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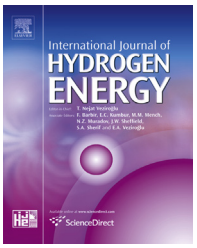

On the structure and stability of supersonic hydrogen flames in channels

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ABSTRACT

The paper considers trans- and supersonic flames propagating through the channels filled with hydrogen-oxidizer mixtures. High-resolution numerical analysis of the flame front propagating in the so-called "chocked" regime allowed us to formulate possible mechanisms of further flame acceleration and successive onset of detonation. It is shown that the following criteria should be satisfied for further flame acceleration after "chocked" flame regime establishment: 1) the reaction rate should rise with pressure; 2) the effect of external gasdynamical and acoustic fields should be reduced to minimum. According to the formulated criteria all of the experimentally obtained regimes of supersonic combustion and onset of detonation can be described generally in terms of "chocked" flame stability towards chemical and gasdynamical factors. The first criterion is satisfied in near stoichiometric hydrogen–oxygen and hydrogen–air mixtures at normal and higher ambient pressures due to peculiarities of the hydrogen oxidation kinetics. The second criterion is satisfied in smooth channels and can be temporary satisfied in obstructed channels of specific widths and blockage ratios. In case of smooth channel filled with highly active mixture subsequent flame acceleration results in a deflagration-to-detonation transition. In case of lower chemical activity of the combustible mixture flame propagation continues in a quasi-steady supersonic regime. In this case oscillations of the flame velocity provoke the non-steady flow perturbations and compression waves emergence that can cause formation of auto-ignition kernels on the surface of contact discontinuity or on the obstacles surfaces.

Introduction

For decades gaseous explosions were of paramount interest due to their hazardous potential. Analysis of accidental scenarios allowed one to extract basic features of the gaseous explosion evolution. Among wide variety of explosion regimes special attention was paid to non-steady accelerating flames inside closed vessels filled with gaseous combustible mixtures. Flame acceleration inside closed vessel is characterized by the increase both in combustion completeness and in compression rate. It is accompanied with generation of compression waves which in turn cause impact on the shell by themselves and in the form of shock waves. Finally the accelerating flame together with the generated shocks can produce self-sustained detonation. Regimes with high energy release such as fast flames, supersonic flames and detonations provide high combustion efficiency and directed

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impulse that is of primal interest in propulsion [1], welding [2], nano- and microparticles implantation [3,4] etc. Without a doubt hydrogen is one of the most perspective fuels for these means. Compare with hydrocarbons hydrogen is rather cheap, it has wide detonability limits and its combustion kinetics is more or less known distinct to the hydrocarbon fuels. The latter allows detailed numerical simulations and quantitative predictions.

To understand the possibilities of supersonic flames and detonation implementation as well as to develop hydrogen safety measures the clear understanding of the non-steady processes evolution should be achieved. In practice the detailed and clear experimental analysis of the fast combustion phenomena occurs to be rather difficult. First because of the limitations of experimental equipment usually used for studying dynamics of the reacting flows. 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. The detonation onset as a result of flame acceleration inside narrow channels or gaps can be obtained only in the highly reactive oxy-fuel mixtures (of hydrogen, acetylene, ethylene etc.) [5–8]. To achieve higher rates of acceleration and increase the probability of detonation onset in slowly reactive mixtures including hydrogen–air it is common to use channels obstruction as a reliable technique of flow acceleration first proposed by K.I. Shchelkin. However even in obstructed channel the flame acceleration causes the detonation onset quite rarely (see e.g. Refs. [9–11]). Instead of detonation two basic regimes are usually observed: (1) trans- or supersonic flame, usually called as "chocked" flame, and (2) so-called "quasi detonation". Both of them are characterized by deficit in propagation speed and thermodynamic parameters compare with self-sustained detonation. These regimes are intrinsic not only to the laboratory scales experiment but also arise in the large-scale experiments [12]. Quasi detonation represents a periodic process of detonation quenching and re-initiation driven by the flow interactions with the obstacles [13]. In experiment using pressure transducers together with ion probes quasi detonation can be distinguished from normal detonation by slight lag between the leading shock and the reaction zone [14]. At the same time chocked flame can be observed as a double–wave complex consisting of the leading shock wave and the flame front noticeably lagging behind. Both propagate with almost equal speed that is supersonic relative to the fresh mixture. Such double wave structures can be also observed in the distinct class of experiments devoted to examine the features of detonation quenching after its diffraction on obstacles [15,16] or after its transmission into the narrow gap [17]. Instantaneous increase in momentum and heat losses causes decoupling of the detonation wave into the shock wave followed by the reaction wave. Expanding detonation products push the reaction front that can cause its acceleration. Similar flow pattern can be observed during flame acceleration in channel, where the flow is also driven by the expanding products. The main distinction is higher rate of compression behind the leading shock in case of detonation decay. Therefore the burning rate is higher as well and the conditions occur to be more comfortable for further chocked flame acceleration and probable onset of detonation. In case of diffraction on multi-dimensional obstacles the flow non-uniformity can trigger detonation re-initiation behind the reflected oblique shocks [16]. Besides, the detonation can arise as a consequence of reflected shock interaction with the side flame surface [18,19]. Mechanisms of such a regime of detonation formation is related with dynamical impact on the mixture inside and ahead the reaction zone that was studied in Refs. [20,21].

Concerning smooth channels, there are two basic mechanisms of deflagration-to-detonation transition after the flame acceleration. According to [6] in stoichiometric hydrogen–oxygen mixture at initial atmospheric pressure (1.0 bar) the detonation arises directly on the flame surface, while in equimolar mixture at initial pressure of 0.11 bar one can observe several distinct regimes involving the birth of new contact surfaces and compression waves and their interactions. The first mechanism was numerically reproduced and analyzed in details in our recent works [22–24]. It was obtained that in this case detonation arises due to self-sustained flame acceleration and combustible mixture compression inside the reaction zone. According to the second mechanism, also called "explosion in the explosion", detonation is formed out from the auto-ignition kernels on the contact discontinuities ahead of the flame front [25]. In Ref. [26] the mechanism of ignition in the system of two contact surfaces and two shocks was reproduced numerically in attempt to visualize and analyze the experimentally obtained emergence of the auto-ignition kernels ahead the primal flame front. Recently in Ref. [27] a two-dimensional variant of the same problem was numerically analyzed that allowed to visualize a role of boundary layer in the shock-contact surface interaction inducing the auto-ignition kernel formation. Both in Refs. [26] and [27] the contact surfaces and the shocks were introduced artificially in the initial conditions and there is still no information about the origins of such contact surfaces and shocks ahead the naturally accelerating flame. However there still no information about the origins of such contact surfaces and shocks ahead of the naturally accelerating flame.

Summing up the large amount of experimental data on chocked flames, quasi detonations, deflagration-to-detonation transition (DDT) and detonation onset via "explosion in the explosion" mechanism one can see qualitatively the same behavior prior to the chocked flame formation. Afterward the process evolves in different ways depending on the mixture compound, initial pressure, geometry of the channel and other external parameters. However chocked flame origins, its structure and stability were not analyzed in details yet. The aim of this paper is to extract and study peculiarities of chocked flame evolution in the most common cases and to formulate the basic mechanisms of possible further flame acceleration and detonation onset. In particular we study numerically the chocked flame structure in hydrogen–oxygen stoichiometric mixture at two different pressures (1.0 bar and 0.1 bar) and hydrogen–air mixtures of different compounds. The first problem allowed us to extract the chocked flame stability towards kinetics peculiarities on the example of two mixtures corresponding to two different

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