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Acceleration of the Deflagration-to-Detonation Transition in Gases: From Shchelkin to Our Days

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Abstract: The development of some Shchelkin's ideas in investigations of the Semenov Institute of Chemical Physics of the Russian Academy of Sciences is described. These ideas include the discovery of different effects of intense and weak turbulence on surface combustion, study of phenomena near the detonation origination point, experimental demonstration of chemical self-preparation of an explosive mixture, and identification of the dominating role of gas-dynamic factors in the deflagration-to-detonation transition.

Keywords: turbulent combustion, acceleration of the deflagration-to-detonation transition, controlled detonation of gases.

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INTRODUCTION

In physics of gas combustion, the name of K. I. Shchelkin is associated with a large number of new ideas and achievements, which include the discovery of different effects of intense and weak turbulence on surface combustion [1], study of phenomena near the detonation origination point [2], experimental demonstration of chemical self-preparation of an explosive mixture [3], and identification of the dominating role of gas-dynamic factors in the deflagration-to-detonation transition (DDT) [4]. These ideas and achievements formed the basis for basic and applied research mainly dealing with explosion safety problems and (today) with practically feasible methods of obtaining controlled detonation in promising industrial pulsed-detonation burners and jet engines for flying vehicles [5]. The paper describes the development of the ideas put forward in [1–4] at the Semenov Institute of Chemical Physics of the Russian Academy of Sciences (ICP RAS) where Shchelkin started his research activities and performed the basic studies described above.

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TURBULENCE AND SURFACE COMBUSTION

The modern classification of various modes of homogeneous combustion of gases in a turbulent flow [6] includes a number of modes determined by the values of the Reynolds number (Re), Damköler number (Da), and Karlovitz number (Ka):

$$\mathrm{Re} = \frac{U_t L_t}{\nu}, \quad \mathrm{Da} = \frac{L_t/U_t}{\delta/u_n}, \quad \mathrm{Ka} = \frac{\delta/u_n}{L_K/U_K}.$$

Here U_t and L_t are the root-mean-square fluctuation of velocity and the turbulence macroscale, ν is the coefficient of kinematic viscosity of the gas, u_n and δ are the normal velocity and thickness of the laminar flame, and U_K and L_K are the velocity and turbulence microscales, respectively. The mode frequently observed in real combustion chambers is surface combustion with $\mathrm{Re} > 1$ (turbulent flow), $\mathrm{Da} > 1$ (fast chemical reactions), and $\mathrm{Ka} < 1$ (weak effect of turbulence on the internal structure of the laminar flame). In this mode of combustion, turbulence only curves the flame surface and does not exert any significant effect on the flame thickness and internal structure; therefore, the local velocity of turbulent combustion u_t can be formally determined from the mass conservation law

$$\frac{u_t}{u_n} = \frac{S'}{S_n} = F\left(\frac{U_t}{u_n}, \frac{L_t}{\delta}, \dots\right),$$

where S' is the surface area of the curved flame and S_n is the area of an equivalent plane flame. Numerous models for the function F have been proposed up to now. Some of them [1, 7–12] are given below:

$$F = 1 + \frac{U_t}{u_n} \quad [7], \tag{1}$$

$$F = \left(1 + \frac{U_t^2}{u_n^2}\right)^{1/2} \quad [1], \tag{2}$$

$$F = 1 + 0.52\left(\frac{U_t}{u_n}\right)^{1/2}\left(\frac{U_t L_t}{\nu}\right)^{1/4} \quad [8], \tag{3}$$

$$F = 1 + 0.62\left(\frac{U_t}{u_n}\right)^{1/2}\left(\frac{u_n L_t}{\nu}\right)^{1/4} \quad [9], \tag{4}$$

$$F = 1 + 0.95\mathrm{Le}^{-1}\left(\frac{U_t}{u_n}\right)^{0.5}\left(\frac{L_t}{\delta}\right)^{0.5} \quad [10], \tag{5}$$

$$F = 1 + 0.435\left(\frac{U_t}{u_n}\right)^{0.4}\left(\frac{u_n L_t}{\nu}\right)^{0.44} \quad [11], \tag{6}$$

$$F = -0.274\left(1 + \frac{u_n L_t}{\nu}\right) + \left[0.076\left(1 + \frac{u_n L_t}{\nu}\right)^2 + 0.547\left(1 + \frac{u_n L_t}{\nu}\right)\frac{U_t}{u_n} + 1.547\right]^{0.5} \quad [12] \tag{7}$$

(Le is the Lewis number).

Along with Damköler's formula (1), formula (2) derived by Shchelkin is referred to the classical formulas. Shchelkin's formula (2) predicts a weaker dependence of u_t on U_t than Damköler's formula and agrees better with the experiment.

An algorithm of explicit flame tracking in a turbulent flow has been recently developed at ICP RAS for modeling homogeneous combustion of gases [13, 14]. With a given initial geometry of the ignition site, the surface separating the fresh mixture from the combustion products is presented as a set of elementary areas of the turbulent flame. In the turbulent flame, each area of the flame front moves with a local velocity equal to the sum of the burning velocity u_t and the flow velocity. The burning velocity u_t is found by using one of the known turbulent flame models (1)–(7), and it depends on local values of u_n and on turbulence parameters. The flow field is determined by solving a system of averaged equations of the flow by the control volume method.

As the flow field is unsteady and inhomogeneous, the ignition site is deformed. The continuity of the combustion front is ensured by a system of heuristic rules eliminating improbable flame configurations from considerations. Electronic tables of the laminar burning velocity as a function of the initial temperature, pressure, and composition of the mixture play an important role in algorithm implementation. Such tables were composed on the basis of solving the problem on the structure of the plane laminar flame with the use of both detailed and semi-empirical kinetic mechanisms. In addition, such tables contain information on the flammability limits.

Using the above-described algorithm, we calculated turbulent combustion in tubes with one open end and in closed volumes. The turbulent flame velocity was determined by Shchelkin's formula. The turbulence parameters including U_t were calculated by the standard k–ε model. The flame front in each computational cell was described by 15 elements or more.

Figure 1 shows the calculated and experimental [15] dependences of the distance covered by the flame in a stoichiometric propane–air mixture in smooth tubes with a square rectangular cross section (the side length is 40 mm) and length of 5.1 and 6.1 m as functions of time under standard initial conditions. As in the experiments [15], the mixture was ignited at the closed end of the tube, and the flame position was determined by the leading point on the flame front. The calculated and experimental results are in excellent agreement, though the gas flow in the tube in the case considered here is complicated by flame interaction with the tube walls and also with expansion and compression waves periodically arising on the open end of the tube. When the flame approaches the open end of the tube, the visible velocity of the flame reaches 400 m/s.

The calculated and experimental [16] dependences of the flame front velocity on the distance covered by the flame in a stoichiometric propane–air mixture in a circular tube with the ratio of channel blockage by regular annular obstacles $f = 0.43$, 0.6, and 0.75 under standard initial conditions are compared in Fig. 2. The tube diameter is 15.2 cm, and its length is 3.1 m. The blockage ratio is determined as the ratio of the cross-sectional area of the obstacles to the cross-sectional area of the tube. The distance between the obstacles is equal to the tube diameter. It is again seen that the calculated results agree with the experimental observations. Good agreement is observed at the initial segment of flame acceleration up to 300–400 m/s. As a whole, the flame accelerates up to velocities of 800–900 m/s, which corresponds to the adiabatic velocity of sound in combustion products (≈890 m/s). At the initial stage, flame acceleration is more intense in the tube with large obstacles because they induce stronger turbulent oscillations. With increasing flame velocity, however, the losses of momentum on the obstacles also increase, and flame acceleration at higher blockage ratios is not so fast. Oscillations of the flame front propagation velocity

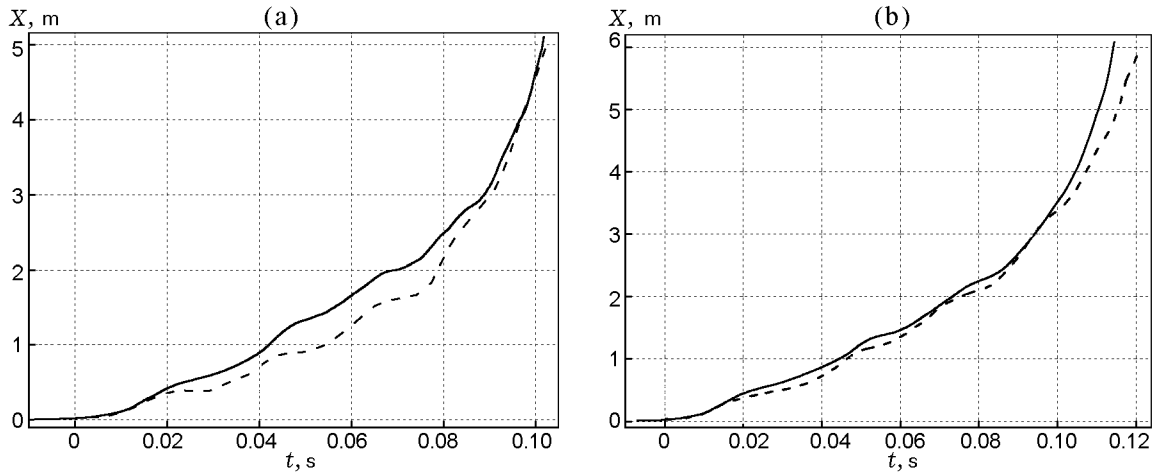


Fig. 1. Comparison of the calculated (solid curves) and experimental [15] (dashed curves) dependences of the distance covered by the flame in smooth tubes with a square cross section and length of 5.1 (a) and 6.1 m (b).

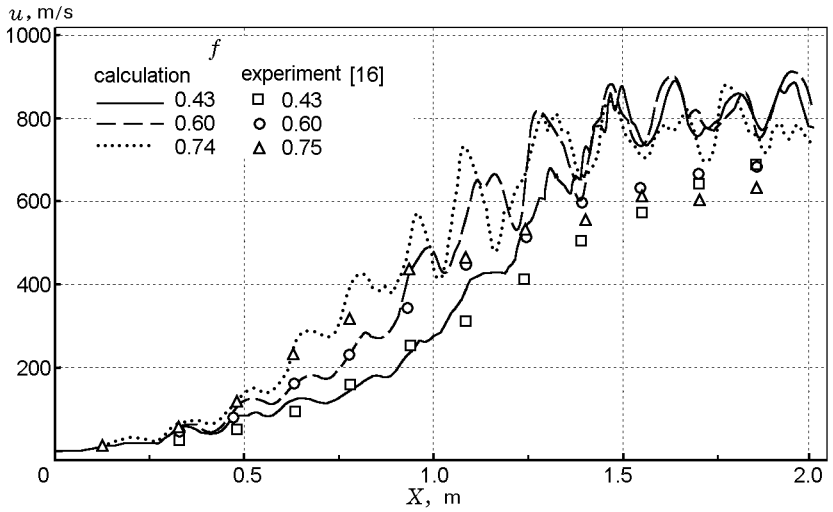
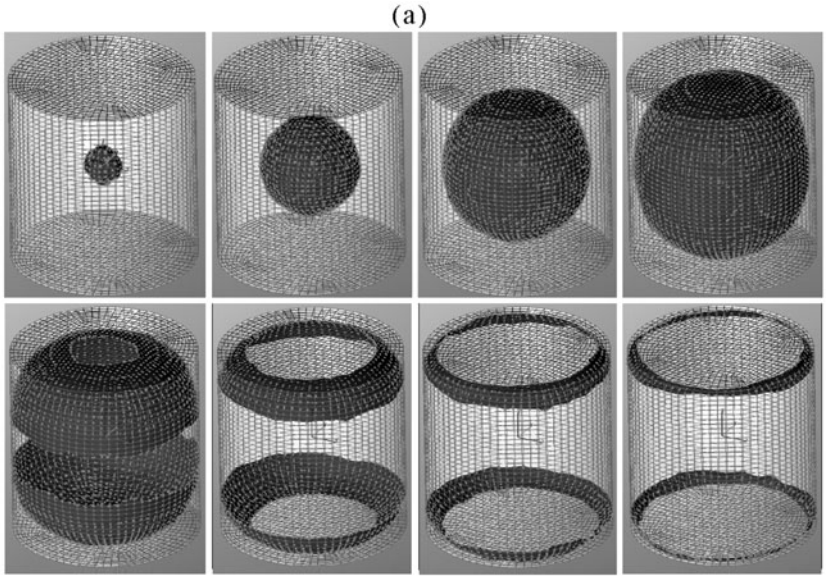


Fig. 2. Comparison of the calculated (curves) and experimental [16] (points) of the visible velocity of the flame front versus the covered distance.

are associated with flow constriction near the obstacles and flow expansion between them.

Figure 3 shows some examples of flame calculations in a closed cylindrical vessel (144.5 mm in diameter and 150 mm high) filled by rich propane–air mixture (Fig. 3a, fuel-to-air equivalence ratio $\phi = 1.1$) and lean propane–air mixture (Fig. 3b, $\phi = 0.8$) with the initial pressure $p_0 = 1$ atm and initial temperature $T_0 = 305$ K. Both in calculations and experiments [17], an initially quiescent mixture was ignited at the center of the vessel by a weak source. It is clearly seen from Fig. 3b that the calculation agrees well with the experiment up to the time $t \approx 80$ ms, when the pressure in the cylinder almost reaches the maximum value. The subsequent changes in pressure in the cylinder are mainly related to heat exchange with the cylinder walls, and fine computational grids should be used for correct modeling of these processes. As the spatial resolution of the grid in the near-wall region in these calculations was insufficient, the curve in Fig. 3b appreciably deviates from the experimental points at $t > 80$ ms.

As a whole, it follows from the above-given examples that Shchelkin's classical formula for u_t ensures a satisfactory description of unsteady combustion under conditions of both intense (flame acceleration in smooth tubes and in tubes with obstacles) and weak (combustion in a closed vessel) turbulence.



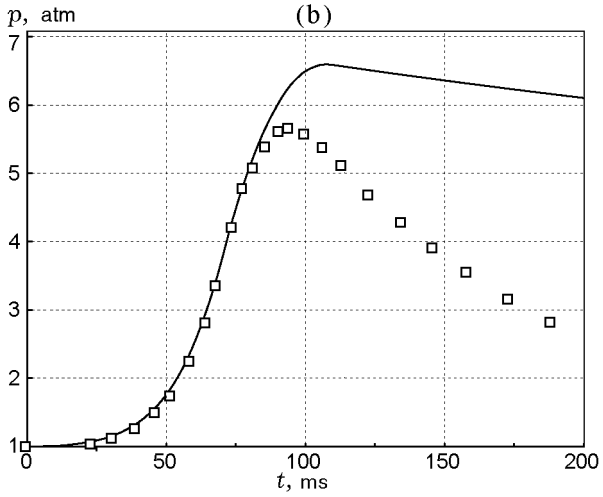


Fig. 3. Calculations of combustion of a propane–air mixture in a closed cylindrical vessel: (a) calculated positions of the flame front in the case of combustion of a rich ($\phi = 1.1$) mixture for the following moments (from right to left): $t = 5$, 15, 25, 35, 45, 55, 65, and 75 ms; (b) calculated (curve) and measured [7] (points) dependences of pressure on time in the case of combustion of a lean ($\phi = 0.8$) mixture.

PHENOMENA NEAR THE PLACE OF DETONATION ORIGINATION

In the course of DDT, self-ignition of the explosive mixture occurs in the fresh mixture ahead of the accelerating flame front, and reaction propagation transforms from the frontal mode (flame) to the volume mode (detonation). Shchelkin paid much attention to phenomena near the place of detonation origination [2]. Analyzing wave diagrams, he explained why detonation almost always occurs in an immediate vicinity of the accelerating flame front rather than at a certain (rather large) distance from it.

A special numerical method was developed at ICP RAS for multidimensional modeling of DDT. Using this method, one can simultaneously consider frontal and volume chemical reactions in a compressible turbulent gas flow [14]. Frontal combustion is described by the method of explicit identification of the flame front, and volume combustion is calculated by the particle method.

In the particle method, the pre-flame zone is presented as a set of Lagrangian elements or "particles," which are realizations of the local instantaneous state of the turbulent flow. The "particles" have their own temperature, density, chemical composition, and ve-

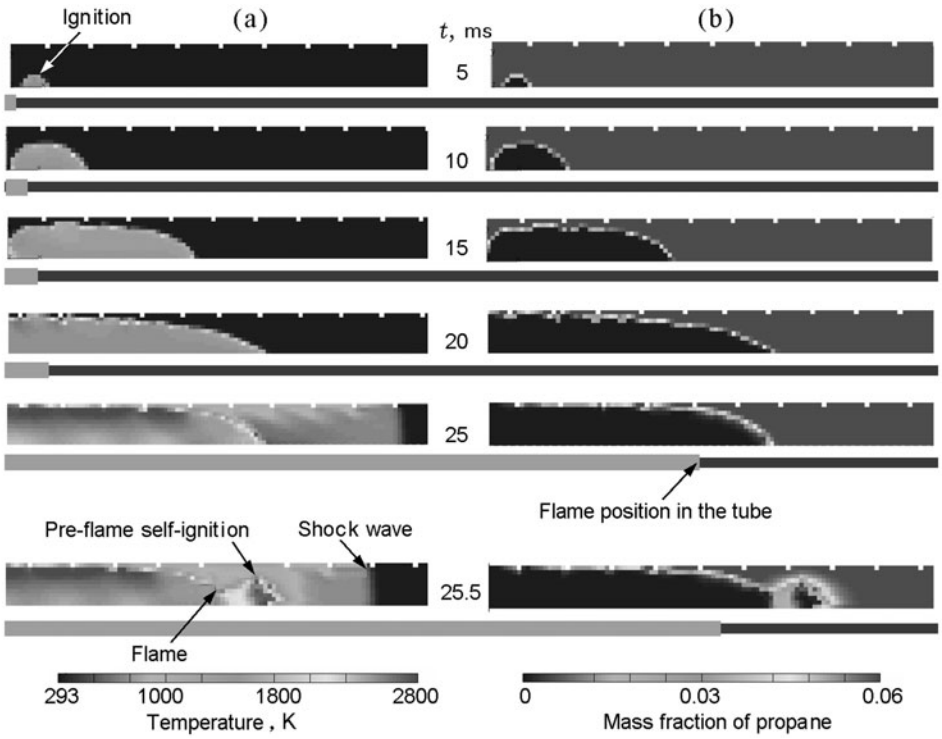


Fig. 4. Calculations of flame acceleration in a stoichiometric propane–air mixture until the instant of pre-flame self-ignition (only the upper half of the channel is shown).

locity; the evolution of these variables in space and time is described by the equation for the joint probability density function (JPDF) for velocity and scalars (concentrations of chemical species and enthalpy) [6]. The JPDF equation is numerically solved by the Monte Carlo method. The main advantage of this approach is the possibility of using some particular kinetic mechanism of self-ignition reactions without involving additional hypotheses about the influence of turbulent oscillations on the mean rate of chemical reactions: the mean reaction rate is determined by averaging over an ensemble of "particles."

Figure 4 shows an example of calculations of flame acceleration in a plane channel 40 mm wide and 3 m long with regular obstacles having a 2×2 mm rectangular cross section (placed with a step of 20 mm). The channel is filled by a stoichiometric propane–air mixture under standard initial conditions. The channel walls are assumed to be isothermal and cold.

The process begins when the mixture is ignited at the closed end (see the time instant $t = 5$ ms in Fig. 4). The flame accelerates to ≈40 m/s during ≈20 ms and up to 950 m/s during the next 5 ms. At the time $t =$ 25 ms in Fig. 4, one can clearly see the bow shock wave moving approximately 60 mm ahead of the extended flame and a series of shock waves attached to obstacles in the pre-flame zone.

By the time of 25.5 ms after ignition of the mixture, a compact set of self-ignition sites is formed in the central part of the flow, at a moderate distance from the flame front. These sites are seen both in the temperature distribution (Fig. 4a) and in the distribution of the propane mass fraction (Fig. 4b). The geometry of the region with self-ignition sites resembles a vortex core ahead of a piston moving in a tube. The instantaneous values of temperature and fuel mass fraction in these sites are noticeably different, which testifies that the explosive reactions in these sites occur at different times. The "detonation" (in accordance with Shchelkin's terminology [2]) ignition of the gas ahead of the flame front first occurs at a certain distance from the front, near the plane of symmetry of the channel, and then "propagates" in the form of a disordered series of self-ignition events in the streamwise direction and predominantly in the transverse direction, not reaching the cold wall. In our opinion, under conditions of intense turbulence in the pre-flame zone, we can talk only about self-ignition events rather than a self-ignition waves because the formation of ordered spatial structures with a macroscopic gradient of the self-ignition induction period is little probable and was not predicted by calculations. It is important to note, however, that explosions of individual sites generate secondary shock waves in the medium, which is already prepared to self-ignition

as a whole. Collisions of such waves can give rise to secondary sites, etc., i.e., the process is escalated.

In the numerical example considered here, the detonation in the channel occurred at the time of 25.7 ms, i.e., 200 μs after the first events of pre-flame self-ignition.

CHEMICAL SELF-PREPARATION OF THE EXPLOSIVE MIXTURE

The effect of self-preparation of the explosive mixture on DDT was first demonstrated in the experiments of Shchelkin and Sokolik [3]. They showed that preliminary thermal preparation of the combustible mixture before spark ignition can reduce the pre-detonation distance almost by 50%. The experiments [3] were performed in a closed glass tube 110 cm long, which had an inner diameter of 20 mm. The tube was placed into an electric furnace with a slot for recording flame propagation and DDT onto a moving photographic film. A spark plug was placed at one of the tube ends. The examined explosive was a homogeneous mixture of vapors of petroleum ether (fraction with a boiling point at 38–40°C, which was conventionally given the name of pentane in [3]) at $\phi \approx 1.1$. The mixture was composed in a reservoir by the method of partial pressures and was then fed to a tube heated to a temperature $T_0 = 598$–673 K. The duration of the mixture motion from the reservoir to the tube was 0.4–0.6 s. The pressure and temperature of the mixture in the experiments [3] were chosen in such a manner that the mixture experienced cold-flame oxidation, but did not reach self-ignition. Such a situation was ensured by reduced pressures $p_0 = 0.33$–0.49 atm. The cold flame induction period τ (time from the instant when the mixture arrived in the tube until a small pressure peak was detected by a high-sensitivity membrane manometer) was measured in preliminary experiments (without spark ignition). The occurrence of the cold flame was accompanied by an increase in temperature by 200–300° and by weak glowing of the gas. Depending on the temperature and pressure of the mixture in the tube, the cold flame induction period varied in the interval $\tau = 0.4$–3.6 s. In the main series of experiments with spark ignition of the mixture, three parameters were varied: ignition delay t_i (time between the instant of arrival of the mixture in the tube and the instant of ignition), initial temperature T_0, and initial pressure p_0 of the mixture.

When the mixture was ignited at the closed end of the tube, accelerated flame propagation was first observed in the experiments [3]. The detonation occurred in the region between the shock wave and the flame front. In the photographic records, it was identified with the emergence of a new front of bright luminosity with a significantly different slope and also with the emergence of a retonation wave propagating in the opposite direction. The pre-detonation distance S was determined from the photographic records of the process as the distance between the ignition plug to the point of a drastic change in the luminant front slope.

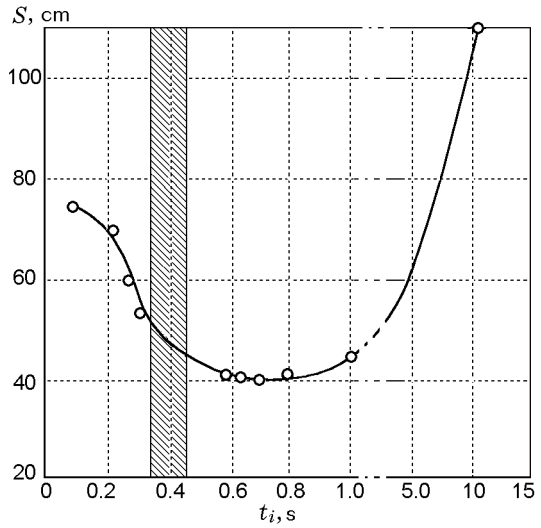


Fig. 5. Pre-detonation distance S versus the ignition delay t_i [3]: $C_5H_{12} : 8O_2$ mixture, $T_0 = 608$ K and $p_0 = 0.42$ atm; the hatched area shows the time of cold flame occurrence.

The results of the experiment [3] at $T_0 = 608$ K and $p_0 = 0.42$ atm are presented in Fig. 5 as the dependence of S on the ignition delay t_i. Because of the errors in measurements of τ, the instant of cold flame occurrence is marked in the figure as a hatched band, which covers a time interval of approximately 0.2 s. The main result of the experiments [3] was the drastic reduction of the pre-detonation period length in the case with the mixture ignited at an instant directly after the cold flame occurrence and, vice versa, extension of the pre-detonation period in the case with the mixture ignited after a considerable time after cold flame occurrence (the pre-detonation distance can become so large that no detonation occurs at all).

The effect (which is now called the Shchelkin–Sokolik effect) of drastic reduction of the pre-detonation distance was attributed in [3] to significant changes in the reactive and kinetic properties of the mixture at the cold flame stage of the oxidation process. On the one hand, active products of oxidation (such as hydroperoxides) appear in the mixture during the cold flame induction period. Subsequent decomposition of these products in the cold flame leads to the formation of new ac-

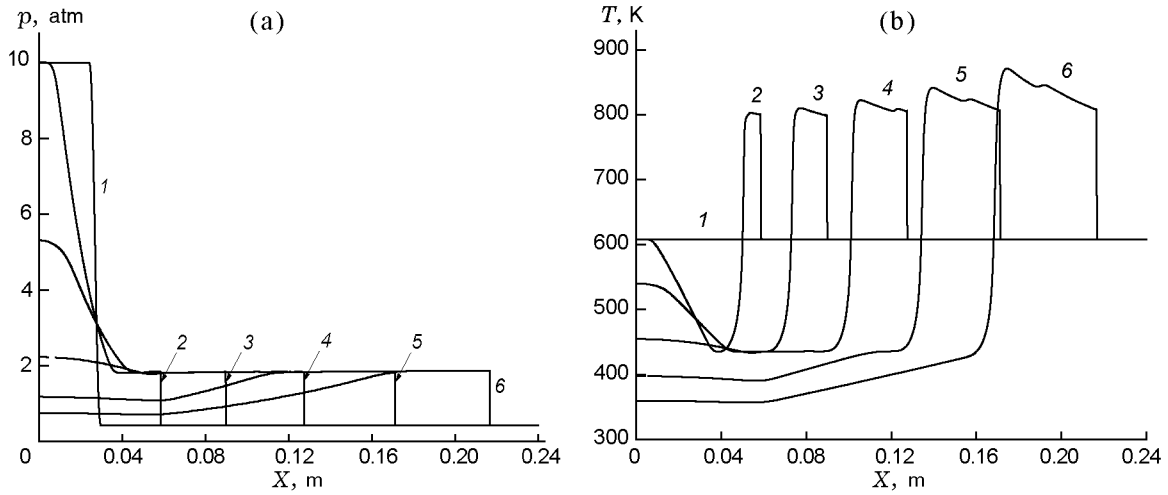


Fig. 6. Calculated profiles of pressure (a) and temperature (b) in the shock wave without preliminary thermal treatment of the mixture ($C_5H_{12} : 8O_2$): $T_0 = 608$ K, $p_0 = 0.42$ atm, $t_i = 0$, and $t = 0$ (*1*), 43.4 (*2*), 87.2 (*3*), 141 (*4*), 204 (*5*), and 270 μs (*6*).

tive centers accelerating oxidation reactions and, therefore, increasing the detonability of the mixture. On the other hand, the decrease in the detonation velocity in the case with the mixture ignited immediately after the cold flame stage, which was noted in [3], testifies to the loss of the portion of the combustion heat released in the cold flame (up to 10%) and, therefore, to reduction of the burning temperature and laminar flame velocity. According to [3], the existence of the minimum on the curve $S(t_i)$ is induced by the prevailing effect of the first factor during the time interval about $t_i - \tau \leqslant 0.5$ s. At $t_i - \tau > 0.5$ s, the second factor starts to dominate. Moreover, as the oxidation process following the cold flame goes on, more stable products (aldehydes and alcohols) appear in the mixture, and its detonation properties degenerate.

To quantify the Shchelkin–Sokolik effect, we posed and solved the following problem [18]. A straight tube of length L was filled by a homogeneous *n*-pentane–oxygen mixture with an initial pressure p_0 and initial temperature T_0. The tube was assumed to be closed on both ends and to be thermally insulated. As the detonation in the experiments [3] occurred in the region between the shock wave and the accelerating flame front, we simplified the problem by eliminating spark ignition of the mixture and accelerated flame propagation from considerations. Instead, we considered propagation of a shock wave with a certain prescribed initial intensity from one of the closed ends of the tube ($X = 0$). The Mach number of the shock wave at elevated initial temperatures (600–900 K in the experiments [3]) was M $\approx$ 1.8–2.4.

In our calculations, we used a semi-empirical kinetic mechanism of two-stage oxidation of *n*-pentane. The kinetic calculation of oxidation of a stoichiometric *n*-pentane–oxygen mixture in a closed reactor under the conditions of the experiments [3] showed that the cold flame occurs in the mixture at a certain time: during the time interval $t \approx 0.15$–0.21 s after the beginning of the process, the substance temperature increases from the initial value of 608 K to the maximum value of 930 K.

Figure 6 shows the calculated profiles of pressure and temperature at different time instances in the case of shock wave propagation in the tube without preliminary thermal treatment of the mixture. It is seen that the pressure profiles in the shock wave do not differ much from the case where the shock wave propagates in an inert gas. The temperature profiles, however, reveal heat release due to cold flame reactions behind the shock wave front: the temperature behind the front increases by 70–80 K prior to wave arrival on the right wall, but no self-ignition occurs behind the shock wave. In accordance with the definition of the pre-detonation distance used in [3], we have $S > L = 0.24$ m in the case considered.

Figure 7 shows the calculated profiles of pressure and temperature in the tube at different time instants for $t_i = 0.2$ s, i.e., with preliminary thermal treatment of the mixture during the time needed for the cold flame to occur in the tube. By the time $t = t_i = 0.2$ s, the mixture is heated by the cold flame up to $\approx$900 K, and its composition changes. At the time $t \approx t_i + 119$ μs, i.e., $\approx$119 μs after the beginning of shock wave propagation (curves 3 in Fig. 7), self-ignition occurs behind the wave front. As a result of self-ignition, two explo-

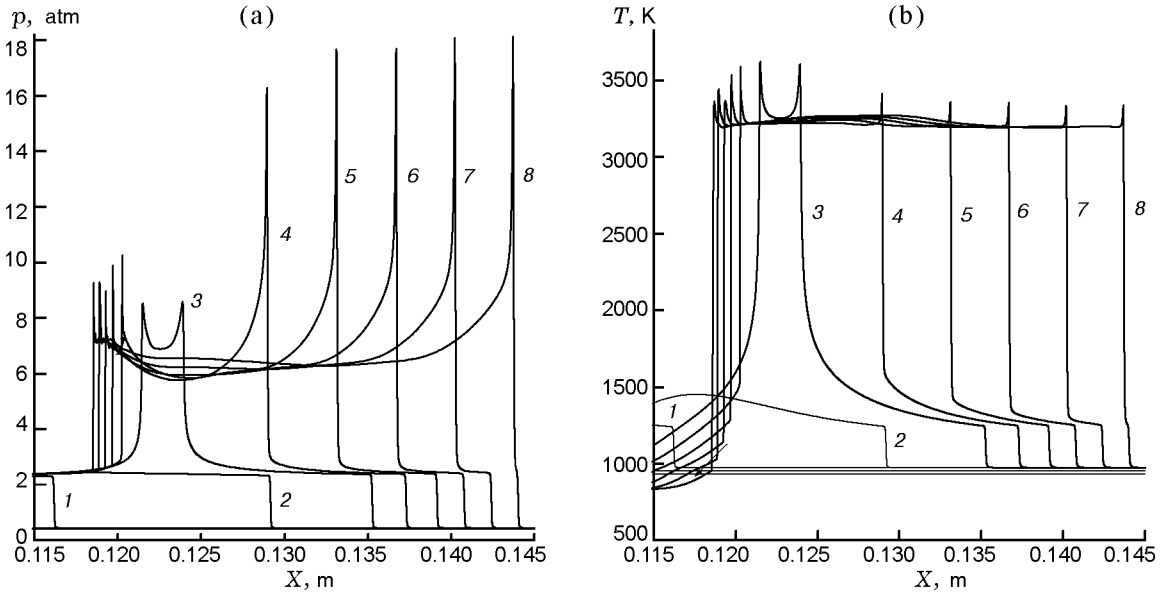


Fig. 7. Calculated profiles of pressure (a) and temperature (b) in the shock wave with preliminary thermal treatment of the mixture ($C_5H_{12}:8O_2$): $T_0 = 608$ K, $p_0 = 0.42$ atm, $t_i = 0.2$ s, and $t - t_i = 98$ (*1*), 112 (*2*), 119 (*3*), 121 (*4*), 123 (*5*), 124.7 (*6*), 126.1 (*7*), and 128.1 μs (*8*).

sive waves are rapidly formed in the shock-compressed gas: an overdriven detonation wave following the primary shock wave and catching up with it and a retonation wave propagating in the opposite direction. At $\Delta t > 129$ μs, a self-sustained detonation wave propagates along the tube toward its right end, and the calculated mean detonation velocity (≈1990 m/s) is fairly close to the measured value of 1970 m/s [3]. In accordance with the definition of the pre-detonation distance, we have $S \approx 0.122$ m in the case considered. Thus, comparing the results in Figs. 6 and 7, we can conclude that preliminary thermal treatment of the mixture in the cold flame improves the conditions for detonation occurrence.

To evaluate the influence of the chemistry of cold flame oxidation and intermediate products on shock wave propagation in a pentane–oxygen mixture, we used a detailed kinetic mechanism with two effective near-wall reactions of recombinations of active radicals (peroxides) and with allowance for heat transfer to the tube walls [18]. The calculations led us to an interesting conclusion. If we take into account heat transfer to the tube walls and ignore recombination of peroxides on the wall, the calculated dependence $S(t_i)$ has no clearly expressed minimum observed in the experiment. For this reason, we can expect near-wall reactions to play an important role in small-diameter tubes with comparatively low pressures (as in the experiments [3]). In tubes with greater diameters and higher pressures, however, the role of near-wall reactions is expected to decrease, and the minimum on the dependence $S(t_i)$ degenerates. New experiments are needed to check this conclusion.

GOVERNING ROLE OF GAS-DYNAMIC FACTORS IN DDT

One of the prominent achievements of K. I. Shchelkin is his discovery of the governing role of gas-dynamic factors in the DDT phenomenon. His classical experiments on flame acceleration and DDT in tubes with wire spirals [4] demonstrated that flow turbulization ahead of the accelerating flame front is the most effective means of acting on combustion acceleration, which allows the pre-detonation distance and time to be appreciably reduced.

In this paragraph, we give a brief description of experimental studies of DDT acceleration in gases, which were recently performed at ICP RAS. The analysis of experimental results of various authors, which were obtained in tubes with different regular obstacles (spirals, annular inserts, etc.), revealed some contradictions concerning the limiting conditions for DDT. Thus, Kuznetsov et al. [19, 20] reported the results of experiments on DDT in methane–air mixtures having different compositions in straight closed tubes of different diameters equipped with regular annular obstacles with the distance between the obstacles being equal to the

tube diameter and with the blockage ratio of 0.3 to 0.6. Under standard conditions, DDT was observed only in tubes 520 and 174 mm in diameter, and the minimum distances from the ignition source to the place of detonation origination were $L_{\mathrm{DDT}} = 15$–17 and 6–8 m, respectively [19]. It is of interest that DDT in the tube 121 mm in diameter was observed only at an elevated initial pressure (2 atm and higher) at the distance $L_{\mathrm{DDT}} > 4$–5 m [20]. The results of Kuznetsov et al. [20], however, contradict the results of Vasil'ev [21] who reported experimental observation of DDT in a stoichiometric methane–air mixture in a tube 100 mm in diameter under standard conditions at an extremely short distance $L_{\mathrm{DDT}} = 2.5$–3 m in the case where patented obstacles of a special shape were used. Moreover, the results of Kuznetsov et al. [20] contradict the known fact that the limiting diameter of a smooth tube in which the methane–air mixture can detonate under standard conditions is close to 100 mm. For instance, recently we successfully initiated detonation in a stoichiometric methane–air mixture under standard conditions in a tube 94 mm in diameter by a comparatively weak shock wave with the Mach number of 3.3, which was diffracted on a single obstacle having a special shape of a convergent–divergent nozzle [22].

Apparently, the reason for these contradictions is different effects of obstacles on the flame and shock wave, which are two most important components of the DDT process. A cascade of regular obstacles or spiral turns, which favors rapid acceleration of the flame owing to intense turbulization of the flow, can interfere with shock wave propagation because of high losses of momentum and, thus, hinder or completely prevent the mere possibility of DDT. This means that the solution of the problem of DDT acceleration should be sought by careful selection of the shape of obstacles and their arrangement, which would provide optical matching of the flame acceleration rate and shock wave amplification. It was this idea that was used as a basis for the fast DDT concept, which was recently proposed at ICP RAS and was successfully validated in experiments not only for gas mixtures, but also for jet-droplet explosive mixtures [5].

Based on this concept [5], the possibility of controlled cyclic DDT in a tube 94 mm in diameter with one open end at very short distances with separate continuous supply of natural gas and air was proved in [23] for the first time. The experimental facility consisted of three connected sections: settling chamber with the ignition source (standard car plugs), device for flame acceleration with a total length of 1200 mm, and tube 3600 mm long accommodating obstacles having a special shape and arranged in a special order.

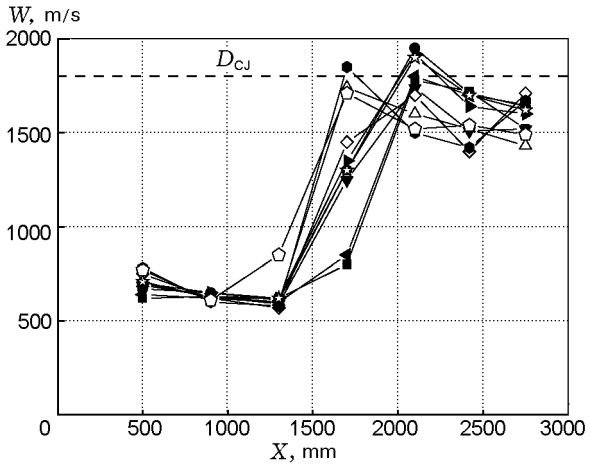


Fig. 8. Deflagration-to-detonation transition in a mixture of natural gas and air in ten cycles of operation of a pulsed-detonation burner with a frequency of 0.03 Hz with individual continuous supply of natural gas and air.

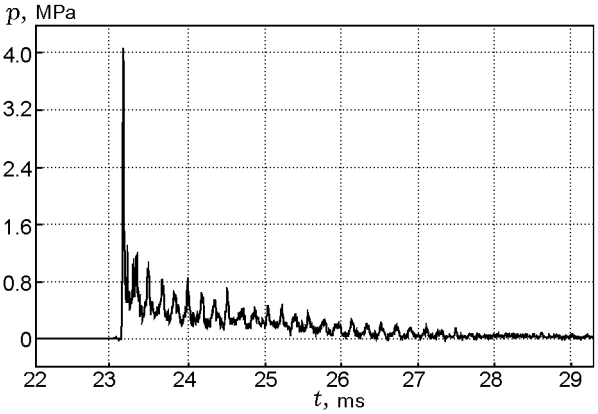


Fig. 9. Oscillogram of pressure in the spin detonation wave.

The tube segment 900 mm long adjacent to the open end was smooth, i.e., there were no obstacles in this segment. Natural gas and atmospheric air were continuously supplied to the pulsed-detonation burner through individual pipelines from receivers with a moderate excess pressure. The flow rates of the gases were chosen to ensure a stoichiometric composition of the mixture. The natural gas used in these experiments contained 98.9% of methane ("motor" gas).

Figure 8 shows the measured shock wave velocity as a function of the distance covered by the wave in the detonation tube in ten cycles with operation at a frequency of 0.03 Hz, which approximately corresponds to two cycles per minute. The distance is counted from

the input section of the detonation tube. It is seen that DDT occurs in the tube at a distance of 1.5–2.0 m from the beginning of the tube, and the arising detonation wave propagates over a length of ≈1–1.5 m quasi-steadily with the mean velocity of 1500–1700 m/s, including the smooth segment.

The observed detonation regime should be considered as a near-critical mode. First, the deficit of the mean velocity with respect to the thermodynamic value for a stoichiometric methane–air mixture ($D_{\mathrm{CJ}} \approx 1800$ m/s) agrees well with the admissible velocity deficit for detonation at the limit of its propagation in a smooth tube. Second, the wave structure in the smooth segment of the tube (Fig. 9) corresponds to the structure of spin detonation with typical, weakly decaying oscillations of the signal with a frequency (≈6 kHz) that agrees well with the known heuristic "rule" $s/d \approx 3$, where s is the spin pitch and d is the tube diameter.

Based on the above-described experimental studies, an experimental prototype of a pulsed-detonation burner was developed, fabricated, and tested. This burner is a pilot version of industrial burners of a new generation, which combine the shock wave (mechanical) and thermal effects on objects located in the flow of combustion products. Emissions of nitrogen oxides NO_x were measured on the experimental prototype of this burner in experiments with single DDT [24]. The samples of the detonation products were collected by a probe with a check valve and a perforated tube for scattering the detonation products to avoid their directed motion. The probe tube was inserted into the tube of the pulsed-detonation burner along the axis to a depth of 500 mm from the output section. The fraction of nitrogen oxides in the detonation products were measured by a Testo 335 gas analyzer (produced by Testo AG, Germany). For the detonation wave propagating over a stoichiometric mixture of natural gas and air at $p_0 = 0.1$ MPa and $T_0 = 293$ K, the mean fraction of nitrogen oxides obtained in the experiments was $[NO_x] \approx 210$ ppm ($[NO] \approx 203$ ppm).

Note that NO_x emissions in existing burners with slow combustion (deflagration), intense forced injection of the species, and high burning temperature reaches 500–700 ppm [25]. Even with the use of the most advanced schemes of multistage combustion, NO_x emissions in such burners can be reduced only to a level of 400 ppm, which is 1.5–2 times higher than the values obtained in the pulsed-detonation burner.

CONCLUSIONS

K. I. Shchelkin's ideas are developed in the fast DDT concept [5] proposed and actively used at ICP RAS. The concept is based on combining various methods of DDT facilitation, in particular, on choosing an appropriate shape of tripping obstacles and their arrangement to ensure optimal matching of the flame acceleration rate and shock wave amplification, chemical self-preparation of the explosive gas mixture, etc. An algorithm and a computational code were developed to search for the ways of DDT acceleration, which allows us to consider simultaneously the frontal and volume chemical reactions in a multidimensional compressible turbulent gas flow.

Test calculations with Shchelkin's formula for the turbulent burning velocity revealed reasonable agreement with available experimental data on the flame velocity as a function of time and of the covered distance both for smooth tubes and for tubes with regular annular obstacles of different height and different step between them, as well as for closed volumes. Based on numerical simulations of phenomena near the place of detonation origination, it was found that the "detonation" ignition of the gas ahead of the flame front is distributed in time and in space and occurs in the form of a compact set of self-ignition sites. The numerical studies of Shchelkin and Sokolik showed that preliminary thermal treatment of the mixture in the cold flame improves the conditions for detonation occurrence, and this effect is better expressed at higher pressures and in tubes having greater diameters, because the role of near-wall reactions is not that important in such cases. Based on the concept [5], an experimental prototype of a pulsed-detonation burner was developed, fabricated, and tested at ICP RAS. This burner is a pilot version of industrial burners of a new generation, which combine the shock wave (mechanical) and thermal effects on objects located in the flow of combustion products.

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