Fundamentals of Deflagration to Detonation Transition in Gases.*

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Keywords: deflagration, detonation, pulse detonating devices, transition scenario, control, numerical models

Deflagration to detonation transition (DDT) is, undoubtedly, the most intriguing phenomenon among those relative to combustion processes. DDT in gases is relevant to gas and vapor explosion safety issues, as well as to creating pulse detonating devices. Knowing mechanisms of detonation onset control is of major importance, on one hand, for creating effective mitigation measures addressing the two major goals: to prevent the DDT in case of mixture ignition, or to arrest the detonation wave in case it was initiated. On the other hand, it is important for developing reliable pulse detonating devices for PDE and other practical applications. Being very widely spread in practice hydrocarbon fuel-air mixtures are of great interest from the point of view of DDT and detonation arrest.

The goal of the present paper is to discuss fundamentals of DDT processes in hydrocarbon - air gaseous mixtures and to reveal the influence of major governing parameters (geometrical characteristics of the confinement, flow turbulization, mixture temperature and fuel concentration) on the onset of detonation.

Introduction

First 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. Different 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. 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; Zeldovich et al., 1988; Smirnov et al., 1989, 1995). 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 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.

To promote DDT in tubes effective measures were suggested: introducing the Shchelkin spiral in the ignition section (Shchelkin, Troshin, 1963), incorporating wider turbulizing chambers in the ignition section (Smirnov et al. 1986, 1999), blocking the initial part of the tube with orifice plates (Knystautas et al. 1998). To bring detonation to a decay detonation arrestors are used (Fischer, 1999). Wider turbulizing chambers were discovered to provide for DDT both promoting effect and inhibiting effect depending on their number and location (Smirnov et al. 2002). The present investigation was aimed at revealing the effects of wider turbulizing chambers in DDT and its control.

Theoretical investigations

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.(Smirnov et al., 2002). The production and kinetic terms were modeled using the Gaussian quadrature technique. 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 (Fig.1).

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 on the contact surface. That explosion can bring to either deflagration or detonation waves propagating from the exothermic center. Following the gradient

* Russian Foundation for Basic Research, US Office of Naval Research and European Program INTAS (00-0706) are acknowledged for financial support.

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.

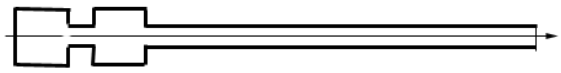

Fig.1. Two-chamber detonation tube.

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. 1) 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. 2 shows reaction zone trajectory (left) and mean flame front velocity (right) variation in the tube versus time for the cases of tube incorporating two chambers in the ignition section (Fig. 2,a), and a tube without any chambers (Fig. 2,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.

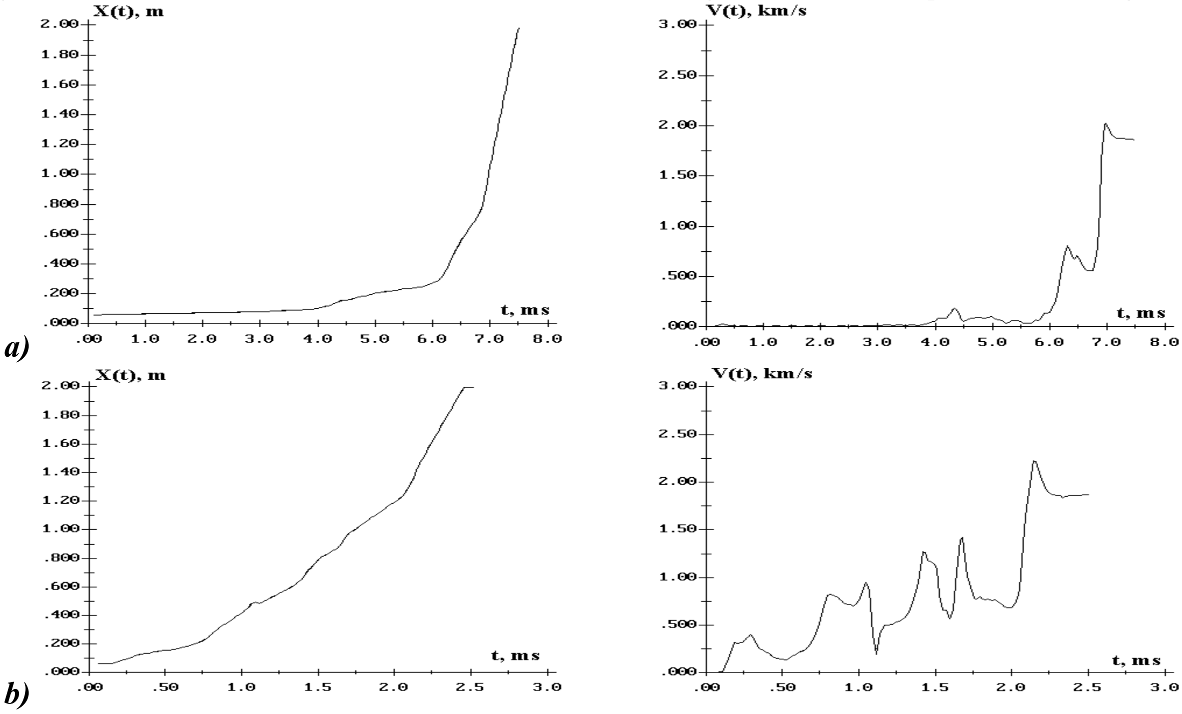

Fig. 2. Reaction zone trajectory (left) and mean flame front velocity (right) variation in the tube versus time for fuel concentration C_{fuel}=0.012: ***a*** - tube incorporating two chambers in the ignition section, ***b*** - tube without any chambers.

The 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 (Fig. 1), but symmetrical in respect to 180° rotation (equivalent t ignition performed at the opposite side). 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. 3 illustrates reaction front trajectory and velocity variation versus time for the detonation onset and degeneration in a tube with two chambers at the end (fuel concentration was 0.012).

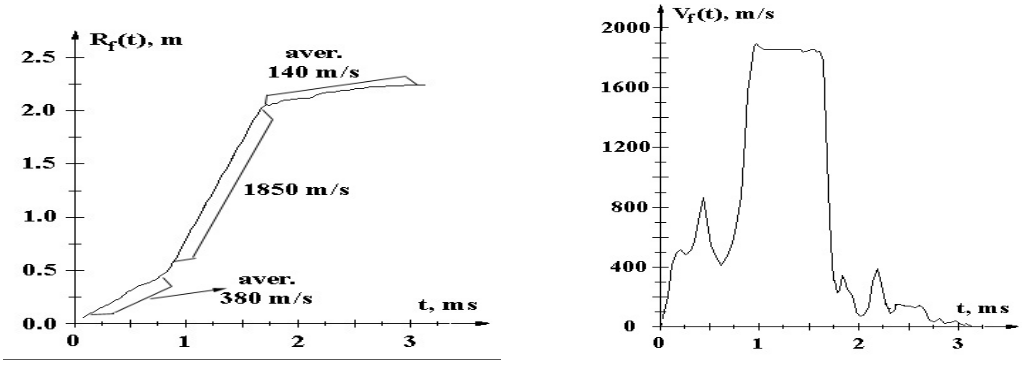

Fig. 3. Reaction front position and velocity for fuel volumetric concentration 0.012

Thus similar chambers of wider cross-section incorporated in the end of the detonation tube bring to an arrest of the detonation wave.

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. 4. 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.5.

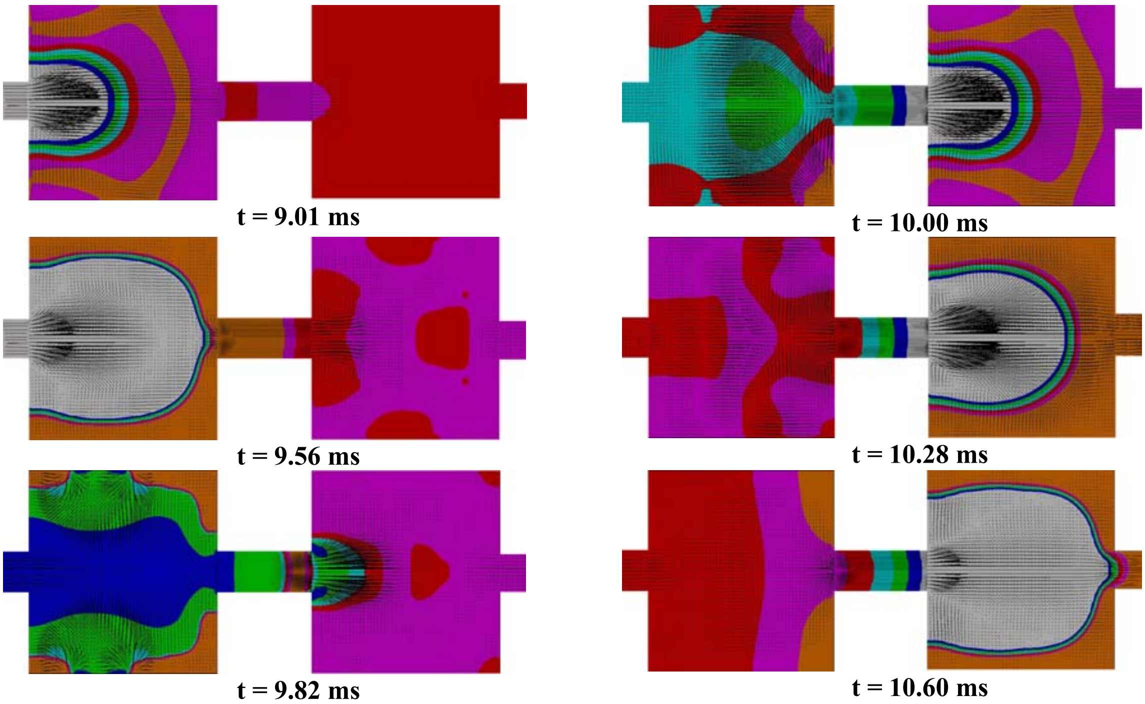

Fig. 4. Density maps in the 6-th – 7-th chambers. Expansion ratio β_{ER}=0.96 , fuel volume concentration 0.012

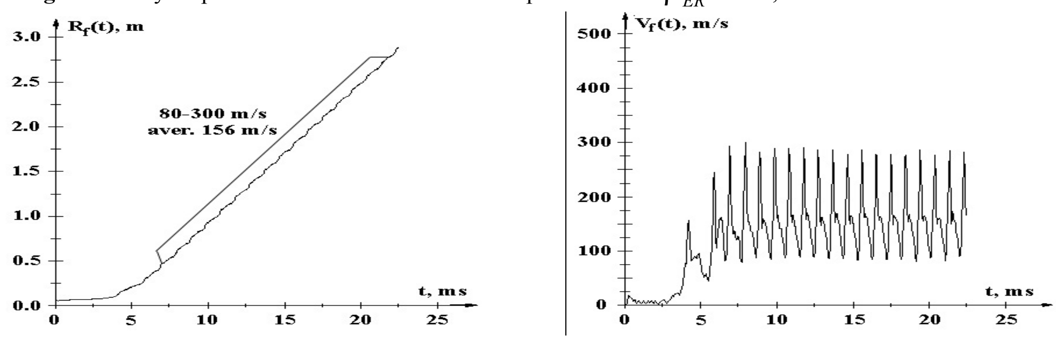

Fig. 5. Reaction front position and velocity in a multi-chamber tube.

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. 2, *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. Investigations of the sensitivity of self-sustaining combustion modes to expansion ratio parameter show that for small expansion ratios low velocity galloping detonation was established for large expansion ratios self-sustained galloping high speed combustion took place, the transient values of the expansion ratio, which characterize the transition from low velocity detonation to a high speed galloping combustion, increase with the increase of fuel concentration within detonability limits (Fig. 6).

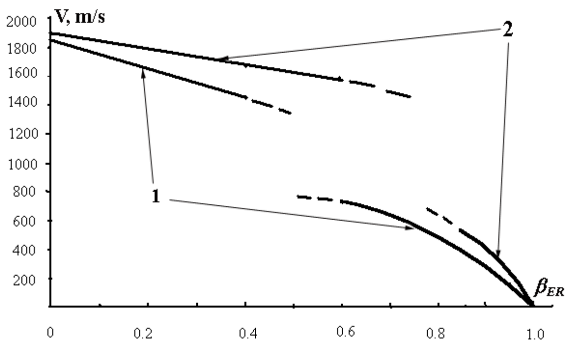

Fig. 6. Mean reaction front velocities in a multi-chamber tube for different expansion ratios:
1 - fuel concentration 0.012; **2 -** fuel concentration 0.015.

The influence of mixture temperature on DDT

In tubes incorporating wide chambers in the ignition section the increase of temperature promotes DDT and shortens pre-detonation length. This effect comes due to 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. The use of these turbulizing chambers neutralizes the effect of sound velocity increase with the increase of temperature. Thus the effect of reduction of chemical induction time with the increase of temperature turns to be predominant.

Conclusions

The undertaken experimental and theoretical investigations show that the onset of detonation wave in DDT process takes place in local exothermic centers ("hot spots") between the accelerating zone of turbulent combustion and the leading shock wave. Those hot spots appear due to flow non-uniformity mostly on the contact discontinuities, formed due to the interaction of shock waves overtaking each other ahead of flame zone.

Depending on hot spots internal structure they could give birth either to deflagration or detonation waves. In case of detonation onset the detonation wave propagates in all directions from the source and finally forms detonation wave propagating ahead and retonation wave propagating backward. The detonation wave overtakes the leading shock and after their interaction a quasi-plane overdriven detonation wave is formed in the unburned mixture, which gradually slows down to a self-sustained Chapman-Jouget mode.

In case the hot spot gives birth to a deflagration wave its propagation in all directions from the exothermic center is much slower, which gives enough time for the other hot spots to reach auto-ignition and in the long run could bring to the onset of detonation.

The presence of one or two turbulizing chambers of a wider cross-section in the ignition section shortens the pre-detonation length for hydrocarbon-air gaseous mixtures and makes the onset of detonation more stable.

The increase of the number of similar chambers uniformly distributed along the tube blocks the onset of detonation: galloping highs speed combustion modes were established for large expansion ratios, or low velocity galloping detonations were established for small expansion ratios. Mean reaction front axial velocity grows with the increase of hydrocarbon fuel concentration in the range of 0.010 - 0.015. For expansion ratios within the range 0.4 - 0.6 the increase of fuel content could bring to a change of propagation regime: galloping combustion mode could be changed for the low velocity detonation regime. Transient values of the expansion ratio, which characterize the transition from low velocity detonation to a high speed galloping combustion increase with the increase of fuel concentration within detonability limits.

The increase of the number of turbulizing fore-chambers in the ignition section promotes DDT until flame velocity on leaving the last fore-chamber surpasses sonic velocity. The further increase of the number of chambers inhibits DDT.

The increase of initial mixture temperature in tubes incorporating turbulizing fore-chambers of wider diameter in the ignition section promotes DDT and shortens pre-detonation length, while in tubes without fore-chambers the effect of temperature increase on DDT could be quite the opposite bringing to the increase of pre-detonation length.

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