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Reduction of the Deflagration-to-Detonation Transition Distance and Time in a Tube with Regular Shaped Obstacles

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Here, we suggest, for the first time, use of regular obstacles of special shape for acceleration of deflagration-to-detonation transition (DDT). As shown by calculations and experiments, such obstacles make it possible to considerably decrease the DDT length and time as compared to regular rectangular obstacles. The new method of acceleration of the DDT can be used for designing compact combustion chambers of air-breathing pulse detonation engines (PDEs).

Detonation has been considered, until recently, only as an extremely undesirable scenario of an accidental explosion, as an inadmissible combustion regime in a piston engine, or as a powerful source of destruction in military operations. However, recently, a new field of study has been initiated and developed that deals with the creation of jet propulsion systems with controlled detonative fuel combustion, PDEs [1]. The key requirement for PDE operation is that detonation be initiated at the shortest distance, in the shortest time, and at a minimal energy of the ignition source. One classical method—direct detonation initiation [2]—ensures detonation at short distances as a result of a rapid concentrated energy release in amounts that are inapplicable to PDEs. Another classical method—DDT [3]—ensures detonation initiation by a weak ignition source but at a long distance and over a long time inapplicable to PDEs even when artificial turbulizing elements like the Shchelkin spiral or regular orifice plates are used.

In [4, 5], another method of detonation initiation was developed; namely, detonation in a tube with a gaseous or drop explosive mixture was initiated by a traveling ignition pulse. In this case, the mixture was ignited by several, rather than one, electric dischargers mounted along the tube. The careful synchronization of the electric discharge with the shock wave (SW) arrival at the cross section of each discharger ensured detonation in a smooth-walled tube at very short distances, with the overall ignition energy being considerably lower than the energy of direct detonation initiation by a single discharge. In [6], based on a survey of the experiments in [4, 5], an important conclusion was drawn: classical experiments on DDT in tubes with regular obstacles can also be considered as detonation initiation by a traveling ignition pulse, at least, at the final stages of the process after the SW has formed. In this case, the forced ignition of a mixture near the SW front is not necessary; rather, the autoignition of the mixture takes place due to SW reflection from the obstacles. The ignition delay, determined by the SW intensity and the SW compression phase duration, plays the same role as the forced ignition delay in the experiments in [4, 5]. Thus, the closer to the SW front the autoignition region is ("synchronization" of autoignition with the SW arrival) and the larger this region is, the more favorable the conditions for fast DDT in a tube with regular obstacles. Such an interpretation of the classical experiments on DDT opens up new possibilities for reducing the detonation run-up distance and time. One such possibility was considered for the first time in [7]. In the present work, the results of calculations of DDT in channels with regular obstacles were described and compared with experimental results.

In calculations, the final stage of DDT in a flat channel of height H with regular obstacles was considered after a relatively weak SW, with the Mach number M_0 and the compression phase duration τ, has formed capable of initiating ignition of the mixture when reflecting from the obstacles. The work dealt with the search for the shape of regular obstacles ensuring fast shock-to-detonation transition (SDT) by the mechanism described in [6]. For definiteness, the shape of obstacles

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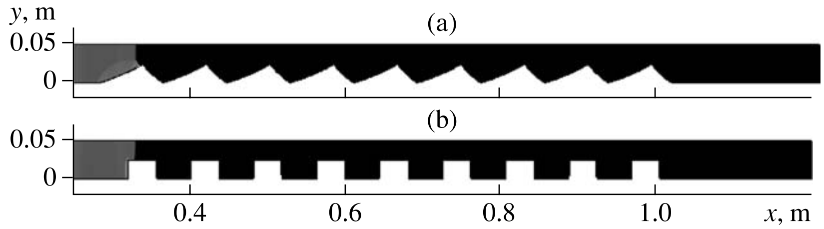

Fig. 1. Geometry of a flat channel with regular obstacles shaped as (a) a combination of parabolas and (b) rectangles. Only the lower portion of the channel is shown. The SW propagates from left to right (light region).

was taken to be a combination of two parabolas $x_1 = a_1y^2 + b_1y + c_1$ ($a_1 > 0$) and $x_2 = a_2y^2 + b_2y + c_2$ ($a_2 < 0$) with the foci lying in the plane of symmetry of the channel. The points of intersection of the parabolas corresponded to the apices of obstacles of height h located on the opposite walls of the channel. In the test section of length L of the channel, several identical obstacles were mounted at a distance $\delta = c_1 - c_2$ from each other (Fig. 1a). Smooth-walled sections of length L_- and L_+ were located, respectively, upstream and downstream of the test section. For comparison, the channel in which the test section had rectangular obstacles was considered, the values of H, L, δ, h, L_-, L_+, M_0, and τ being the same (Fig. 1b). It was assumed in all cases that, at the initial instant, the channel was filled with a quiescent explosive mixture at temperature T_0 and pressure p_0.

Numerical simulation of SW propagation in the channel with obstacles was performed on the basis of the two-dimensional Navier–Stokes equations for a viscous compressible gas coupled with equations of energy and chemical kinetics and by the equation of state of the ideal gas. The chemical transformation was described by a single-stage reaction with the Arrhenius dependence of the rate constant K on temperature T: $K = kp^n\exp\left(-\frac{E}{RT}\right)$, where R is the gas constant. The kinetic parameters of the rate constant—the activation energy E, the preexponential factor k, and the exponent n at the pressure p (in atmospheres)—were preliminarily calibrated against known experimental data on ignition delays for the selected fuel–air mixture. Integration of the set of equations was performed by the finite volume method with the Godunov convective flux approximation [7]. Calculations were performed on a structured grid with up to 200000 cells, with a maximal cell size of 500 μm and a maximal time step of integration of 10 ns.

Calculations were carried out for a stoichiometric propane–air mixture at the following values of governing parameters: $E = 190.3$ kJ/mol, $k = 7 \times 10^{14}$ cm^3/(mol s), $n = -0.2264$, $L_- = 0.25$ m, $L = 0.76$ m, $L_+ = 0.19$ m, $H = 0.1$ m, $h = 0.025$ m, $T_0 = 298$ K, $p_0 = 0.1$ MPa, $M_0 = 3$ (initial SW velocity $D \approx 1020$ m/s), and $\tau \approx 800$ μs. An SW was generated assuming that, at the initial instant, the section L_- contained a high-pressure region filled with air at $T_- = 1159$ K and $p_- = 6.06$ MPa. In calculations, only the parameters determining the shape of obstacles were varied. It is worth noting that, in a straight smooth-walled channel, no autoignition of the mixture occurred during the time while the SW was traveling the length of the channel.

At the specified governing parameters, the shortest detonation run-up distance was achieved for the parabolic obstacles shown in Fig. 1a, with local common focus coordinates $x_1 = x_2 = 0.065$ m and $y = 0.05$ m and coefficients $c_1 = 0.08$ m and $c_2 = 0$. Autoignition of the mixture occurred over the fifth obstacle (at a distance of about 0.4 m) about 490 μs after the SW entered the test section of the channel (Fig. 2a). As is seen, detonation occurred before the seventh obstacle about 100 μs after the first autoignition event: the shock wave front and the reaction front were coupled. After that, the resulting detonation wave propagated through both the section with obstacles and the smooth-walled section with a constant average velocity close to the Chapman–Jouguet detonation velocity. When parabolic obstacles of another shape were used, detonation either took place at a longer distance or did not occur at all.

For the channel with rectangular obstacles, calculations showed a lack of detonation, although hot-spot ignition at obstacles occurred earlier (at the second obstacle). Additional calculations showed that, in the channel with rectangular obstacles, detonation occurred at a considerably higher intensity of the initiating SW.

A specific feature of the SW propagation in the channel with regular parabolic obstacles with the best shape found is the periodic gas-dynamic focusing of reflected pressure waves into the central part of the SW front in the free flow core. Therefore, the local temperature in the central part of the flow behind the SW stepwise increased (a kind of pumping) up to ignition of a rather large gas volume in the flow core over the fifth obstacle. Calculations showed that, at the instant of ignition, a region of a shock-compressed fresh mixture, 10 × 3 mm, with a temperature above 2000 K formed in the central portion of the channel. Autoignition in this region led to the formation of a secondary explosion wave, the reflection of this wave from an obstacle, and its further accelerated propagation through the fresh precondi-

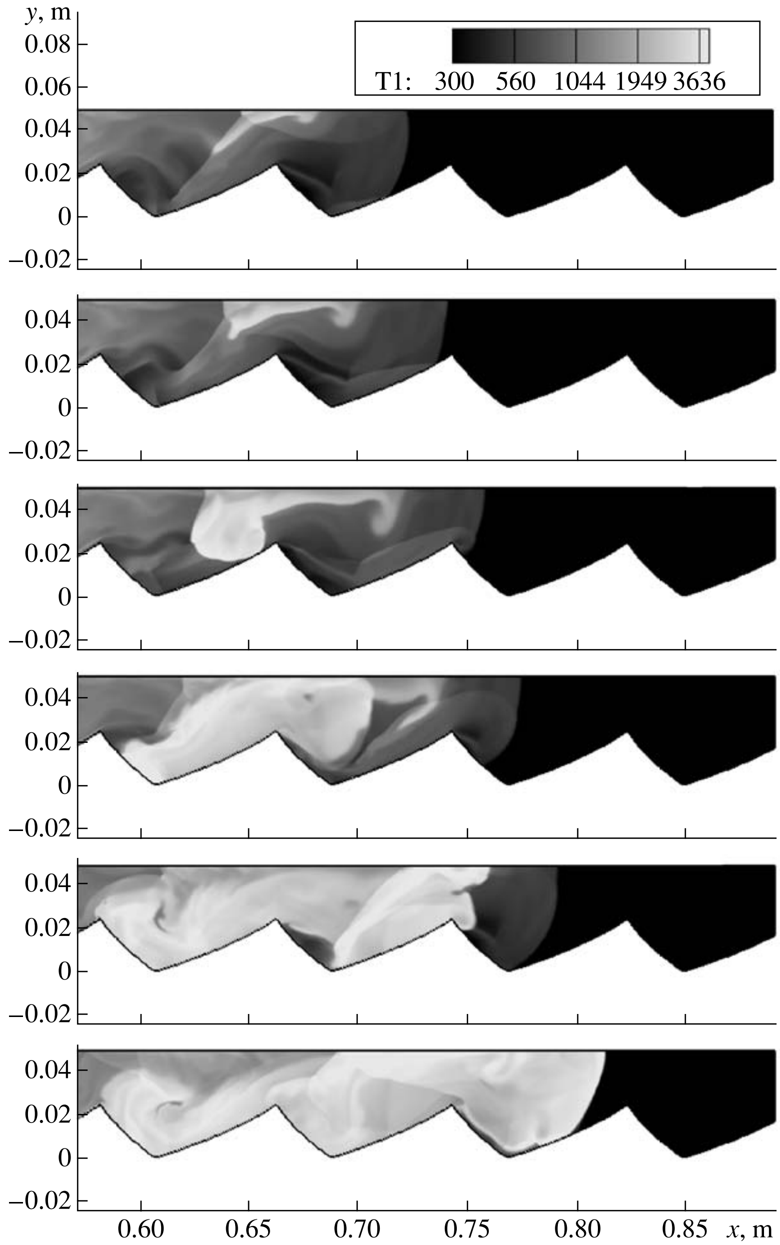

Fig. 2. Calculated temperature fields in the channel with regular parabolic obstacles after ignition over the fifth obstacle (top) about 490 μs after the SW entered the test section with obstacles. From the top down, the fields are plotted with an interval of 20 μs.

tioned mixture. Coupling of this wave with the analogous secondary explosion in the focal region over the sixth obstacle led to detonation. When a parabolic obstacle had a "nonoptimal" shape, the autoignition region occurred far from the central part of the SW front and was subjected to the action of rarefaction waves arising from diffraction of SWs on the obstacles. Upon SW propagation in the channel with rectangular obstacles, ignition occurred on the upstream side of obstacles, rather than in the free flow core, and was subjected to a strong action of rarefaction waves. Therefore, in the channel with such obstacles, detonation did not occur.

To check the calculation results, we carried out two series of experiments with parabolic and rectangular obstacles. The experimental setup was a laboratory shock tube of the diaphragm type 2.5 m in length with a high-pressure chamber (HPC) intended for generation of the initiating SW and a low-pressure chamber (LPC) with a test section equipped with regular obstacles. The HPC, 70 mm in diameter and 0.1 m in length, which was separated from the LPC by a bursting diaphragm, was filled with a stoichiometric propylene–oxygen mixture at different initial pressures (up to 0.8 MPa). The LPC included a buffer section—a smooth-walled tube 70 mm in diameter and 0.6 m in length filled with

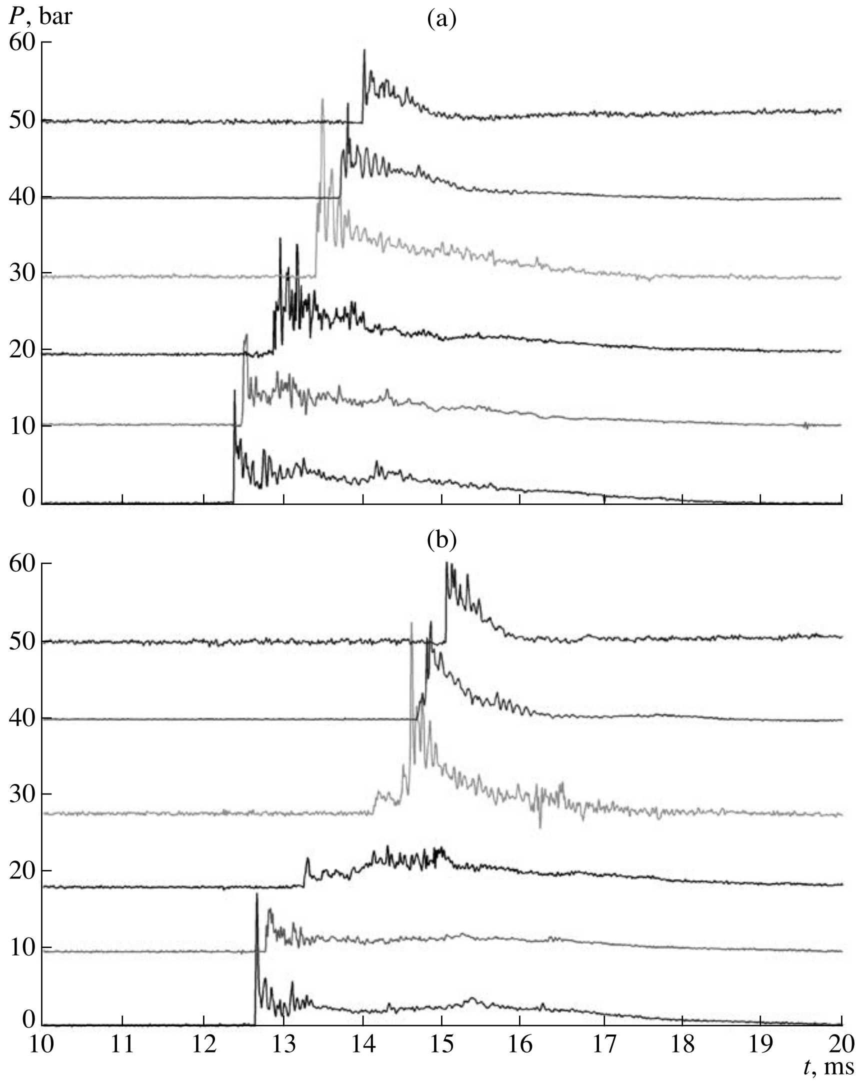

Fig. 3. Pressure records in the experiment with SDT in the channel with regular parabolic obstacles at an initiating SW velocity of (a) 1070 ± 30 and (b) 920 ± 30 m/s.

air; a test section of square cross section (100 × 100 mm) 1 m in length; and an exit section—a smooth-walled tube 70 mm in diameter and 0.8 m in length. The last two sections were filled with a stoichiometric propylene–air mixture. The buffer section was separated from the test section by a thin film. All experiments were carried out in an armored chamber at the normal initial pressure of the test mixture (0.1 MPa) and a temperature of 290 ± 2 K. The regular obstacles used were of the same shape and size as in the calculations corresponding to Figs. 1a and 1b. The obstacles were cut to templates from a plywood sheet 7 mm thick. The pieces were connected to each other with pins to form packs 100 mm thick, which were mounted on the upper and lower walls of the test section. The SW was initiated by fusing a wire in the HPC, which led to rapid combustion of the propylene–oxygen mixture and to bursting of the diaphragm. The SW parameters were measured with the use of six DDZ-026M high-frequency tensoresistive pressure transducers mounted at distances of 0.57, 0.695, 1.095, 1.605, 1.925, and 2.255 m from the bursting diaphragm. All transducers were equipped with signal followers with an individual power supply and were interfaced with a personal computer through

Comparison of SW velocities measured in a tube with regular parabolic and rectangular obstacles

Segment, mm	SW velocity, m/s	
	parabolic	rectangular
570–695	1070 ± 30	1070 ± 30
695–1095	1061 ± 30	714 ± 20
1095–1605	836 ± 25	637 ± 20
1605–1925	1025 ± 30	1000 ± 30
1925–2255	1590 ± 50	970 ± 30

an analog-to-digital converter. The error of measurement of the SW velocity was no more than 3%. To apply rapid video recording (5000 frames/s), two Plexiglas windows, 350 × 110 mm in size and 40 mm thick, were installed on one wall of the test section.

The table presents the results of two experiments with the same (within the error of measurements) initial SW intensity for obstacles of different shape. As is seen, when parabolic obstacles are used, detonation occurs in the tube segment between the two last pressure transducers (1925–2255 mm) and propagates at a velocity of 1590 ± 50 m/s, whereas, in the tube with rectangular obstacles, the SW velocity in the same segment is 970 ± 30 m/s (detonation is lacking). This fact confirms the results of the numerical simulation: shaped obstacles are more efficient for SDT than rectangular obstacles.

Figure 3 shows the pressure records obtained in the experiments with parabolic obstacles at the initial SW velocities 1070 ± 30 m/s (Fig. 3a, table) and 920 ± 30 m/s (Fig. 3b). In both cases, SDT was observed. In Fig. 3b, the pressure transducer located at the distance 1.605 m from the bursting diaphragm recorded a strong secondary explosion wave rapidly overtaking the primary shock front. This phenomenon was predicted by the numerical simulation of the SDT.

Thus, we suggested and experimentally confirmed a new method of decreasing the DDT distance and time. The method implies the use of regular obstacles of special shape that ensure the autoignition of the shock-compressed gas in the free flow core near the central part of the initiating SW front followed by rapid SDT due to a series of secondary explosions. The SDT mechanism resembles the mechanism of detonation initiation by a traveling pulse of forced ignition where the secondary explosions behind the SW front are initiated by an external source. It should be emphasized that, for DDT in round tubes, orifice plates are as efficient as the Shchelkin spiral [1]. Hence, we showed that regular-shaped obstacles are more efficient for SDT than rectangular obstacles and the classical Shchelkin spiral.

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REFERENCES

1. Frolov, S.M., *Impul'snye detonatsionnye dvigateli* (Pulse Detonation Engines), Moscow: Torus Press, 2006.
2. Zel'dovich, Ya.B., Kogarko, S.M., and Simonov, N.N., *Zh. Tekh. Fiz.*, 1956, vol. 26, no. 8, pp. 1744–1752.
3. Shchelkin, K.I., *Bystroe gorenie i spinovaya detonatsiya gazov* (Fast Combustion and Spin Detonation of Gases), Moscow: Voenizdat, 1949.
4. Frolov, S.M., Basevich, V.Ya., Aksenov, V.S., and Polikhov, S.A., *Dokl. Phys. Chem.*, 2004, vol. 394, part 1, pp. 16–18 [*Dokl. Akad. Nauk*, 2004, vol. 394, no. 2, pp. 222–224].
5. Frolov, S.M., Basevich, V.Ya., Aksenov, V.S., and Polikhov, S.A., *Dokl. Phys. Chem.*, 2004, vol. 394, part 2, pp. 39–41 [*Dokl. Akad. Nauk*, 2004, vol. 394, no. 4, pp. 503–505].
6. Frolov, S.M., *J. Loss Prevention*, 2005, vol. 19, nos. 2–3, pp. 238–244.
7. Semenov, I.V., Frolov, S.M., Markov, V.V., and Utkin, P.S., *Pulsed and Continuous Detonations*, Roy, G., Frolov, S., and Sinibaldi, J., Eds., Moscow: Torus Press, 2006, pp. 159–169.