Deflagration to detonation transition in meta-stable systems.

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Abstract

Experimental and theoretical investigations of gaseous flames propagation in combustion chambers of complex geometry showed that flow induced instability could cause rapid acceleration of flame propagation and could even bring to a change of the combustion mode from deflagration to detonation. Knowing mechanisms of detonation onset control is of major importance for creating effective mitigation measures.

The paper contains the results of theoretical and experimental investigations of deflagration to detonation transition (DDT) processes in hydrocarbon - air gaseous mixtures. The influence of geometrical characteristics of the confinement, flow turbulization, temperature and fuel concentration in the unburned mixture on the onset of detonation and its possible arrest are discussed.

Introduction

In 1881 Mallard et Le Chatelier [1] and Bertelot et Vieille [2] were the first to face deflagration to detonation transition process. On investigating flame propagation in homogeneous gaseous mixtures they unexpectedly detected the onset of a supersonic mode of combustion wave traveling at velocities of thousands meters per second. This combustion mode got the name of “false” or “out of tone” combustion, which sounds in French like “detonation” being originated from the French verb “détonner’. The existence of two alternative velocities for the combustion process needed theoretical explanation, which was given in 1993 by an Associate Professor of Moscow University V.A.Mikhelson in his paper “ On normal combustion velocity of explosive gaseous mixtures”[3]. Based on having been published by that time papers by Rankine [4] and Hugoniot [5] Mikhelson was the first to explain that the mechanism of flame propagation in detonation was not the heat conductivity, but “adiabatic heating up to the ignition point in shock waves”. That was the birth of the classical theory of detonation, which found its further development in the papers by Chapman [6] and Jouget [7].

Investigations of deflagration to detonation transition (DDT) in hydrogen -- oxygen mixtures [8-11] and later in hydrocarbons - air mixtures [12-14] 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 [9, 11] and the gradient mechanism of "spontaneous flame" by Zeldovich [15].

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 [16-22]. 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 [23]. 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 [23]. The fundamental experimental and theoretical investigations [24, 25] of the reflected shock - laminar flame interactions bringing to the onset of detonation 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.

Analyzing a detonation initiation by means of local heat release, one can distinguish three scenarios. The first takes place when a strong shock wave develops in gas, and activation of chemical reactions increases behind the wave due to the increase of temperature and pressure. The second scenario of detonation initiation can take place when the shock wave developed after a local heat release not strong enough to activate the chemical reactions before it fades away; however, the temperature increase in the heat release core is enough to activate chemical reactions there. In this case, a

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normal combustion wave propagates from the heat release core (ignition location). Heating from burnt layers due to thermal conduction, not compression in a shock wave, is the primary mechanism of the wave propagation. Developing in gas, the combustion wave accelerates and disturbs the flow ahead of the front; this brings to further acceleration of the flame. Compression waves ahead of the combustion front converge into one or several shocks overtaking each other. Finally, either stabilization of the flame velocity, or detonation developing is possible; in the last case the velocity of detonation wave propagation stabilizes on the level of self-sustaining detonation. This process of detonation onset is known as deflagration to detonation transition (DDT). Many theoretical and experimental studies are devoted to an intermediate case, which is characterized by stabilization of normal combustion wave being affected by additional small shock wave interaction: both effects being too weak to cause detonation, but their combination bringing to the detonation onset[24, 25]. To promote DDT in tubes effective measures were suggested: introducing the Shchelkin spiral in the ignition section [26], incorporating wider turbulizing chambers in the ignition section (Smirnov's cavities) [12, 23], blocking the initial part of the tube with orifice plates [27]. To bring detonation to a decay detonation arrestors are used [28]. Wider turbulizing chambers were discovered to provide for DDT both promoting effect and inhibiting effect depending on their number and location [29]. The present investigation was aimed at revealing the effects of geometrical characteristics of combustion chambers in flame acceleration and changing the combustion modes.

Mathematical model

Numerical investigations of the DDT processes were performed using the system of equations for the gaseous phase 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 [30]. The production and kinetic terms were modeled using the Gaussian quadrature technique.

The governing equations include mass balance in the gas phase, mass balance of components, momentum balance and energy balance respectively. The term responsible for chemical transformations, is very sensitive to temperature variations, as it is usually the Arrhenius law type function for the reactions' rates. The temperature was regarded as a stochastic function with mean value and mean squared deviate.The model was closed then by the equations for turbulent kinetic energy, dissipation and mean squared deviation of temperature.

The procedure for averaging non-linear functions was described in details in [30].

The system of gas-dynamics equations was split in three parts due to three different physical processes: chemistry, source terms, turbulence production formed the "local part" of the equations; convective terms formed the "hyperbolic part" of the equations; and diffusive, viscous and thermo-cunductive terms formed the "parabolic part" of the equations.

The local part was solved implicitly using an iterative algorithm independently for each grid node. The hyperbolic part was solved using explicit FCT techniques [31]. The parabolic part was solved implicitly using 3-diagonal matrix solvers for linear equations [32]. The techniques removed viscosity from the time step criterion and reduced it to the Courant-Friedrichs-Lewy criterion.

To solve the system of equations splitting by coordinates was used according to MacCormack [33]. Validation of the numerical scheme was performed by comparing the results of test runs with the exact gas-dynamics solutions and with model experiments on turbulent flames propagation in confined volumes.

Results of numerical modeling

Numerical modeling made it possible to explain the scenario of flame acceleration and the onset of detonation on the contact surface ahead of the flame zone (Fig. 1). In flame acceleration weak shock waves in gas precede the deflagration wave. The interaction of shock waves 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 on the contact surface. That explosion can bring to either deflagration or detonation waves propagating from the exothermic center. 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 Chapman-Jouget speed.

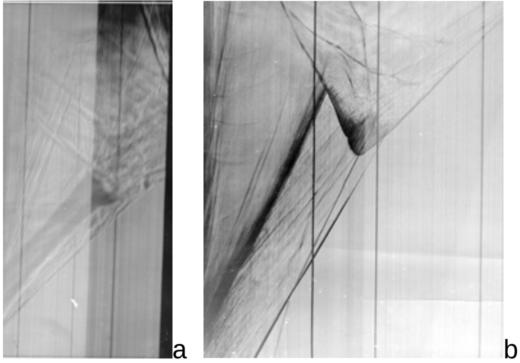
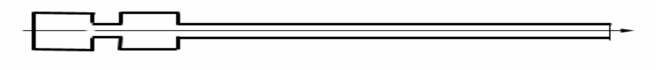


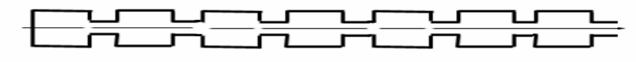
Fig. 1. Schlieren pictures of detonation onset in flame zone (a) and on the contact surface ahead of flame.

Experimental investigations of the deflagration to detonation transition in combustible gases testified that the presence of different turbulizing elements in the initial sections of detonation tubes promotes DDT by shortening the pre-detonation length and pre-detonation time. Turbulizing chambers (cavities) of a wider cross-section were found to be one of the most effective geometrical promoters for the DDT. Numerical experiments were undertaken for comparative studies of the role of different turbulizing elements and their location in the tube (Fig. 1). Ignition of mixture was performed by a concentrated energy release in the center of the first chamber or the tube itself in the left hand side near the closed end. The number of chambers was varied from one to twenty. Simulations were performed for the following cases:

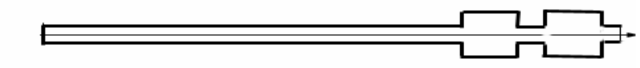
1) the initial section had two incorporated turbulizing chambers of a wider cross-section;
2) the far end section had two similar incorporated turbulizing chambers of a wider cross-section;
3) turbulizing chambers were located along the whole tube.



a) two chambers in the ignition section;



b) chambers incorporated into the tube along the whole length;



c) two chambers in the far end section of the tube.

Fig. 2. Geometry of the computational domain.

The role of chambers in the ignition section.

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 containing a detonation tube with two chambers of a wider cross-section (Fig. 2) filled in with combustible gaseous mixture at ambient pressure. Ignition of the mixture was performed by a concentrated energy release in the center of the first chamber. The results show the process of flame propagation that in the first chamber is rather slow and is determined mostly by initial turbulization of the mixture. 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 Fast combustion in the second chamber brings to a sharp pressure increase that pushes the flame further into the tube, which gives birth to strong flow nonuniformity and shock wave formation in the tube ahead of the flame zone. At some place the detonation arises from a hot spot within the combustion zone, which gives birth to strong detonation and retonation waves. Fig. 3 shows mean flame front velocity variation in the tube versus time for the cases of tube incorporating two chambers in the ignition section (Fig. 3,a), and a tube without any chambers (Fig. 3,b). It is seen that the onset of detonation in a tube without chambers is an unstable stochastic process, and each pulsation of velocity depending on some additional disturbance could result in the onset of detonation. The increase of the number of chambers incorporated into the ignition section to one or two makes the DDT more stable and brings to the decrease of pre-detonation length.

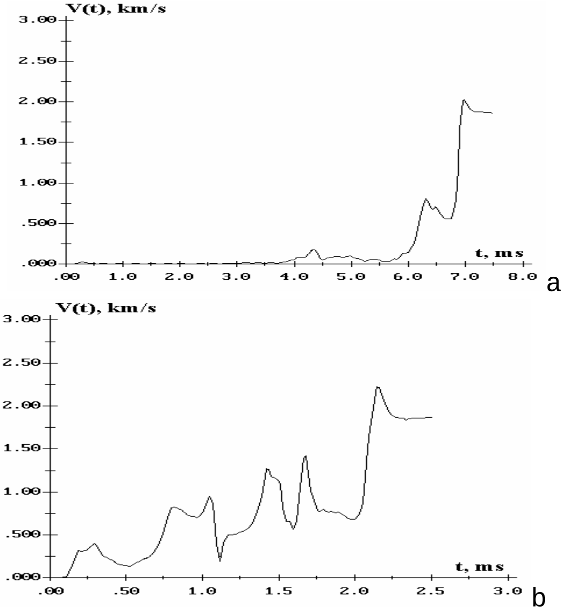
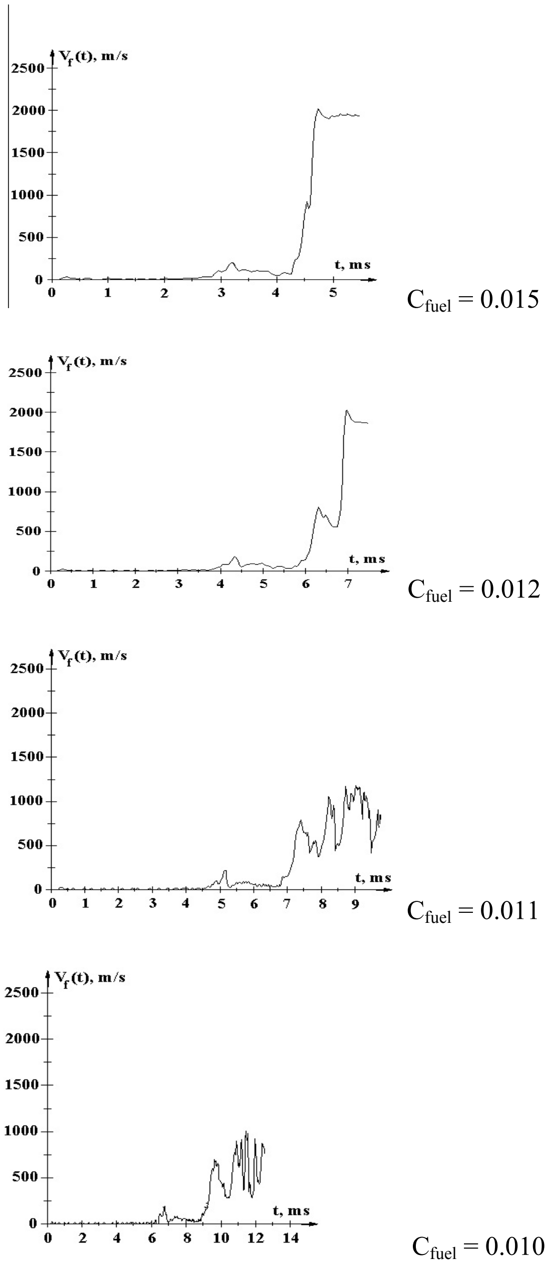


Fig. 3. Mean flame front velocity variation in the tube versus time for fuel concentration C_{fuel}=0.012: ***a*** - tube incorporating two chambers in the ignition section, ***b*** - tube without any chambers

The influence of fuel concentration.

Fig.4 *a-d* shows the mean flame front velocity variation in the tube for different values of fuel concentration, but for one and the same tube geometry. It is seen that flame accelerates on entering the second chamber, then it slows down. A high speed combustion wave enters the detonation tube, where the transition takes place. Analysis of results present in Fig.4 shows that on decreasing the fuel content of the mixtures its detonability via DDT decreases. The pre-detonation time increases (Figs.4*a,b*), but once the onset of the detonation takes place it propagates at a practically constant velocity. Velocity diagrams testify, that in both cases the onset of detonation takes place via an overdriven regime.

The decrease of fuel molar concentration below C_{fuel} = 0.011 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 peaks) and in the center and bring to flame zone accelerations. The reaction zone trajectories and velocities shown in Fig.4 *c,d* allow to evaluate oscillations. For fuel concentration 0.011 the galloping combustion regime propagates with velocity oscillations within the range of 420 – 1200 m/s. The onset of detonation does not take place within the 2.25 m length of the tube. The average velocity of the galloping combustion mode here was 760 m/s. For fuel concentration 0.010 the galloping combustion begins later and propagates with a lower velocity: oscillations within the range 270 - 1000 m/s, average velocity 435 m/s.



C_{fuel} = 0.015

C_{fuel} = 0.012

C_{fuel} = 0.011

C_{fuel} = 0.010

Fig. 4. Reaction front velocity for different fuel concentrations in a two-chamber device.

The role of chambers at the end of the tube

To provide a comparative data we investigated the role of two chambers of a wider cross-section incorporated in the far end of the tube. The tube was identical to that used in previous numerical experiments but symmetrical in respect to 180° rotation (equivalent to ignition performed at the opposite side) (Fig. 2c). Numerical results showed that after ignition in a narrow tube (ignition energy was increased) acceleration of flame zone accompanied by a number of oscillations brought to formation of the detonation wave propagating with mean velocity 1850 m/s. On entering the first chamber decoupling of the shock wave and reaction zone took place and the mean velocity of reaction zone propagation decreased to 200 m/s, then in a narrow bridge flame accelerated up to 400 m/s, and slowed down in the second chamber to 100 m/s. Fig. 5 illustrates flame velocity variation versus time for the detonation onset and degeneration in a tube with two chambers at the end (fuel concentration was 0.012). Thus similar chambers of wider cross-section incorporated in the end of the detonation tube bring to an arrest of the detonation wave.

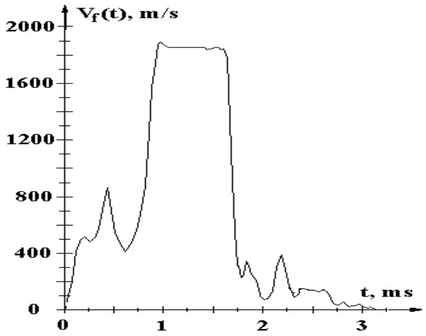
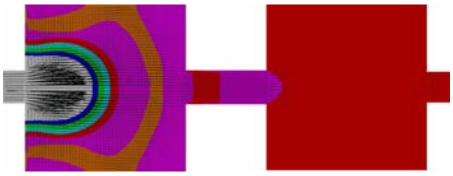


Fig. 5. Reaction front position and velocity for fuel volumetric concentration 0.012.

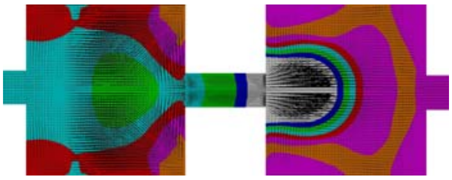
The effect of chambers incorporated in the tube along the whole length

The geometry of the test vessel was the following: the detonation tube 2.95 m length incorporated 20 similar turbulizing chambers uniformly distributed along the axis. The results showed that for the fuel concentration 0.012 the DDT process did not take place at all. The galloping combustion mode was established characterized by velocity oscillations within the range 80 - 300 m/s, average velocity of flame front 156 m/s. The maps of density and velocity for successive times in the section of the tube incorporating chambers number 6 and 7 are shown in Fig. 6. It is seen that in each chamber combustion passes through similar stages: flame penetration from the tube, expansion and slowing down in the chamber, being pushed into the next tube accelerating due to continuing combustion in the chamber. Reaction zone trajectory and velocity for fuel concentration 0.012 are shown in Fig.7.

The results of numerical experiments show, that increasing the number of turbulizing chambers did not promote the DDT for the present configuration, but just the opposite, it prevented from the onset of detonation and brought to establishing of the galloping combustion mode. The effect took place due to very sharp jumps of the cross-section area in the chambers and periodical slowing the flame down due to its expansion. (In the present numerical experiment the expansion ratio parameter $\beta_{ER} = (S_{chamb} - S_{tube}) / S_{chamb}$ was equal to 0.96.) Why does the increase of the number of chambers up to two promote DDT, while further increase inhibits the process? To answer the question let us regard the flame dynamics in DDT in a two chamber tube (Fig. 3, *a*) keeping in mind that the necessary condition for the DDT is turbulent flame acceleration up to a speed surpassing sonic velocity. Analysis of results shows, that the piston effect of expanding reaction products in the chamber brings to a rapid flame acceleration on entering a narrow tube. After the first chamber flame acquires velocity ~200 m/s, which is less than sonic velocity. After the second chamber flame is pushed into the tube with a velocity 500 - 700 m/s, which surpasses the sonic velocity. Thus further increase of the number of chambers is not necessary as it would not increase chamber exit velocity. However, investigations of different mixture composition and geometry of cavities [34] showed optimal number of cavities to be four.



t = 9.01 ms



t = 10.00 ms

Fig. 6. Density maps in 6-th – 7-th chambers, ratio β_{ER} =0.96 , fuel volume concentration 0.012

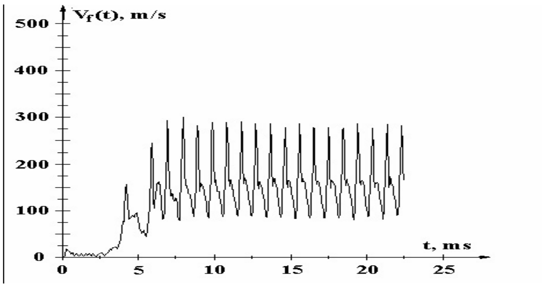


Fig. 7. Reaction front position and velocity in a tube with multiple cavities.

The influence of mixture temperature on DDT

The influence of temperature on the DDT in gases is one of intriguing issues. The available experimental data on the influence of initial mixture temperature on the DDT process in gases is contradictory. The experiments on DDT in stoicheometric hydrogen-oxygen mixtures in tubes of a constant cross-section at a constant pressure showed the increase of the pre-detonation length with the increase of temperature [35]. On decreasing the content of hydrogen the essential influence of initial mixture temperature on the pre-detonation length was not detected within the temperature range 311K—473K [36]. Investigations of DDT in hydrocarbon fuel-air mixtures [12] in tubes incorporating cavities in the ignition section demonstrated the decrease of pre-detonation length with the increase of initial mixture temperature.

Contradictory results are due to two opposite effects: on one hand, the increase of temperature promotes chemical reactions thus promoting the flame acceleration due to kinetic reasons, on the other hand, transition to the detonation takes place after turbulent flame propagation relative velocity surpasses the speed of sound in gas, which increases with the temperature increase, thus inhibiting the transition process. Probably, due to the competition of these opposite effects the available data on the influence of initial mixture temperature on the DDT process in gases is contradictory.

As it has been already mentioned, in stoicheometric hydrogen-oxygen mixtures the increase of temperature brought to the increase of pre-detonation length [36].

In our investigations of the DDT in tubes incorporating chambers of a wider cross-section [12, 14, 23] we rely heavily on the role of a piston effect of the expanding reaction products, which penetrate the narrow tube from a wide chamber thus pushing the turbulent flame in the tube assisting it in achieving high velocities surpassing the velocities of sound. Thus the influence of temperature on sonic velocity brcomes relatively small. The use of turbulizing cavities neutralizes the negative effect on DDT of sound velocity increase with the increase of temperature. Thus the effect of reduction of chemical induction time with the increase of temperature could turn to be predominant. (Fig. 8)

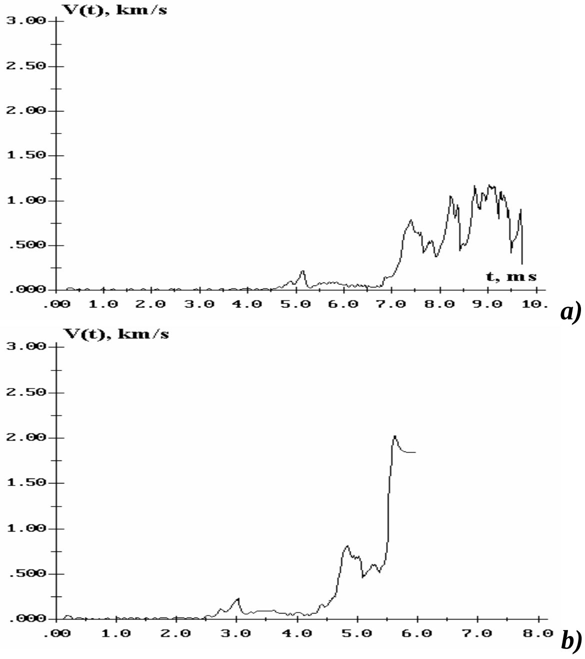


Fig. 8. Flame velocity in a tube with 2 cavities, C_{fuel}=0.011, β_{ER}=0.96, for normal and elevated temperatures: ***(a)*** - T_0=300 K; ***(b)*** - T_0=353 K .

Acknowledgements

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