Peculiarities of Deflagration to Detonation Transition in Gases.

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Investigations of deflagration to detonation transition in gases are relative to both explosion safety issues, and pulse detonating devices. For both applications the control of detonation onset is of major importance, though the purposes of the control are just the opposite. In explosion safety issues the main goal is to prevent the DDT, while in pulse detonating devices the advantages of detonation over constant pressure combustion bring to the necessity of promoting the DDT and shortening the pre-detonation length.

The paper contains the results of theoretical and experimental investigations of control of the DDT processes in hydrocarbon - air gaseous mixtures relative to propulsion applications. The influence of geometrical characteristics of the ignition chambers and flow turbulization on the onset of detonation and the influence of temperature and fuel concentration in the unburned mixture are discussed.

Introduction

Investigations of deflagration to detonation transition (DDT) in hydrogen -- oxygen mixtures (Oppenheim et al., 1966; Salamandra, 1959; Soloukhin, 1969) and later in hydrocarbons - air mixtures (Smirnov et al., 1986, 1995) showed the multiplicity of the transition processes scenario. The various modes of the detonation onset were shown to depend on particular flow pattern created by the accelerating flame, thus making the transition process non-reproducible in its detailed sequence of events. By now, there exist different points of view on the DDT mechanism: the "explosion in explosion" mechanism by Oppenheim (1966) and the gradient mechanism of "spontaneous flame" by Zeldovich (1970).

The later theoretical analysis showed that micro-scale non-uniformities (temperature and concentration gradients) arising in local exothermic centers ("hot spots") ahead of the flame zone could be sufficient for the onset of detonation or normal deflagration (Merzhanov, 1966; Borisov, 1974; Kailasanath and Oran, 1983; Smirnov et al., 1989, 1995, 1997; Frolov, 1992). Analysis and comparison of theoretical and experimental results showed that self-ignition in one or in a number of hot spots ahead of the accelerating flame followed by the onset of either detonation or deflagration waves brings to a multiplicity of the transition scenarios (Smirnov et al., 1999). The common feature of all those scenarios is the formation of local exothermic centers according to stochastic Oppenheim mechanism followed by the onset of detonation at a micro-scale in one of the exothermic centers according to spontaneous Zeldovich mechanism (Smirnov et al., 1999). The investigations of the reflected shock - laminar flame interactions bringing to the onset of detonation (Brown and Thomas, 1999; Khokhlov and Oran, 1999) showed, as well, that the transition to detonation in a hot spot takes place through the gradient mechanism, while the shocks and flames interactions were important for creating the proper conditions for the hot spots to occur.

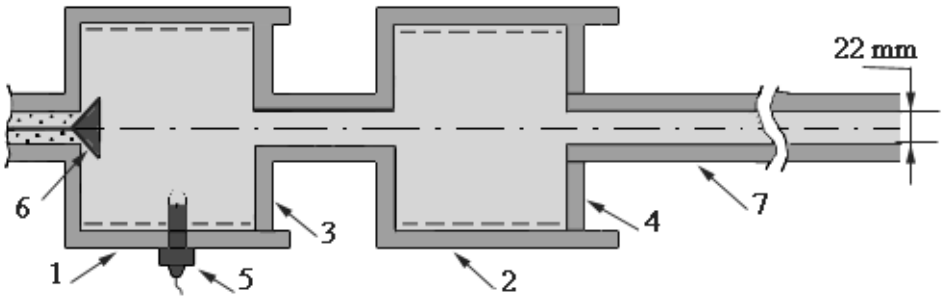
Experimental investigations of the sensitivity of DDT processes to mixture parameters variation have a natural limitation on the precision of the results, because various modes of detonation onset depend on stochastic flow pattern created by accelerating turbulent flames thus minor uncontrolled changes of flow parameters could bring to a different transition mode. Besides, it is hardly possible to vary different parameters independently in physical experiments. That increases the importance of numerical modeling for investigating the detonation initiation sensitivity to governing parameters' variations.

Numerical investigations of transition processes provide a unique possibility to vary each parameter independently and monotonously.

The paper presents the results of theoretical and experimental investigations of the deflagration to detonation transition in homogeneous gaseous mixtures and its sensitivity to variations of governing parameters.

Experimental investigations

Experimental investigations of pulsed detonation regimes initiation in gaseous mixtures of hydrocarbon fuels with air were undertaken. A detailed description of the experimental procedure and apparatus could be found in (Smirnov et. al., 1999). Here we'll just give a brief summary of results. Physical experiments were undertaken for comparative studies of the role of different turbulizing elements: Shchelkin spiral, orifice plates, turbulizing chambers c ated into the



ignition sections of the tube (Fig. 1) promoted the onset of detonation by shortening essentially the pre-detonation length for hydrocarbon fuels – air mixtures.

Figure 1. Pulse detonating device with variable volume chambers.

The optimization of the size of turbulizing chambers was performed using the chambers of variable volume in experiments. The side walls of the chambers (1) and (2) (Fig. 1) having a thread on the inner surface, made it possible to screw the cylindrical plates (3) and (4) more or less deep into the chambers thus varying the volume. The mixture was ignited in the chamber (1) by a spark plug (5). The gas flow induced by the flame expansion was highly turbulized due to geometry of the vessel: a thoroidal vortex appeared in the chamber (2) causing a rapid expansion of the flame area on entering the second chamber. The increase of pressure in both chambers kept the valve (6) closed. Expansion of the reaction products into the narrow tube (7) produced an additional piston effect thus increasing the flame acceleration and promoting the DDT. The investigations made it possible to determine the optimal structure of the initiating section shortening the pre-detonation length in pulse detonation devices.

For air - gasoline gaseous mixture the pre-detonation length was shortened to 1.5 - 2.0 m in tubes 22 mm in diameter. The Schlieren pictures illustrating the variety of scenario of the transition process were published before (Smirnov et al, 1995, 1999). The Figs.2-4 illustrate the types of flow patterns at different distances from initiating section. The flame is propagating from the left to the right, time increasing from bottom to top. Thus the Schlieren pictures give the x-t diagrams of the process. The x-axis gives the actual coordinate along the axis of the tube (the valve (6) was assigned to be the zero point). The t-axis provides only the time scale, but not the actual point (the zero point is adjusted to the beginning of the registration).

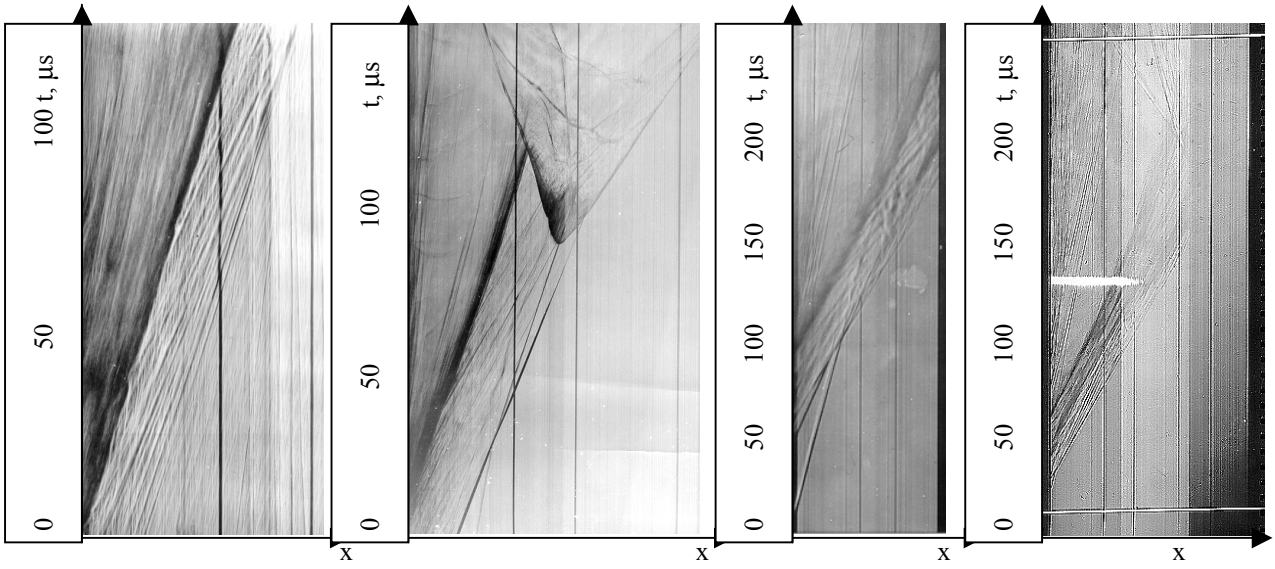


Fig.2. Compression waves ahead of an accelerating turbulent flame.

Fig.3. The onset of detonation ahead of turbulent flame on a contact discontinuity.

Fig.4a. Auto-ignition in a hot spot ahead of the flame giving birth to a new flame zone.

Fig.4b. Auto-ignition in a number of hot spots ahead of the flame

Fig.2 shows the flow pattern before the onset of detonation. The presence of turbulizing chambers contributes to flow irregularity ahead of the flame, that could promote the onset of detonation. The piston effect of the expanding reaction products formed on burning out the mixture in the chambers brings to formation of several primary shock waves propagating in front of the turbulent flame. Other shock waves were formed by coalescing compression waves due to acceleration of turbulent flame. The flame velocity is 950 m/s. The later shock waves overtake the primary ones until a strong shock wave supported by the flame induced compression waves is formed ahead of the flame (Figs.3, 4).

The detonation wave occurs after ignition in local exothermic centers ("hot spots") ahead of the flame. The transition scenario illustrated in Fig.3 is characterized by the hot spot formation in the high enthalpy zone on the contact surface resulting from two primary shock waves interaction. Fig. 4a illustrates the transition scenario characterized by formation of the secondary combustion zone between the flame and the leading shock due to auto-ignition in a local exothermic center. Combustion zone expands in all directions, the onset of detonation

takes place 180 μs later. Fig. 4b illustrates the transition scenario under which ignition takes place subsequently in a number of hot spots ahead of the flame. Those ignitions do not lead directly to formation of detonation waves. Flames propagating in all directions from the ignition centers expand in both directions leading to formation of volume combustion and further compression of the mixture behind the leading shock. The detonation wave arise in one of subsequent exothermic centers more close to the leading shock beyond the limits of the photographic zone. The retonation wave moving backward at a speed of 1350 m/s in the upper part of Fig.4b testifies that.

The available experimental data on the DDT process sensitivity on gas temperature variations were contradictory. Thus, special experimental investigations of the influence of initial mixture temperature on pre-detonation length and the time were undertaken for the pulse detonation device shown on the Fig. 1. The pre-detonation times for mixtures of air with gasoline of different detonability are shown in Fig. 5.

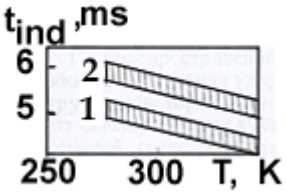


Figure 5. Pre-detonation time in air - gasoline mixtures: 1 - A-76; 2 - A-93.

The results show that for air - gasoline mixtures all the induction times decrease on increasing the initial mixture temperature. The increase of the octane number of gasoline from 72 to 93 brought to a 15% – 20% increase of the pre-detonation length. For low temperatures, the DDT process was more stable for enriched mixtures while for T>320 K the DDT in lean mixtures was also very stable.

Theoretical investigations

The system of equations for the gaseous phase was obtained by Favre averaging of the system of equations for multicomponent multiphase media. The modified *k-epsilon* model was used. To model temperature fluctuations the third equation was added to the *k-epsilon* model to determine the mean squared deviate of temperature.(Smirnov et al., 2000). The production and kinetic terms are modeled using the Gaussian quadrature technique.

Numerical modeling made it possible to explain the onset of detonation on the contact surface. In case weak shock waves precede the deflagration wave their interaction gives birth to a rarefaction wave moving backward to the flame front and the contact discontinuity that exists between the leading shock and the flame zone. The zone between the leading shock and the contact surface has a higher temperature. Thus the induction period in this zone is less than between the flame front and the contact surface. The first thermal explosion takes place in the layer of gas that has been at the higher temperature for the longest time, i.e. in the gas layer very on the contact surface. That explosion can bring to either deflagration or detonation waves propagating from the exothermic center. Following the gradient mechanism detonation waves propagating in opposite directions could be formed in this zone. The intensity of the retonation (reverse detonation) wave falls down on entering the reaction products. The detonation wave overtaking the leading shock forms an overdriven detonation in the uncompressed mixture that gradually slows down to the Chapman-Jouget speed.

To investigate the influence of turbulizing chambers of a wider cross-section on the onset of detonation numerical modeling was performed for a test vessel shown in Fig.1. The vessel contains a detonation tube with two chambers of a wider cross-section filled in with combustible gaseous mixture at ambient pressure. Ignition of the mixture is performed by a concentrated energy release in the center of the first chamber. Five model reactions in the gas were taken into account: hydrocarbon decomposition, carbon monoxide oxidation, carbon dioxide decomposition, hydrogen oxidation, water vapor decomposition. The tube has 20mm in diameter with two chambers 100mm in diameter and 100mm long incorporated in the ignition section. The bridge between the two chambers is 20mm in diameter and 50mm long.

The results (Figs. 6, 7) show that on mixture ignition in the first chamber the process of flame propagation is rather slow and is determined mostly by initial turbulization of the mixture. The flame being initially spherical changes its form for cylindrical on approaching the walls of the chamber. The flame accelerates and penetrates the bridge between the two chambers due to a gas flow caused by the expansion of reaction products. A high velocity jet penetrating the second chamber brings to a very fast flame propagation both due to additional flow turbulization and the piston effect of the expanding reaction products supported by the continuing combustion in the first chamber. The line segments in Fig.6 characterize the values of velocities in gas.

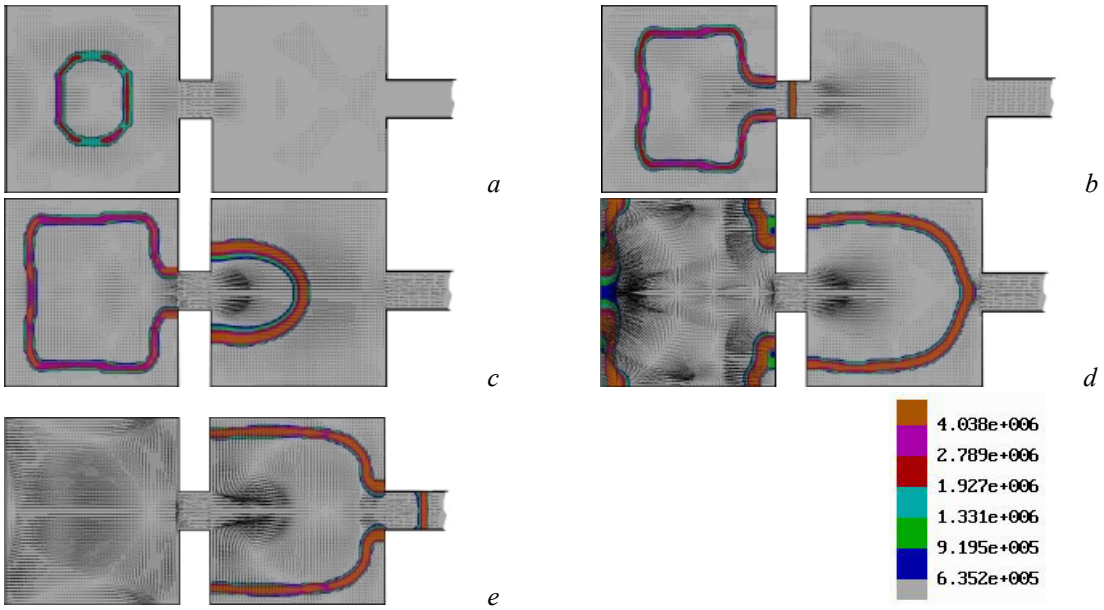


Figure 6. Chemical reaction zone evolution for successive times after ignition: *a*- 1ms, *b*- 3.1ms, *c*- 3.7ms, *d*- 4.2ms, *e*- 4.4ms.

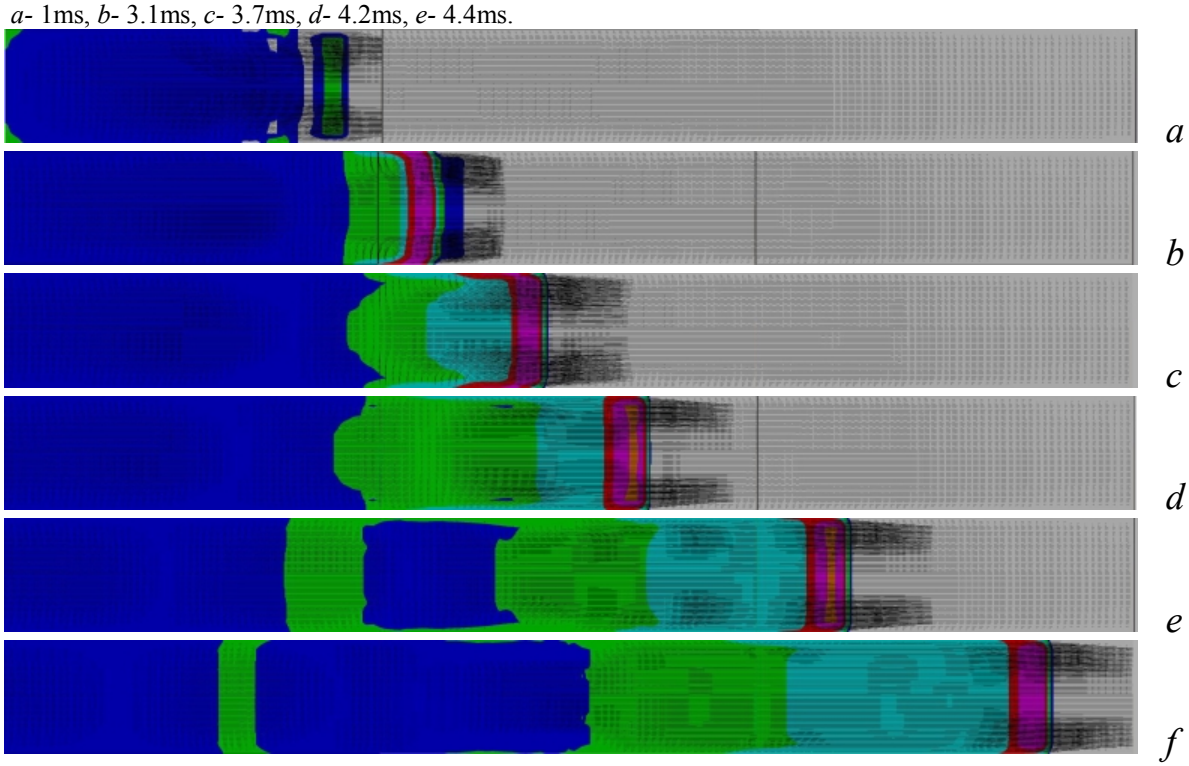


Fig.7. Pressure evolution in the detonation tube in the transition zone for successive times: *a*- 4.593 ms, *b*- 4.628 ms, *c*- 4.643 ms, *d*- 4.657 ms, *e*- 4.683 ms, *f*- 4.709 ms.

Fast combustion in the second chamber brings to a sharp pressure increase that pushes the flame further into the tube(Fig.7). A shock wave is formed in the tube ahead of the flame zone. Pressure waves generated by continuing combustion in the chambers overtake the flame and the leading shock wave. That causes nonuniformities in the combustion zone and formation of transverse waves. At some place the detonation arises from a hot spot within the combustion zone. For the present scenario of the process the onset of detonation takes place at a distance of about 1 m from the ignition section. Before the onset of detonation hot spots appearing in the combustion zone bring to formation of compression waves irradiated form the reaction zone in all directions.

Those waves support the leading shock and propagate backwards as well until the onset of detonation waves in one of successive hot spots gives birth to strong detonation and retonation waves.

The decrease of fuel molar concentration brings to formation of galloping combustion regimes. Those galloping combustion regimes are not caused by numerical instability as one cycle of the process develops within 150 – 200 time steps. The hot spots occur alternatively near lateral walls (higher pressure pikes) and in the center and bring to flame zone accelerations.

The increase of initial temperature of the combustible hydrocarbon – air mixture brings to shortening the pre-detonation time for lean mixtures especially. However, parametric studies show that for high energy density gaseous mixtures (fuel – oxygen) the dependence could be quite the opposite under certain conditions.

The decrease of the number of chambers incorporated into the ignition section to one chamber, and then to zero chambers brings to the increase of pre-detonation length and time. The further increase of the number of the chambers up to more than two does not bring to any essential variations of the pre-detonation length. Thus one or two chambers could be considered as an optimal configuration to promote the onset of detonation.

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