

# On the mechanisms and criteria of deflagration-to-detonation transition in gases

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**Abstract.** The origins of different supersonic combustion regimes in channels are discussed. It is shown that the evolution of supersonic flames including the formation of quasi-steady supersonic flames, transition to detonation directly at the flame front and auto-ignition inside the kernels at some distance ahead the flame front are fully determined by the same gasdynamical effects and peculiarities of combustion kinetics. Three basic criteria are formulated aiming to establish correlation between the initial state of the gaseous combustible mixture and the possibility of deflagration-to-detonation transition. Formulated criteria are in an adequate agreement with the data on combustion of hydrogen-based mixtures.

## 1. Introduction

One of the most important unresolved questions of contemporary theory of combustion and detonation is the determination of criteria for deflagration-to-detonation transition (DDT), which is of primal interest for perspective technical systems design as well as for the safety control of their operational regimes. It is known that in most active gaseous mixtures such as hydrogen-oxygen, acetylene-oxygen, ethylene-oxygen etc. the flame propagating through the channel with acceleration is able to cause detonation onset on relatively small spatial-time scales even in short and narrow channels (see e.g. [1, 2, 3]). In less reactive mixtures, including hydrogen-air and hydrocarbon-air mixtures, the sufficient flame acceleration becomes possible only inside wide obstructed channels and only on rather large distance [4, 5]. However, it should be noted that even in such conditions the DDT is not intrinsic to all the mixtures. The resulting regime alternative to detonation onset is a quasi-steady flame propagation with trans- or supersonic speed. Such regimes are experimentally observed in lean and rich mixtures [4, 5] as well as in mixtures under low pressure [6]. In addition, in low-reactive mixtures [7] and high-reactive mixtures at low pressure [8] one can also observe the formation of auto-ignition kernels at the distance ahead the propagating flame. In number of cases such localized auto-ignition becomes origin of detonation wave formation that is one of the mechanisms of DDT together with the mechanism of detonation onset directly on the flame front observed in high-reactive mixtures. Earlier in [9] the mechanism of DDT directly on the flame front was formulated and described on the example of stoichiometric hydrogen-oxygen mixture on the basis of available experiments interpretation and high-precision numerical simulations. Further investigations partly reviewed in [10] allowed us to understand physical and chemical mechanisms determining the evolution of combustion waves propagating through the channels, including



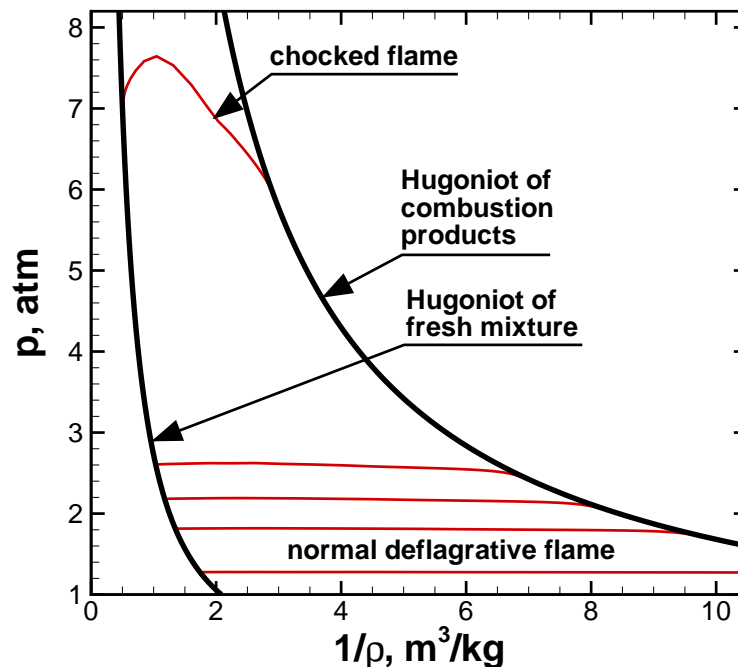
flame acceleration up to sonic and supersonic speeds and two mechanisms of DDT. The present paper represents the basics of quantitative DDT criteria elaboration on the basis of recent work. All the considerations concerning DDT criteria discussed below are proved by means of high-precision numerical simulations. The calculations are carried out using one- and two-dimensional reactive CFD codes elaborated and approved in our previous papers (see e.g. [10, 11, 12] and citations within).

## 2. On the scenarios and criteria of DDT

Consider the primary features of flame propagation through the channel filled with combustible mixture under given temperature and pressure. Independently on the channel geometry, the main mechanism of flame acceleration is the combustion products expansion that cause the formation of compression waves transferring the energy and momentum to the flow. The accelerating flow drags the flame and cause its corresponding acceleration and stretching, that in turn determine the increase of the mass of combustible mixture burning per time unit. Independent on the channel geometry and the concrete mechanism of flame stretching, the positive feedback between flow acceleration and flame acceleration is establishing, that determine averagely exponential character of acceleration. However, according to the Vulis law of “inverse actions” [13] the acceleration of the flow inside the channel, with the continuous energy release inside the reaction zone, is limited by the velocity value equal to the sonic speed. Thus, on the basis of fundamental gasdynamical concepts it can be concluded that the maximal flow velocity of the reactive flow cannot exceed the sonic speed in the combustion products ( $\max(u_f) = a_b$ ). The corresponding upper limit for the flame speed (relative to the channel walls) is  $\max(U_{f,L}) = U_f + a_b$ , where  $U_f$  is the burning velocity (or the flame speed relative to the fresh mixture). It should be noted that at corresponding time instant the state of fresh mixture ahead of the flame is determined by the set of compression waves irradiated from the propagating flame during the whole process of flame acceleration before reaching the discussed limit ( $\max(u_f) = a_b$ ). Herewith depending on the mixture the burning velocity  $U_f(T, p)$  can vary sufficiently compare with one at initial conditions ( $T_0, p_0$ ).

As soon as the flame speed relative to the channel walls becomes supersonic ( $U_{f,L} > a_f$ , where  $a_f$  - sonic speed in the fresh mixture), the acoustic perturbations occur to be choked by the supersonic flow formed ahead. Due to this, such a regimes of flame propagation with supersonic speed are usually called “choked flames”. After a choked regime is established, the flow begins to decelerate according to the Vulis law, and this in turn provides additional compression of the fresh mixture inside the flame front. In such conditions the burning velocity changes ( $U_f = U_f(T, p)$ ), that can cause either additional flame acceleration or flame deceleration depending on the mixture chemical features. Generally the burning velocity  $U_f$  increases with temperature and is a non-monotonic function of pressure  $U_f \sim p^{(n-2)/2}$ , where  $n$  is a global reaction order changing with mixture composition, pressure and temperature. Therefore, an additional compression of the fresh mixture can cause progressive or intermediate flame acceleration or even deceleration of the flame. In first case, the additional acceleration causes corresponding compression on the scales of the reaction zone. A shock wave is forming, which together with a reaction front forms a detonation wave as it was reported in [9]. In case of insufficient burning velocity growth or its decrease, the gasdynamical mechanisms play the leading role and the flow velocity stagnates in the vicinity of gasdynamical limit ( $\max(u_f) = a_b$ ). Thereby experimentally observed oscillations of the flame speed are determined by the competition between gasdynamics and chemistry. This non-steady behavior of the flame propagation causes discrete generation of the compression waves driven by the pockets of compressed gas, outrunning from the flame front on the deceleration stages of choked flame evolution [12]. On the x-t diagrams illustrating this regime, one can observe sequence of shocks and contact surfaces propagating ahead the flame front [7]. In number of cases one can also

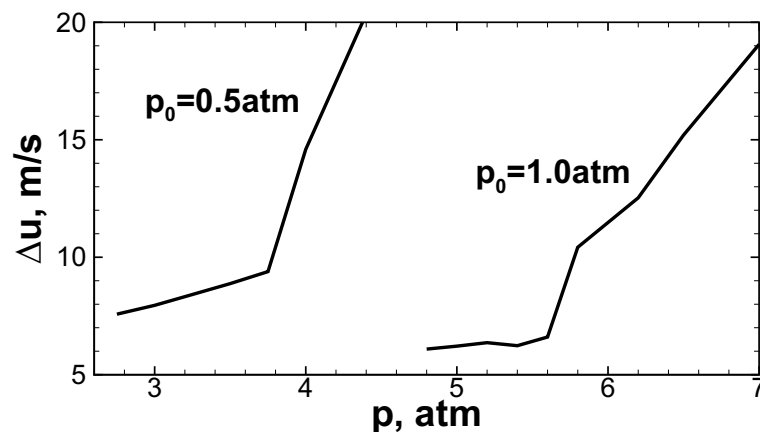
observe the auto-ignition kernels arising at these contact surfaces.



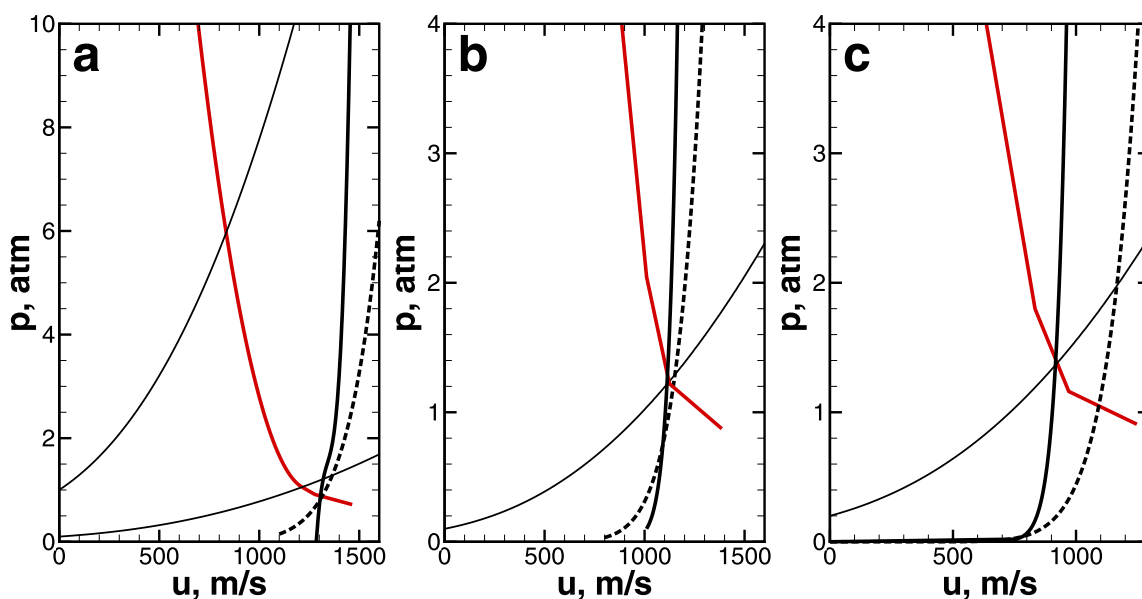
**Figure 1.** Hydrogen-oxygen flame front in  $p$ - $V$  coordinates at different stages of flame acceleration (red lines, presented at equally distant time instants). Thick black lines represent the Hugoniot curves for fresh mixture and combustion products.

The overall pattern described above includes all the regimes observed experimentally such as quasi-steady supersonic flames, DDT and auto-ignition kernels formation ahead the flame front. According to this, it can be concluded that all these phenomena have the same nature and can be described by the same basic mechanisms. Consider now the evolution of fresh mixture state during the whole process of flame acceleration. Figure 1 shows the calculated evolution of the hydrogen-oxygen flame acceleration through the two-dimensional channel in  $p$ - $V$  coordinates. The presented profiles illustrate the flame structures on the stages of normal deflagration and chocked flame propagation through the compressed medium. One can see, that the compression of the fresh mixture during the whole process takes place along the Hugoniot curve that can be also observed experimentally. Thus in [14] a rather wide review of experimental measurements of fresh mixture state for different mixtures is presented, that confirms the known fact, that the state of medium compressed by the sequence of compression waves corresponds to the state at Hugoniot curve. As the state of fresh mixture during the whole process of flame acceleration is described adequately by the shock-wave compression, we have assumed that it is rather convenient to elaborate the DDT criteria along the Hugoniot curve that will allow us to get correlation between the initial state  $(T_0, p_0)$  of the considered mixture and the probability of DDT.

As it was already discussed above, the additional compression of the fresh mixture ahead of the chocked flame causes the change of the burning velocity and as a result the additional acceleration of the flow. Herewith, additional compression of the fresh mixture results in increase of local sonic speed that in turn determines the critical flow velocity. Taking this issue into account it can be shown that the criterion exists beyond which the flame acceleration mechanism due to chemical reaction begins to play the leading role in contrast with the gasdynamical one. If



**Figure 2.** Values of flow velocity variation due to combustion kinetics depending on the pressure characterizing the state on the Hugoniot curve. Two curves represent data for two different initial conditions ( $p_0=0.5$  and  $1.0\text{atm}$ ).



**Figure 3.** Diagram for determination the possibility of different supersonic combustion regimes of stoichiometric hydrogen-oxygen (a), equimolar hydrogen-oxygen (b) and stoichiometric hydrogen-air (c). Thick black lines - gasdynamical velocity limits. Red lines - criteria of additional supersonic flame acceleration due to peculiarities of chemical kinetics. Dashed lines - “crossover”. Thin lines - Hugoniot curves corresponding to different initial pressures: (a) - 1.0 and 0.1atm, (b) 0.11atm, (c) 0.2atm.

the variation of burning velocity ( $\Delta U_f$ ) under additional compression becomes greater than the corresponding variation of sonic speed ( $\Delta a_f$ ), the leading role in the following flame acceleration will switch to the mechanism of reaction intensification with compression. If this criterion is not satisfied, the flow will accelerate via gasdynamical mechanism up to the critical gasdynamical velocity scale equal to  $a_b$ . Note that due to the additional compression the sonic speed is rising

with temperature as  $a_f \sim \sqrt{T}$ , while the burning velocity is defined by non-monotonic function of temperature and pressure. Thus, for example, in hydrogen-oxygen mixture compressed via shock Hugoniot from the initial normal conditions ( $p_0 = 1\text{atm}$ ,  $T_0 = 300\text{K}$ ) as well as from the state with lower pressure the function  $U_f(T, p)$  changes its rate of increase at some critical state realized along the Hugoniot compression curve (see figure 2). Therefore, along every Hugoniot curve built for different initial conditions one can obtain the criterion beyond which the features of chemical reaction determine additional flame acceleration even if the flow velocity has reached the gasdynamical threshold. To obtain this criterion quantitatively, it was proposed to solve the following problem. We studied numerically the stability of converging initially supersonic flow with combustion front propagating in it. The numerical setup was as following. A spherically symmetric domain was initially divided in three regions: (1)  $r < R_0$  - fresh mixture at initial temperature and pressure ( $T_0$  and  $p_0$ ), (2)  $R_0 < r < R_1$  - ignition kernel containing the fresh mixture at elevated temperature, (3)  $r > R_1$  - high pressurized driver gas at pressure  $p_1$  and temperature  $T_0$ . Discontinuity decay at  $r = R_1$  provided a converging flow of compressed gas. A reaction front was formed in the vicinity of the contact surface and propagated from the ignition kernel towards the fresh mixture. The solution of considered problem qualitatively reproduces all the features intrinsic to the supersonic reactive flow in channel. In both cases, the flow is continuously decelerating, that provides compression of the fresh mixture before burning inside the flame front. Criteria obtained numerically in such a way for hydrogen containing mixtures are presented in figure 3 by thick red lines. Thin lines represent some characteristic Hugoniots and thick black lines represent the gasdynamical criterion  $u_f = a_b$ . According to the obtained diagrams it can be concluded, that there are two basic opportunities: 1) if the flow accelerates up to the gasdynamical criterion prior the moment of reaching the state for which kinetics induces further acceleration of the choked flame than a quasi steady supersonic combustion regime will establish, 2) otherwise DDT can occur.

An important criterion for gaseous combustibles is the transition from so-called non-degenerate explosion to the degenerate one characterized by sufficiently fast induction period compared with the period of exothermal stage. In literature this criterion is also known as a “crossover” determining the balance between the chain branching and chain termination reactions. As the mixture state transits into the region of degenerate explosion, the burning rate of the fresh mixture can become of the order or even higher than that inside the flame front. In such a case, the mechanism of flame propagation switches from the normal deflagration to the combustion of the mixture reacting at the initial conditions [15]. Set of such “crossover” states is presented in fig. 3 by the dashed lines. According to the presented diagrams, there are two basic opportunities of supersonic combustion in the vicinity of “crossover”. In the first case, the supersonic flow continues to accelerate due to the features of chemical kinetics and achieves the state beyond the “crossover”. The independent ignition of the mixture ahead the flame front becomes possible, that can be observed experimentally as a local “spontaneous” acceleration of the flame front sheet. The auto-ignition kernel in such conditions is located in the gas directly ahead the contact surface pushing the flow, where the mixture occurs to be the most heated. In the considered case the role of this contact surface belongs to the flame front, and therefore the ignition visually almost cannot be separated from the primal flame front. The second scenario is realized when the flow first achieves the “crossover” state and then the gasdynamical velocity limit, however the chemical activity of the mixture is not enough to provide additional acceleration of the supersonic flow. In such conditions a quasi-steady regime of supersonic flame propagation takes place which is characterized by the downwind propagating shock waves followed by contact surfaces. As the state of mixture corresponds to the so-called degenerate explosion the contact surfaces driven by the additionally compressed gas can become the sources of auto-ignition kernels at some distance from the primal flame. Both regimes were obtained experimentally in [8] in the equimolar hydrogen-oxygen mixture at lowered pressure ( $\sim 0.11\text{atm}$ ).

It is interesting to note, that the regime with DDT on the flame front was also observed in this mixture that defines some instability which was not observed in stoichiometric hydrogen-oxygen mixture at normal initial conditions, also considered in [8], and for which only regime with DDT on the flame front was observed. As it can be concluded from fig. 3b, in case of equimolar hydrogen-oxygen mixture at pressure of 0.11atm, the flow achieves the gasdynamical velocity limit in the vicinity of intersection of all the three limits discussed above. Therefore because of experimental errors the possibility of three different regimes becomes possible. In stoichiometric mixture at higher pressures this instability was not observed experimentally [1, 2, 8, 16], that correlates with the results presented in fig. 3a. It should be also noted, that in less reactive mixtures and even in hydrogen-air mixture, there is no such a region in which the intersection of all the three criteria is observed. Thus in fig. 3c one can clearly see the limit between two possible regimes of DDT and quasi-steady supersonic flame propagation. According to fig. 3c quantitatively criterion equals to 0.2atm, that from our point of view agrees adequately with available experimental data. For example, in [17] an asymptotic increase of the pre-detonation distance was observed with the pressure decrease down to 0.3atm.

### 3. Conclusion

Three basic criteria were formulated aiming to establish correlation between the initial state of the gaseous combustible mixture and the possibility of DDT and the mechanism of its arising in channel. The first one is the gasdynamical velocity limit - the maximal flow velocity which can be achieved due to the flame acceleration through the channel. The second one is the critical state in which the features of combustion kinetics allow additional acceleration of the supersonic flow even if it has already exceeded the gasdynamical velocity limit. The third one is the so-called "crossover" determining the critical state in which the pre-flame kinetics starts to play a sufficient role, and alternative mechanisms of DDT become to be possible. Formulated criteria have demonstrated an adequate compliance with the data on combustion of hydrogen-based mixtures.

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