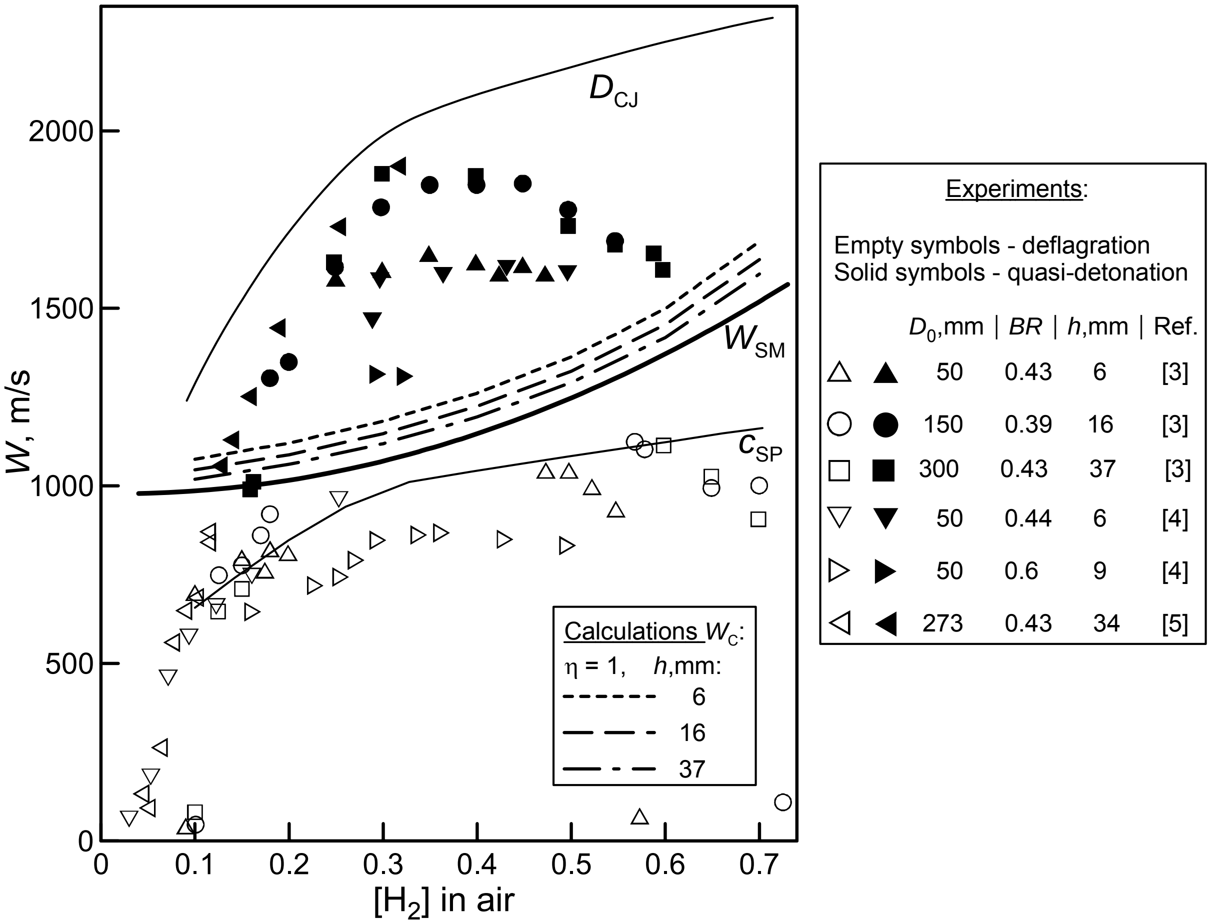

Fig. 1

the most sensitive to DDT. In spite of the fact that the reflection of a planar shock followed by accelerating flame presents someway idealized situation, the application of Thomas' criterion clearly demonstrate fundamental difference between choking regime of flame propagation and quasi-detonation. Overall spectrum of quasi-detonation velocities fall into the area where the fresh mixture will be ignited due to shock reflection, while characteristic speeds of the choking regimes are not high enough to provide ignition at reflection of a shock supported by flame.

The critical velocity W_c (and, correspondingly, critical Mach number) slightly decrease with the increase of the obstacle height. However, this decrease has clear physical limit. As it is known, weakening of the (reflected) shock wave leads to the change of the self-ignition mode, namely, from strong to mild ignition. Meanwhile, strong ignition mode plays a crucial role in the propagation mechanism of quasi-detonation. For description of the boundary between mild and strong ignition modes we will use criterion suggested in [6]:

$$\left(\partial\tau_{\mathrm{i}}/\partial T\right)_p = -2\mu\mathrm{sec}/^\circ\mathrm{K} \tag{5}$$

This known criterion was developed for stoichiometric hydrogen-oxygen mixtures at pressure less than 3 bar. However, we checked that it works rather well for hydrogen-air mixtures at pressures between 20 and 50 bar, i.e. in the range under investigation. At the first stage of the evaluation procedure the Eq.(2) is used for determination of the value T_R meeting the condition given by Eq.(5). Then the obtained T_R parameter is considered as temperature under the reflection of the shock wave of velocity W_{SM} i.e. critical velocity for transition between strong and mild ignition regime. The dependence of W_{SM} velocity on hydrogen concentration is shown in Fig.1 by heavy line. Note, that the W_{SM} parameter can be interpreted in two ways. On the one hand it can represent a minimum velocity of a quasi-detonation. On the other hand the value W_{SM} offers the criterion for DDT as a velocity of leading shock wave that should be attained for radical modification of the flow pattern and transition to quasi-detonation.

4 Concluding Remarks

The criterion on the detonation initiation by shock reflection from obstacles suggested by Thomas et al. [2] was applied to analysis of hydrogen – air experiments on DDT in obstructed tubes. For the sake of convenience it was developed analytical procedure of the estimation of critical intensity of shock wave for ignition of combustible mixture under shock reflection. The Thomas' criterion was added by the analytical procedure of estimation of the boundary between mild and strong ignition modes expressed in terms of critical shock wave speed. It was demonstrated that all criteria adequately describe the boundary between choking regime of flame propagation and quasi-detonation. The developed procedure can be used for evaluation of DDT conditions and propagation of quasi-detonation in an obstructed tube.

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