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HYDROGEN COMBUSTION REGIMES IN CONFINED VOLUMES

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Among various problems of gaseous combustion theory the investigations of non-steady combustion regimes are of special interest due to efficiency of control at such non-steady phase. Particularly control of deflagration-to-detonation transition (DDT) is in the center of attention. Some aspects of DDT were investigated in 50th-60th years of the past century [1, 2]. However interest towards DDT problem remains up to date. This issue is conditioned by topical problems of propulsion and fire safety. Besides the fundamental problem is to develop clear comprehensive pattern of flame evolution in case of strictly non-linearity of combustion processes. The different physical mechanisms of the flame acceleration and corresponding DDT are known. Each of these mechanisms is based on the acceleration of the energy release due to chemical reactions. Chemical and hydrodynamic factors and their interaction are fundamentals that determine the process. One of these mechanisms is a deformation and acceleration of the flame due to the hydrodynamic instability of the flame front - the Darieus-Landau instability (DLI) [3]. Most vividly DLI is observed in the flames that propagate in channels and tubes with smooth walls [4]. The deformation of the flame front at such conditions is developed due to the flame-boundary layer interaction near the walls. Under certain physical and chemical conditions the compicated wrinkled flame structure can be generated [5]. Wrinkled flame is characterized by availability of deep folds in its structure. Within the folds, the "hot spots" with the heightened temperature and reaction velocity may appear. With agreement to the Zel'dovich theory [6] the DDT occurs within these "hot spots".

In spite of the big interest of numerous researchers to the problem the major of aspects remain not enough examined. The main reason is the usage of the simplest thermodynamic dependencies in the equations of state and transport coefficients and one-step chemical kinetics (described by one Arrhenius equation). Such approach is widely applied in the contemporary papers [3-5, 7] dedicated to the examination of the phenomena. Results of such numerical simulations allow to reveal many typical properties of non-linear combustion processes. However excessive simplification of mathematical models makes impossible to predict even qualitatively development of these properties in case of real mixtures combustion.

This paper examines the influence of the mixture composition on the DLI evolution, flame acceleration and DDT. Among variety of exothermal reactions in gases the hydrogen-oxygen reaction has been chosen. The influence of neutral component presence on non-linear combustion processes was examined. Comparative analysis of hydrogen combustion in oxygen and in air was carried out. The nitrogen of air assumed to be neutral because of small influence of its oxidation on the exothermal process. All the results are received by methods of numerical simulations using mathematical models describing process sufficiently detail. The solver is based on a two-dimensional model of hydrogen bearing mixture combustion. This model includes the gas dynamic transport of viscous gas, the hydrogen oxidation kinetics, multi-component diffusion, and heat conduction. For multi-component mixture and combustion products the equations of the

real gas state were used. The reduced model of chemical kinetics includes nine reactions. Numerical method is Lagrange-Euler method [9]. Computational grid cell sizes was $0,05 \times 0,05 mm^2$ (variation of cell sizes from $0,01 \times 0,01$ to $0,10 \times 0,10 mm^2$ gave flame speed variation never exceeded value of 4%). Chosen model was widely used by authors and described for example in [10]. The dynamics of flame propagation in the semi-closed channel was examined. The flame was initiated in the preheated layer on the closed end of the channel. The flame front - boundary layer interaction (the nonslip boundary condition at the walls) was considered. After ignition the flat flame front was formed. Perturbations were born into the boundary layer and redistribute along the flame front surface. The further perturbation evolution was determined by the DLI evolution. In two variants the channel was initially filled with premixed stoichiometric hydrogen-oxygen and hydrogen-air mixtures.

Expansion coefficient is about 7 for most gaseous combustible mixtures including hydrogen-oxygen and hydrogen air. Therefore estimations from [8] give relative flame speed increasing due to pure DLI (within channels with slip walls). It is counted as 16%. Obviously so little flame speed increase cannot result in DDT. Taking boundary layer and corresponding nonuniformity of the flow within channel into account gives more realistic model. Non-uniform flow additionally distorts flame surface. Collective effect of DLI and flame-boundary layer interaction can considerably overcome stabilizing factors influence and cause additional flame acceleration.
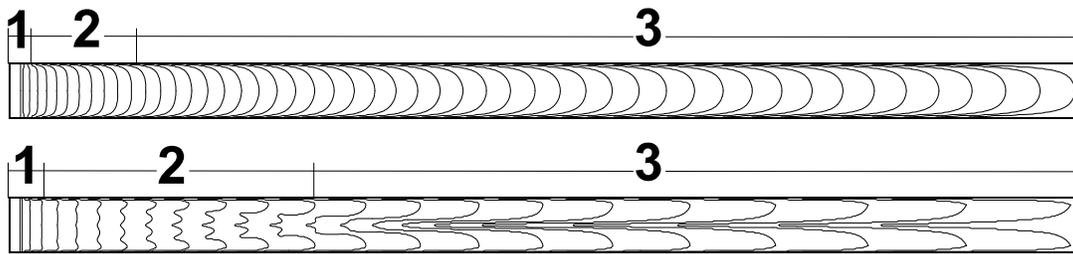
Fig. 1. Flame front evolution in the hydrogen-air (upper) and hydrogen-oxygen (bottom) mixtures. The isolines of hydrogen concentration show the flame front position at different time instants (over every 1.25ms in hydrogen-air and 0.25ms in hydrogen-oxygen). Numerals show space scales corresponding to different DLI evolution stages.

In two different mixtures (hydrogen-air and hydrogen-oxygen) two distinct combustion regimes take place. Fig. 1 shows not only quantitative differences as linear theory predicts but qualitative differences too. Formally for both variants scenario of flame evolution can be described in four stages: 1) birth of the small perturbations and initial distortion of the flame front due to non-perturbed front interaction with boundary layer; 2) the organizing of quasi stable flame structure out of the fastest growing modes; 3) quasi linear instability growth conditioned by the fastest growing modes; 4) non-linear perturbations interaction causing instability growth rate.

At first stage a wide spectrum of small-amplitude perturbations was born as a result of planar front local distortion near side walls. Further at the second stage the long-wave perturbations grew with the highest rate (similar to the regimes in slip-walled channels). For hydrogen-oxygen mixture growth rate is higher than for hydrogen-air one. In latter case the first harmonic becomes dominant. Thereby flame front becomes convex-shaped. Tangential velocity component on flame surface appears and perturbations of smaller wave length are carried to the

walls forced by this velocity. Further flame front elongates and tangential velocity remains relatively big. Therefore perturbations vanish on the walls faster than their amplitude becomes sufficient. As a result at the third stage hydrogen-air flame front has approximately single-mode structure. It's amplitude grows according to exponential law distinct to the linear solution (see fig. 2). Within channels width of 5 and 10mm in hydrogen-air mixture the fourth stage wasn't observed. Estimations show that acceleration formed at the third stage is not enough efficient to generate DDT. The shock generated by such accelerating flame can transit to detonation only on scales of 2-3 meters. However this issue wasn't observed in any experiments.

In case of hydrogen-oxygen mixture the growth rates of first three harmonics are sufficiently high. As a result the short-length perturbations are able to distort flame front before they are carried to the walls. A deep cusp in the flame shape is generated. This cusp captures all the higher harmonics. Calculations shows this structure to be stable and permanently grow during the third stage. At the fourth stage flame speed reaches value that is enough to generate relatively strong shock wave ahead the front. Corresponding warming up of the mixture behind this shock generates DDT in vicinity of the front leading point. Transition to detonation in this case occur according to the scenario described in [1].

Comparing two scenarios of flame acceleration one can conclude that presence of additional neutral component in combustible mixture decreases specific energy release and reduce instability growth rate. In turn this growth rate reducing qualitatively changes flame front structure during process non-steady phase. This factor can become an obstacle for DDT generation.

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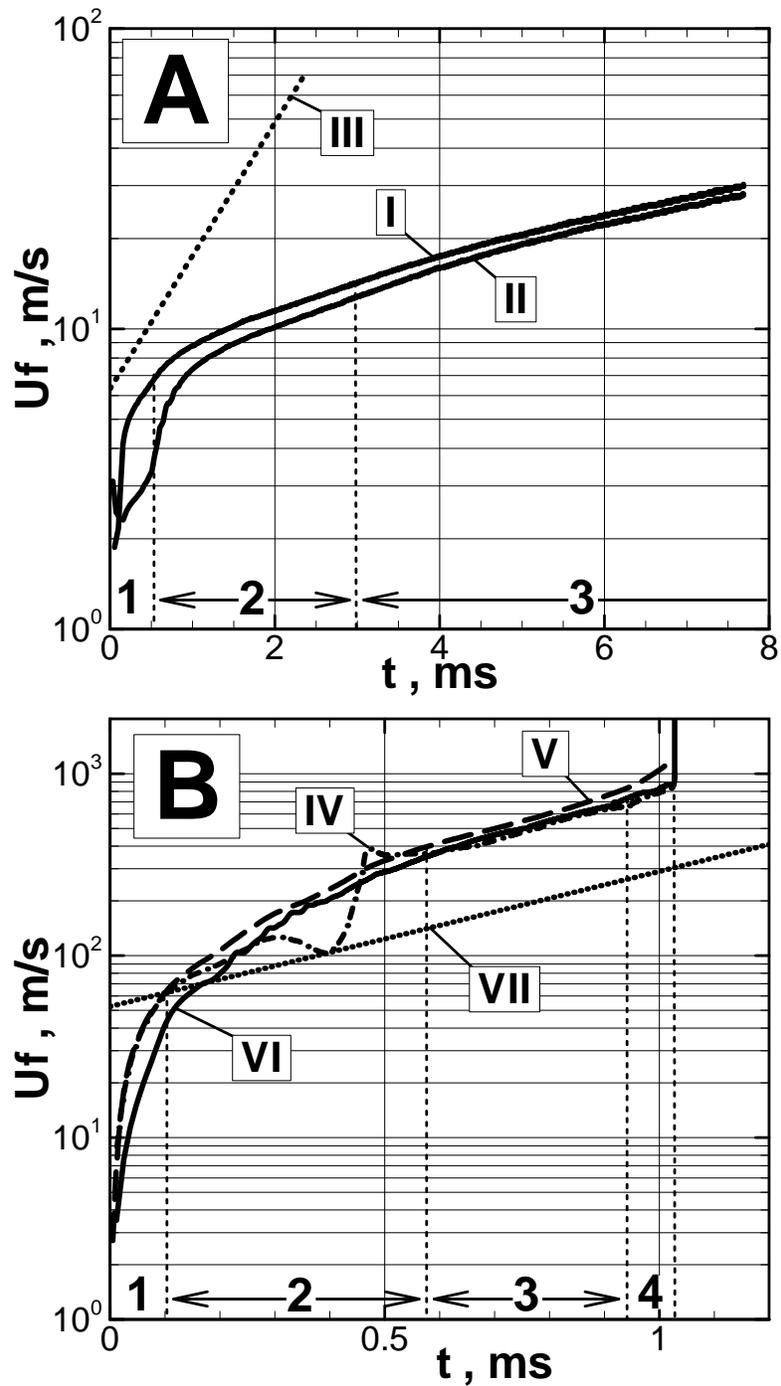
Fig. 2. Evolution for the velocities of the flame surface points in the hydrogen-air mixture (A): I - point on the axis, II - point on the wall, III - linear solution; and hydrogen-oxygen mixture (B): IV - point on the axis, V - leading point, VI - point on the wall, VII - linear solution. Numerals show time scales corresponding to different DLI evolution stages.