Criteria for Deflagration-to-Detonation Transition in Hydrogen-based Gaseous Mixtures

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ABSTRACT

The paper proposes a technique for assessment of critical conditions determining the possibility of deflagration-to-detonation transition (DDT) inside confined vessels filled with hydrogen-based gaseous mixtures. It is known that the chocked flame regime is the necessary step to the deflagration-to-detonation transition in channels. Here the analysis of the chocked flame structure allows defining its stability conditions on the basis of a simple parametric study. The evolution of chocked flame in the stable mode leads to additional flame acceleration finalised with DDT taking place at the flame front. The unstable mode determines the formation of the quasi-steady flame propagating with near-sonic speed. It is found that the proposed parametric study allows assessment of the critical conditions with a fine enough accuracy for the case of smooth channels. However, in flame acceleration inside obstructed channels, the stable mode of chocked flame propagation is limited in time, due to the multidimensionality of the flow patterns formed inside the channel. As a result, one does not observe DDT at the flame front under such conditions. The main scenario of DDT developed inside an obstructed channel is self-ignition in the region of deceleration of supersonic flow by the obstacles. Due to this, to obtain good enough predictions of DDT possibilities inside obstructed channels one should jointly apply the parametric analysis of the chocked flame stability with the geometric criterion (such as the Thomas criterion). This paper demonstrates that such an approach provides good enough predictions of DDT limits for a given mixture, its state and geometry of the vessel.

KEYWORDS: transient combustion, flame acceleration, detonation, hydrogen safety.

INTRODUCTION

Uncontrolled release of hazardous combustible mixtures of gases often leads to emergency situations. To provide adequate risk assessments and confirm the reliability of elaborated mitigation concepts one should understand all the possibilities related to the gaseous explosions. The simplest and most probable scenario of gaseous explosion evolution in well-stirred mixtures is the deflagration. The crucial feature of the deflagration regime is that the hot combustion products expansion causes compression and motion of the fresh mixture. Inside closed volumes, this leads to the increase in pressure and the non-stationary dynamics of the flame. The most hazardous scenarios of non-steady deflagration are associated with significant flame acceleration and corresponding generation of shock waves or even the onset of detonation [1]. In this regard, it is important to predict the limits of different combustion regimes for explosive safety issues.

The main goal of this paper is to formulate the classification of hazardous regimes resultant from flame acceleration including deflagration-to-detonation transition (DDT) and to determine the critical conditions for their successful establishment. For this, the analysis of possible transient combustion regimes taking place in confined vessels filled with gaseous combustible mixtures was carried out. The paper presents the classification of conditions appropriate for the formation of

Proceedings of the Ninth International Seminar on Fire and Explosion Hazards (ISFEH9), pp. 314-320
Edited by Snegirev A., Liu N.A., Tamanini F., Bradley D., Molkov V., and Chaumeix N.
Published by St. Petersburg Polytechnic University Press
ISBN: 978-5-7422-6496-5 DOI: 10.18720/spbpu/2/k19-139

different high-speed combustion regimes, including DDT on the basis of the structure and stability analysis of the flame at different stages of its evolution. The technique for estimation of DDT criteria is formulated and approved in an example of hydrogen-based mixtures filling the smooth and obstructed channels [2].

FUNDAMENTALS

It was recently demonstrated in [3] that the necessary condition for successful DDT is the formation of the so-called chocked flame in the process of flame acceleration. The structure of the chocked flame is determined by the gas-dynamic conditions of its formation and characterized by a permanent compression in the reaction zone at the stage of significant flame acceleration up to trans- or even supersonic speeds [3].

There are two possibilities of chocked flame development: stable and unstable. The evolution of chocked flame in the stable mode leads to additional flame acceleration finalized with DDT taking place at the flame front. The unstable mode determines the formation of the quasi-steady flame propagating with near-sonic speed. In view of this, it becomes possible to propose a parametric problem setup allowing estimation of a DDT possibility, depending on the stability condition for the chocked flame evolved in the mixture of given composition, at a given initial state. Since the mixture state directly ahead of the accelerating flame front changes in time almost via Hugoniot curve [3, 4], there is a simple relation between the initial conditions and those established at the stage of flame chocking. According to this, one can obtain an unequivocal criterion of DDT, knowing only the initial conditions [5]. Such a criterion by its essence is not related with the outer factors such as geometry (purely chemical criterion) and therefore can be fully utilized only for simple cases, such as flame acceleration inside a smooth channel.

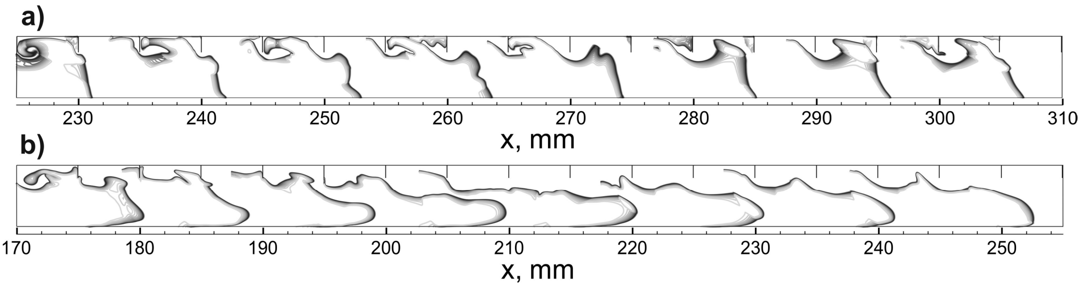

Fig. 1. Flame front evolution in the process of accelerated flame propagation through the obstructed channel filled with 32.5 % hydrogen-air mixture. Channel width – 1 cm, (a) BR = 0.25, max($U_{f,L}$) = 1100 m/s, t = 300-370 μs, Δt = 10 μs, (b) BR = 0.2, max($U_{f,L}$) = 1300 m/s, then DDT takes place, t = 320-390 μs, Δt = 10 μs. The results of 2D numerical simulations are presented for the upper half of the channel.

The stable mode of chocked flame propagation through the obstructed channel is limited in time due to the multidimensionality of the flow patterns formed inside the channel [3]. Thus, for example, in the case presented in Fig. 1b the stage of the chocked flame lasts only ~60 μs. During this period a quasi-steady flow pattern in the vicinity of the flame front is established [3] that determines the negligible effect of transversal flows on the leading edge of the flame front. After this short period, the transverse waves generated by the accelerating chocked flame begin to affect the flame propagation. The stage of chocking flame propagation ends. Due to this, as a rule, one does not observe DDT at the flame front in such conditions. The main scenario of DDT developed inside the obstructed channel is self-ignition in the region of deceleration of supersonic flow by the obstacles. In the case presented in Fig. 1a no conditions for chocking flame propagation is established. The flame propagation is strongly affected by the transverse flows, so permanent oscillations are observed at of the leading edge in the transverse direction. In wider channels, this effect decreases and one can observe DDT [2, 6, 7] for the same mixture via the mechanism in the case presented in Fig. 1b.

The possibility of self-ignition on the obstacle surface is related to the mixture state achieved in the region of flow deceleration after interaction with the obstacle. In [8, 9] it is demonstrated that the so-called Thomas criterion [10] is applicable for the estimation of DDT possibility as a result of shock wave reflection from the obstacle surface. According to this criterion, the self-ignition becomes possible if the induction delay (τ_{ind}) occurs to be shorter than the characteristic time of gas-dynamical rarefaction (h/a, where h is a characteristic height of the obstacle and a is the local sonic speed). In the three-dimensional case considered experimentally the characteristic height of the obstacle was calculated as a function of tube diameter (D_0) and blockage ratio (BR).

Joint application of the parametric analysis of the chocked flame stability, the geometric criterion for chocking conditions in obstructed channels, and the geometrical criterion of successful DDT (such as the Thomas criterion) and should provide good enough predictions of DDT limits for a given mixture, its state and geometry of combustor.

NUMERICAL TECHNIQUES

In the framework of this paper, three types of calculations were carried out. The parametric study of the chocked flame stability was carried out using the one-dimensional calculations of the one-dimensional flame freely propagating through the reactive mixture of given composition at given thermodynamic state. For analysis, the following parameters were determined from the one-dimensional steady solution: burning rate (u_f) and sonic speed in the combustion products (a_b). To analyze the peculiarities of flame evolution at the final stage of its acceleration a set of two-dimensional axisymmetric calculations were carried out. According to the considered problem setup the flame was initiated at the closed end of cylindrical channel and then propagated towards its opened end with acceleration. To estimate the possibility of deflagration-to-detonation transition inside the obstructed channel the induction periods were calculated according to the zero-dimensional problem setup.

More details for each set of calculations are presented below. All three types of calculations (one-dimensional, two-dimensional and zero-dimensional) were carried out, employing the same software platform. The gas-dynamical solutions were obtained with the use of Euler-Lagrangian numerical technique which allows accurate solution when using high enough spatial resolution of the computational domain. This technique has been frequently utilized by the authors for one-, two- and three-dimensional analyses of the phenomena of transient flame propagation [3]. To reproduce chemical kinetics of hydrogen oxidation a contemporary kinetics model [11] was applied.

RESULTS

Parametric study

According to recently established patterns concerning the chocking flame structure [3], the stability of the chocked flame can be formulated in the following way. As soon as the compression inside the reaction zone begins to provide a faster burning rate growth than the corresponding increase in the local sonic speed the flame starts to outrun the compression waves irradiated from the reaction zone. Here, the flame speed $U_{f,L} = u + u_f$, where u is the flow velocity ahead of the flame front and u_f is the burning rate, herewith according to the chocking condition u ~ a_b, where a_b is the sonic speed in the combustion products [3]. The variation of the flame speed under the compression inside the front of the chocked flame can be assessed as $\Delta U_{f,L} \approx \Delta u_f$. At the same time, the forward propagation of compression waves, generated in the reaction zone, is characterized by the speed ~ ($a_b + u_b$), where u_b is the flow velocity inside the flame front. Here it should be noted that there is a change in the flow direction at the flame front. The flow ahead of the flame front is pushed by the expanding combustion products in the forward direction, while the combustion products expand in the opposite direction. Due to this u_b is has a value close to zero, or at least $u_b << a_b$. Hence the maximum speed of compression waves propagation can be estimated as a_b, and its variation under the compression is Δa_b. According to this, as soon as the chocked flame is formed ($u \sim a_b$) and Δu_f becomes larger than Δa_b the additional flame acceleration joint with the compression inside the reaction zone takes place. As a result, the shock wave is formed on the scales of the reaction zone, that triggers the detonation onset. If the criterion $\Delta u_f > \Delta a_b$ is not satisfied when the chocking conditions are set, then such additional acceleration is not possible, and further flame propagation is characterized by a quasi-steady flame speed of the order of a_b.

According to the formulated above, the DDT becomes possible only if the criterion $\Delta u_f > \Delta a_b$ is achieved before the criterion $u = a_b$ does. As mentioned above, the compression can be treated by the Hugoniot relation. Therefore, a simple parametric study can be formulated. Let us calculate the values of burning rate (u_f) and sonic speed in the combustion products (a_b) along the Hugoniot curve corresponding to the mixture of given composition at given initial state: $p = p_H(u) = p_H(u, p_0, T_0)$. The calculations can be taken from the one-dimensional numerical analysis of the laminar flame propagating through the mixture at the thermodynamic state calculated along Hugoniot curve: p_H, T_H. As a result, the following diagram (Fig. 2) in coordinates (p, u) can be plotted. The dash-dotted line represents the criterion $u = a_b$, while the solid line represents the criterion $\Delta u_f = \Delta a_b$. Therefore, all the initial states above the Hugoniot curve (1) correspond to the stable regimes of chocking combustion and as a result, the DDT can take place in the considered mixture at a given initial thermodynamic state. All the initial states below this curve correspond to the unstable choking flames that lead to the formation of quasi-steady supersonic flames. According to this analysis, it is found for a stoichiometric hydrogen-air mixture, that there is a critical initial pressure p_0 = 0.04 MPa (or 0.4 atm), at which the DDT becomes possible. This result correlates well with the critical pressure p_0 = 0.042 MPa value obtained experimentally in [12].

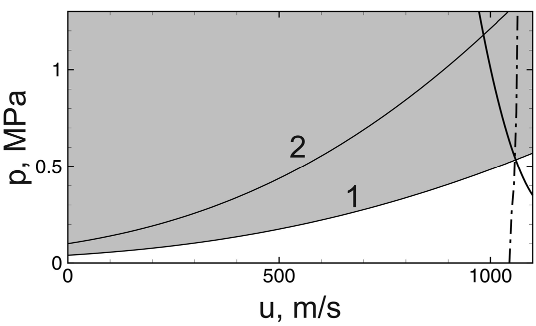

Fig. 2. Diagram of possible regimes in stoichiometric hydrogen-air mixture at initial temperature 300 K and different initial pressures. Solid line – criterion $\Delta u_f = \Delta a_b$. Dash-dotted line – $u = a_b$. 1 – critical Hugoniot curve passing through the initial state point with p_0 = 0.04 MPa. 2 – Hugoniot curve passing through the initial state point with normal pressure (p_0 = 0.1 MPa). Grey region – stable chocked flames, DDT is possible. White region – unstable chocked flames and quasi-steady supersonic flames.

Analysis of numerical results for flame acceleration in a smooth channel

Consider the behaviour of the multidimensional solution for an accelerated hydrogen-air flame obtained in two-dimensional calculations in the conventional problem setup (see e.g. [3]). The flame acceleration is studied in the stoichiometric hydrogen-air mixture at 300 K initial temperature, and different pressures above and below the criterion obtained from the analysis of Fig. 2. Figure 3 presents the regimes of flame propagation at initial pressures 0.02 and 0.1 MPa. As can be seen, at the normal initial conditions the formation of stable chocked flame in the process of flame acceleration inside the smooth channel is possible. As a result, the DDT occurs during ≈ 100 μs after choking conditions are established (Fig.3a).The parameters of the flow evolve along the Hugoniot curve, as can be seen from Fig. 3b. In case of low initial pressure below the above mentioned criterion of 0.04 MPa one can observe the formation of quasi-steady high-speed flame propagating with the flame speed ~1100 m/s (Fig. 3a). Flow parameters change in time periodically (Fig. 3b) along the corresponding Hugoniot curve, with pressure oscillations of magnitude ~0.01–0.02 MPa, and velocity oscillations of magnitude ~40 m/s.

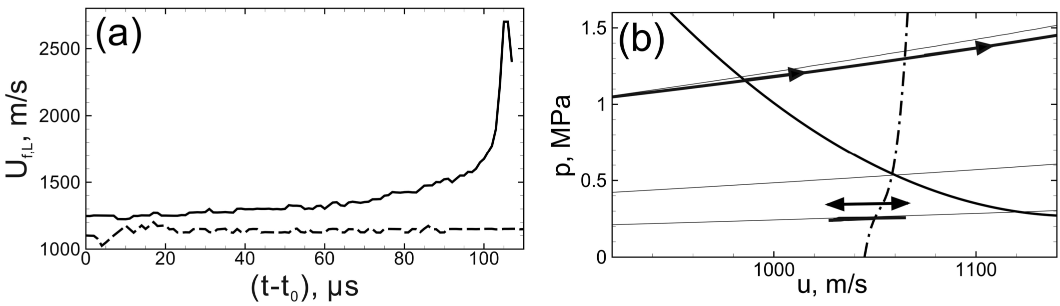

Fig. 3. (a) Histories of the flame speed at the stage of chocked flame starting at time instant t = t_0. Solid line – DDT, initial pressure 0.1 MPa. Dashed line – quasi-steady high-speed flame, initial pressure 0.02 MPa. (b) Evolution of flow parameters (pressure at the flame front and flow velocity exactly ahead of the flame front) at the background of criteria presented in Fig. 2. Solid line – criterion $\Delta u_f = \Delta a_b$. Dash-dotted line – $u = a_b$. Thin lines are the Hugoniot curves for initial pressures 0.02, 0.04, and 0.1 MPa. Results of 2D calculations are presented by red lines.

Geometrical criterion for obstructed channels

Now let us consider the concentration limits of chocked flame stability. Figure 4 demonstrates the flame speed diagram for hydrogen-air mixtures with various hydrogen contents. It is obvious that the DDT region obtained in the process of parametric study (thick solid line) is much narrower compared with experimental data. However, it should be noted that experimental data represented in Fig. 4 correspond to the flame propagation through the obstructed channel while the parametric study concerns only chemical criteria independent of channel geometry. According to the presented data, one can only conclude that as soon as the chocking conditions realized in the obstructed channel the further flame acceleration and DDT are possible only in the relatively narrow range of hydrogen content. Out of this range only quasi-steady transonic flame can be formed.

Actually, the data presented by a thick solid line in Fig. 4 provides hydrogen content at which the chocked flame can be additionally accelerated, that subsequently can cause detonation onset directly at the flame front. However, such a scenario of DDT is at least quite rare in obstructed channels. In most of the cases considered experimentally, one can observe independent self-ignition events taking place at the surface of obstacles ahead of the flame front that in turn can cause DDT [3, 13]. The possibility of self-ignition is related to the mixture state achieved in the region of flow deceleration after interaction with the obstacle [8-10].

For both possible regimes (of stable and unstable chocking flames) the parametric analysis provides the data on the mixture state directly ahead of the flame. Moreover, this state is rather close to that calculated via Hugoniot relations. Due to this one can estimate the particular mixture state exactly ahead of the flame front via Hugoniot relations for the state u = a_b. Taking this into account it is easy to estimate the mixture state in the region of flow decelerated by the obstacle. Afterwards, the induction delay (τ_{ind}) and sonic speed (a) can be calculated. And finally taking into account the data on the tubes width and blockage ratio one can estimate the Thomas criterion and assess the limits where the chocked flame can produce self-ignition ahead of its front in the process of flame propagation through the obstructed channel.

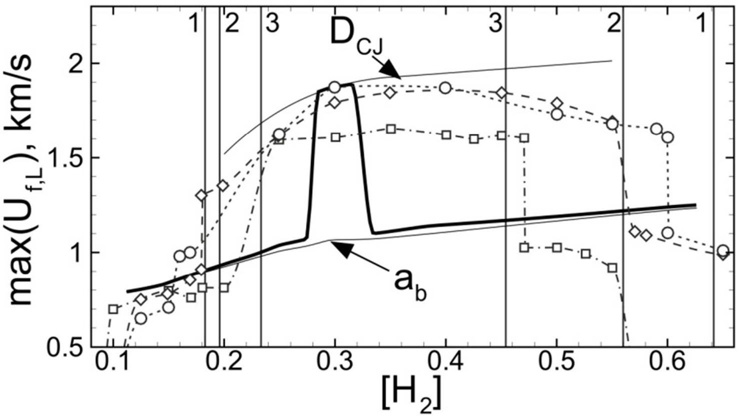

Fig. 4. Diagram of high-speed flame regimes in hydrogen-air mixtures with different hydrogen content. Signs connected with thin dashed lines represent the experimental results [2]. Thick solid line – maximal flame speeds estimated on the basis of the proposed set of chemical criteria. Vertical lines represent the joint implementation of chemical criterion with geometrical one.

The criteria estimated with the formulated technique are plotted in Fig. 4 along with the experimental data. One can clearly see that the obtained critical conditions are in a good agreement with the available experimental data that confirm the correctness of the proposed technique. Without a doubt, there are uncertainties in experimental setups and measurements, and there could be uncertainties in chemical kinetics models and calculations used for the parametric study. However, the predictions are in a rather good accordance with the experimental data, so it can be concluded that all the basic features of the flow and the flame evolution are described accurately. Thus, for example, in recent work [7], for specific geometry, the DDT concentration limits are reported as 19 % and 57 % of hydrogen in the mixture. Proposed technique provides the values of 20 % and 51 % correspondingly.

CONCLUSION

To conclude let us formulate the main ideas underlying the basis of the proposed technique for the estimation of DDT criteria.

- The chocked flame regime is the necessary step to the deflagration-to-detonation transition in channels and other confined vessels filled with gaseous combustible mixtures.
- Analysis of the chocked flame structure allows defining its stability conditions on the basis of the simple parametric study. The evolution of chocked flame in the stable mode leads to additional flame acceleration finalized with DDT taking place at the flame front. The unstable mode determines the formation of the quasi-steady flame propagating with near-sonic speed.
- The stable mode of chocked flame propagation through the obstructed channel is limited in time due to the multidimensionality of the flow patterns formed inside the channel.

Therefore, as a rule, one does not observe DDT at the flame front in such conditions. The main scenario of DDT developed inside the obstructed channel is the self-ignition in the region of deceleration of supersonic flow by the obstacles.

- Joint application of the parametric analysis of the chocked flame stability and the geometric criterion (such as Thomas criterion) provides good enough predictions of DDT limits for given mixture, its state and geometry of the vessel.

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