Modes of chocked flame instability and transition to detonation defined by the peculiarities of combustion kinetics at rising pressure

A.D. Kiverin, I.S. Yakovenko
Joint Institute for High Temperatures of RAS
Moscow, Russia

1   Introduction

For decades clear understanding of the non-steady and transient regimes of gaseous combustion remained to be a topical unresolved problem of the combustion theory. A large variety of combustion regimes can be observed experimentally, but the fast flames and detonations are of the primal interest because of their hazardous impact on the environment and their prospective implementation in the gas-combustion engines. The dynamics of combustion wave depends on the large number of factors of different physical and chemical nature that complicates setting the experiment and interpreting its results. The detailed and clear analysis is difficult first because of the limitations of experimental equipment usually used for studying dynamics of the reacting flows (pressure transducers, ion probes, one- and two-dimensional interference patterns). And second because of the difficulties in reproduction of the combustion regimes being investigated in different mixtures and/or different external conditions (initial pressure, temperature, channel geometry etc.). Thus in most of air-fuel mixtures or even in oxy-fuel mixtures at low pressures it is almost impossible to obtain flame acceleration up to the transition to detonation on the laboratory scales. To achieve higher intensities of acceleration and increase the probability of detonation onset in such mixtures it is common to use channel obstruction as a reliable technique of flow acceleration first proposed by K.I. Shchelkin. However as it can be observed in slowly reacting mixtures (see e.g. [1, 2]) the flame acceleration causes the detonation onset quite rarely. On the other hand, in highly reactive oxy-fuel mixtures (of hydrogen, acetylene, ethylene etc.) the detonation can be obtained even in smooth channels of relatively small width [3-6].

For today a large amount of experimental data on the different cases of accelerating flames evolution has been accumulated including data on deflagration-to-detonation transition, onset of the so-called chocked flames, quasi detonations, slow detonations etc. One should expect similar physical origins of all the possible transonic and supersonic combustion regimes as they arise in the quite close conditions: first the flame accelerates in the flow like a piston-driven one and then achieves the transonic chocked regime, which further evolution in some cases can provide the onset of the detonation. The analogy with the piston-driven flow seems to be adequate for almost all the experimentally studied cases. In the case of the flame propagation through the smooth channel out from the closed-end wall the flow is generated by the expansion of the hot combustion products behind the propagating flame front [7-9]. The compression waves irradiated out from the reaction zone

determine the peculiarities of flame-flow interactions and consequential flame acceleration. On the first stage the flame front is subjected to the continuous influence of the compression waves travelling through the combustion products and reflected from the closed-end wall, that determines the exponential manner of flame acceleration. The multidimensional gasdynamical effects are also of great importance on this stage defying the flame surface adaptation to the established flow field. Characteristic time scales of the first stage with multidimensional factors evolution and flame adaptation can be estimated as 0.1–1.0ms in order of magnitude (see e.g. [10-12]). Thereafter the second sub-exponential stage of flame acceleration begins. As the flame has passed relatively far away from the closed-end wall the influence of the compression waves coming from the closed-end wall becomes discrete. The reflected compression waves interact with each other and achieve the flame front in a form of stronger compression waves or even weak shocks [8] that in turn causes oscillatory flame propagation regime with high rate of flame stretching [9]. Finally the flame speed achieves the sonic speed in the mixture just ahead of the flame front and the chocked regime establishes. The chocked flame can also be formed in the smooth channel after the preliminary acceleration inside the obstructed region [13]. In such a case the pressurized combustion products as well as the reacting unburned packets of fresh mixture inside the obstructed region act like a piston providing flame propagation with a transonic speed or even further flame acceleration. One more interesting example is the flame emerged after the detonation diffraction or failure [14]. In this case the expanding detonation products act like a piston supporting further flame propagation. It should be mentioned that the last two cases can cause much more complicated flow patterns with multidimensional interference of the compression waves and shocks that in turn may trigger ignition of either deflagration or detonation in the fresh mixture independent on the primal flame front [15].

The aim of this paper was to study numerically and systematize the features of chocked flames formed in the piston driven flow depending on the mixture reactivity. We considered stoichiometric hydrogen-oxygen mixture at varying pressures as it was done before experimentally in [4] where different mechanisms of transition to detonation was observed in stoichiometric hydrogen-oxygen mixture at initial normal pressure (1.0bar) and in equimolar mixture at low pressure (~0.11bar).

2   Problem setup

As it was formulated above the chocked flames originate from the flames accelerated in the piston-driven flow. Therefore the intrinsic problem setup excluding complex multidimensional flow patterns is the flame propagating in the one-dimensional co-flow driven by the piston. In case of constant piston speed such a flame propagation regime is quasi stable as it was shown in [16]. The acceleration and formation of the chocked flame can be achieved by including two- or three-dimensional perturbations that cause the increase of the flame surface and its corresponding acceleration [9] (it can be achieved in simulations by applying the non-slip boundary conditions on the side walls). Such conditions can be established in the shock tube where the high pressure chamber is filled with inert media, the low pressure chamber is filled with reacting media and the ignition is initiated in the very vicinity of the diaphragm section between two chambers. The expansion of the inert gas drives the flow of the reacting gas together with the flame front. One may face some difficulties with the synchronization trying to reproduce such an experimental setup however in numerical simulations such a problem setup is rather simple and flexible.

As it was shown recently in [12] the pattern of the process evolving in two-dimensional channel is qualitatively similar to the real three-dimensional one. Therefore here we present results of two-dimensional modeling inside the channel with non-slip walls. To resolve chemical kinetics we used reduced kinetic scheme from [17]. Nitrogen was used as a chemically neutral driver gas at pressures of 5-50bars inside high pressure chamber whereas the low pressure chamber was filled with stoichiometric hydrogen-oxygen mixture at different initial pressures from 0.1 to 1.0 bar. The details of computational model and method can be found in our previous papers (see [10-12] and references within).

3   Results and discussions

3.1 Pressure-dependent stability of the chocked flames

Recently [11, 12] it was shown that the mechanism of combustion wave transition to detonation in channels filled with hydrogen-oxygen mixture is defined by the pressure increase inside the reaction zone. It can be explained in the terms of chocked flame structure. As the compression waves irradiated from the reaction zone occur to be chocked by the locally supersonic flow on the flame tip they start to compress the mixture inside the flame front. At the same time the flame front propagating with the subsonic speed relatively to the moving fresh mixture acts like a piston and the compression of the mixture ahead of the flame front continues. Therefore further flame evolution is determined by two mechanisms: 1) compression of the fresh mixture and 2) compression of the mixture inside the reaction zone. The first mechanism provide burning velocity increase, the second one can either accelerate or decelerate reaction depending on the pressure range. While the flame speed is less than the adiabatic sonic speed in the hot combustion products there is also influence of the compression waves travelling in the gap between flame front and closed-end wall (or piston surface). The competition of all the mentioned mechanisms determine the further flame dynamics: i) the flame speed saturates and one can observe stable supersonic flame or as it sometimes called "quasi detonation", ii) the flame accelerates and transition to detonation takes place, iii) the chocked flame decays transforming into the subsonic deflagration wave.

For better understanding of the phenomena it is useful to discuss the features of combustion kinetics at different pressures. Figure 1 represents the induction period dependence on pressure for fixed temperature of 1100K for stoichiometric and equimolar compounds of hydrogen-oxygen mixture. One can observe two regions of reaction acceleration with pressure increase corresponding to low- and high pressure mechanisms of hydrogen oxidation [18] and transient region of negative reaction rate dependence on pressure. This transient region is determined by the competition between low pressure mechanism of chains branching and high pressure mechanism of chain termination. In the high pressure region the pressure increase causes the increase of the energy release inside the reaction zone. Chocked flame evolving in such conditions accelerates and the violent energy release inside the reaction zone results in the shock wave formation on the scales of the flame front that in turn can become the origin of a detonation wave. Such a case was observed in our previous papers and is illustrated in fig. 2 obtained for the problem setup considered here. If the chocked flame evolves at lower pressures which correspond to the transient region than the outcome depends on the competition between burning velocity increase and the reaction quenching at the rising pressure. This transient region complies to the unstable chocked combustion regimes decaying in absence of the sufficient gasdynamical support or continuing to propagate in its presence. Figure 3 shows the histories of the flame speed and the pressure at the flame front for the case when the reaction zone evolves in the conditions of transient region. In both cases the chocked flame is unstable and the onset of detonation can be observed. The typical flow structure in the vicinity of chocked flame is presented in fig. 4.
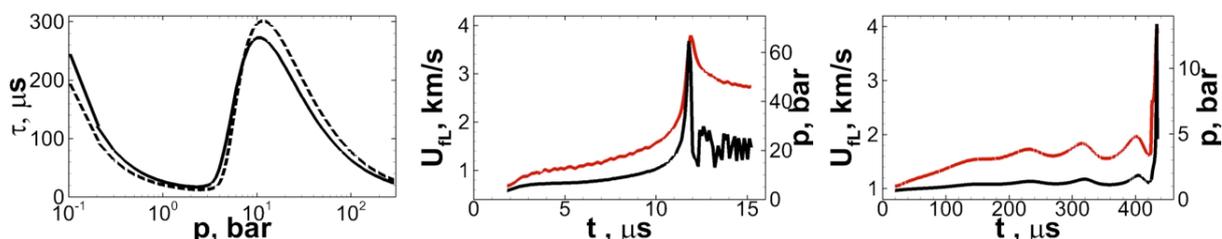
Figure 1. (left) Computed induction periods versus the initial pressure of stoichiometric (solid) and equimolar (dashed) hydrogen-oxygen mixtures.
Figure 2. (middle) Flame speed (red) and pressure (black) histories for the initial conditions: nitrogen pressure p_{N2}=50.0bar, hydrogen-oxygen pressure p_0=1.0bar.
Figure 3. (right) Flame speed (red) and pressure (black) histories for the initial conditions: nitrogen pressure p_{N2}=5.0bar, hydrogen-oxygen pressure p_0=0.1bar.

Figure 4. Flow structure in the vicinity of the chocked flame front (dashed line). Blue color represents the fresh fuel, red one – the combustion products, green – the reaction zone. Solid line represents a sonic line. I – is a supersonic flow, II – combustion products, III – compressed fresh fuel chocked inside the subsonic zone.

3.2 Mechanisms of deflagration-to-detonation transition and autoignition ahead of the flame front

As it was discovered in [4] there are several possibilities of detonation formation in the reacting system with the flame accelerated up to the chocked regime. Chocked flames evolving in the high pressure region determined above result in the deflagration-to-detonation transition (DDT) via the scenario formulated in [10-12]. The flame itself restructures into the detonation wave as soon as the strong enough shock forms inside the reaction zone. Consider in detail the mechanism of this phenomenon. As the perturbations irradiated by the chocked flame do not influence the flow ahead of the flame front the flow cognize the flame's leading edge as a piston moving with the sub-sonic speed equal to the burning velocity $U_f = (U_{fL}-u_f)$, where U_{fL} – is the flame speed in the laboratory reference frame, u_f – is the mass velocity of the flow in the vicinity of the flame's leading edge. The chocked flame continues to accelerate driven by the reaction kinetics at an elevating pressure, the piston surface moves through the reaction zone towards the combustion products. The piston-induced compression of the gas inside the reaction zone (see fig. 5) cause the formation of the shock which birth on the scales of thin reaction zone produces detonation wave as the CJ-conditions of detonation wave formation realize. The lagged perturbations pushed by the expanding detonation products form a retonation shock wave propagating in the opposite direction.
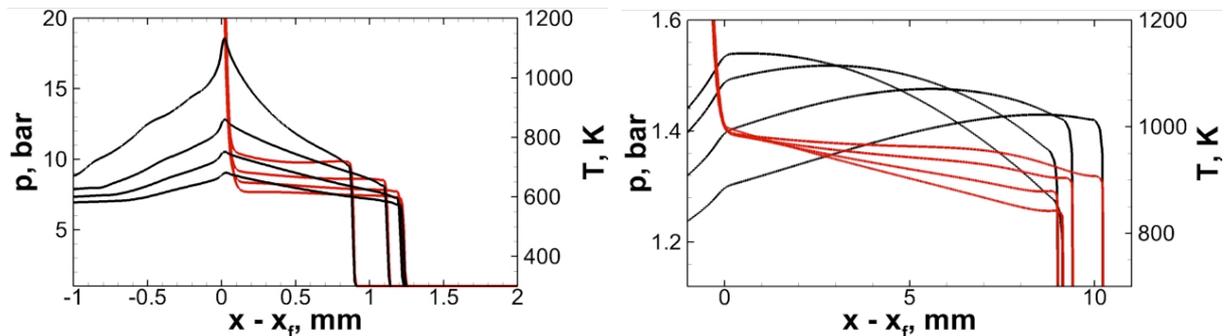
Figure 5. (left) Temperature (red) and pressure (black) profiles in the vicinity of the flame front on the stage prior to the onset of the detonation (conditions of fig. 2). The profiles are presented at different time instants: $t_0 = 8us$, $\Delta t = 1us$.

Figure 6. (right) Temperature (red) and pressure (black) profiles in the vicinity of the flame front on the deceleration stage (conditions of fig. 3). The profiles are presented at different time instants: $t_0 = 320us$, $\Delta t = 5us$.

In case of inverse pressure dependence of the reaction rate the flame front decelerates and becomes sub-sonic. As it happens, the compressed fresh mixture chocked by the supersonic flow in the vicinity of the flame tip (see zone III in fig. 4) flows downstream generating the compression wave ahead (see fig. 6). This packet of compressed mixture acts like a piston on the mixture ahead of its surface. On the other hand the compression waves previously lagged behind the locally supersonic chocked flame overrun the flame front and compress the mixture adjacent to its surface behind the out-flowing contact surface. The flame resumes its acceleration and the cycle repeats. Before the decay of

the chocked flame structure the flame front is the only contact surface and the reaction cannot start independently ahead of it. After the formation of the new contact surface (or surfaces) ahead of the flame front the exothermal reaction can arise on it and initiate independent deflagration wave or even detonation. Depending on the conditions of prior flow evolution the new kernel of auto-ignition can be formed at different distance out from the flame surface. It is useful to extract four cases: 1) the auto-ignition emerges directly ahead of the flame front, 2) between the flame front and the leading shock, 3) directly behind the leading shock, 4) no ignition takes place.

The first case will take place if the out-flowing gas is preheated up to the temperatures providing the induction period shorter than any other characteristic time scale of the problem. When this gas was chocked the supersonic flame consumed it faster than it was able to be ignited. As soon as it separates out from the existing flame front it ignites directly ahead of the front. In this case one could observe seemingly more violent local flame acceleration than the previously observed regimes. In fact it is a new combustion wave arising on the new contact surface and propagating behind the outrunning compression wave generated by the moving contact surface. The temperature between the contact surface and the compression wave front is almost equal in every point, on the other hand the maximum progress of the reaction in such a system is at the contact surface, where the gas propagates with a local sonic speed and therefore the mixture reacts at constant temperature and pressure. The emerged combustion wave propagates via the Zeldovich mechanism of spontaneous ignition so its speed is fully determined by the speed of compression wave that creates the gradient of induction period. It can become detonation wave by itself or after the interaction with the leading shock.

In case of longer induction periods at the contact surface the ignition takes place on larger distances from the flame front. Therefore one can observe ignition between the flame front and the leading shock. The ignition can arise at the contact surface arising as the forming compression wave (or shock wave) intersects the leading shock (such a scenario was considered in [19]).

The most probable location of the autoignition kernel emergence is the region in the vicinity of the wall. This can be explained by the advanced rate of preheating in the boundary layer caused by friction and more intensive preheating inside the fold of the flame surface adjoining the side wall.

4   Conclusions

The systematization of the available experimental and numerical data on chocked flames and DDT allowed us to extract the basic features of the chocked flame establishing and its stability. First it was shown that the origin of chocked flame is the flame acceleration in the piston-driven flow. Further analysis of the chocked flame structure based on our recent works showed that the instability of the chocked flame and transition to detonation is determined by the specific features of chemical kinetics inside the continuously compressing reaction zone. We proposed a numerical model that reproduced the chocked flames driven by the expanding inert gas. The unstable chocked flames were studied for stoichiometric hydrogen-oxygen mixtures at different pressures. The results allowed us to get a clear interpretation of the experimentally observed [4] scenarios of detonation onset: 1) DDT, 2) "violent flame acceleration" and DDT, 3) autoignition on the contact surface at the distance from the flame front, 4) autoignition on the contact surface formed due to the intersection of the formed compression wave (shock) and the leading shock. The kinetic sensitivity to the external conditions should be taken into account while elaborating criterions of chocked flames stability and detonation probability in the real systems.

Acknowledgements

References

[1]   Peraldi O, Knystautas R, Lee JHS. (1986). Criteria for transition to detonation in tubes. Proc Comb. Inst. 21: 1629.

[2]   Alekseev VI et. al. (2001). Experimental study of flame acceleration and the deflagration-to-detonation transition under conditions of transverse venting. J. Loss Prev. Proc. Ind. 14: 591.

[3]   Salamandra GD, Bazhenova TV, Naboko IM. (1959). Formation of Detonation Wave During Combustion of Gas in Combustion Tube. Proc. Comb. Inst. 7: 851.

[4]   Utriew PA, Oppenheim AK. (1966). Experimental observations of the transition to detonation in an explosive gas. Proc. Roy. Soc. A. 295. 1440: 13.

[5]   Kuznetsov M et. al. (2005). DDT in a Smooth Tube Filled with a Hydrogen-oxygen Mixture. Shock Waves. 14: 205.

[6]   Wu M et. al. (2007). Flame Acceleration and the Transition to Detonation of Stoichiometric Ethylene-oxygen in Microscale Tubes. Proc. Comb. Inst. 31: 2429.

[7]   Zeldovich YaB. (1947). On the theory of detonation origin in gases. JTP. 17. 1: 3.

[8]   Kurylo J, Dwyer HA, Oppenheim AK. (1980). Numerical Analysis of Flowfields Generated by Accelerating Flames. AIAA J. 18. 3: 302.

[9]   Deshaies B, Joulin G. (1989). Flame-speed sensitivity to temperature changes and the deflagration-to-detonation transition. Combust. Flame. 77: 201.

[10] Liberman MA et. al. (2010). Deflagration-to-detonation transition in highly reactive combustible mixtures. Acta Astronautica. 67. 7-8: 688.

[11] Ivanov MF, Kiverin AD, Liberman MA. (2011). Hydrogen-oxygen flame acceleration and transition to detonation in channels with no-slip walls for a detailed chemical reaction model. Phys. Rev. E. 83: 056313.

[12] Ivanov MF et. al. (2013). Hydrogen–oxygen flame acceleration and deflagration-to-detonation transition in three-dimensional rectangular channels with no-slip walls. Intl. J. Hydrogen Energy. 38. 36: 16427.

[13] Lee JHS, Knystautas R, Freiman A. (1984). High Speed Turbulent Deflagrations and Transition to Detonation in H2-Air Mixtures. Combust. Flame. 56: 227.

[14] Khomik SV et. al. (2012). Limits and mechanism of detonation re-initiation behind a multi-orifice plate. Shock Waves. 22: 199.

[15] Bhattacharjee RR et. al. (2013). Detonation re-initiation mechanism following the Mach reflection of a quenched detonation. Proc. Comb. Inst. 34. 2: 1893.

[16] Johnson RG, McIntosh AC, Yang XS (2003). Modelling of fast flame–shock wave interactions with a variable piston speed. Combustion Theory and Modelling. 7. 1: 29.

[17] Kusharin AY et. al. (1998). Detonability of H2/CO/CO2/Air Mixtures. Comb. Sci. Tech. 34. 2: 85.

[18] Warnatz J. (1981). Concentration-, Pressure-, and Temperature-Dependence of the Flame Velocity in Hydrogen-Oxygen-Nitrogen Mixtures. Comb. Sci. Tech. 26. 5: 203.

[19] Taki S., Fujiwara T. (1971). One-dimensional nonsteady process accompanied by the establishment of self-sustained detonation. Proc. Combust. Inst. 13: 1119.