SHOCK-TO-DETONATION TRANSITION IN TUBES WITH SHAPED OBSTACLES

I. Semenov*, S. Frolov†, V. Markov‡, and P. Utkin*

*Institute for Computer Aided Design
Russian Academy of Sciences
Moscow 123056, Russia

†N. N. Semenov Institute of Chemical Physics
Russian Academy of Sciences
Moscow 117334, Russia

‡V.A. Steklov Mathematical Institute
Russian Academy of Sciences
119991, Moscow, Russia

Numerical simulation of shock-to-detonation transition (SDT) in the channel with regular obstacles indicates that proper obstacle shaping can be used for a considerable reduction of the SDT distance and time for pulse detonation engine (PDE) applications. In the example considered, the SDT distance and time for the stoichiometric propane–air mixture was about 0.55 m and 590 μs, respectively. The physical mechanism governing fast SDT is closely connected with explosive gas preconditioning by multiple shock compression in the vicinity to the focal points of the parabolic obstacles.

Introduction

Recent review [1] of experimental studies on gaseous and spray detonation initiation by a traveling ignition source indicate that spatially distributed electric dischargers with properly tuned triggering times provide very short distances for SDT in a smooth-walled tube. According to [1], available experiments on deflagration-to-detonation transition (DDT) in tubes with regular or irregular obstacles [2] can also be treated as detonation initiation by a traveling ignition source. In this case, instead of external stimulation of chemical activity behind a propagating shock wave, a localized obstacle-induced autoignition of shock-compressed gas occurs which is closely coupled to the shock wave intensity and compression phase duration. In terms of the ignition delay, the conditions for the coupling between mixture autoignition and the propagating shock wave seem to be equivalent to those found in the experiments with external energy deposition using spatially distributed electric discharges. In case the ignition timing at obstacles is closely coupled with the propagating shock wave, favorable conditions for 'fast' DDT can occur [1]. Otherwise, the propagating shock wave decouples from the ignition pulses and DDT fails or occurs at a later stage due to cumulating of flame-induced pressure waves and "explosion in the explosion" phenomenon. The latter DDT scenario was referred in [1] to as 'slow' DDT.

With this understanding of the DDT phenomena, new approaches to reducing the predetonation distance for PDE applications can be considered. One of such approaches is suggested in this paper. The underlying idea is to promote fast DDT by appropriate shaping of regular obstacles in the detonation tube. It is implied that shock-induced autoignition of the reactive mixture at the obstacles and hence the shock wave – reaction front interaction can be efficiently controlled not only by obstacle blockage ratio and spacing, but also by obstacle shape due to gasdynamic focusing of the propagating shock wave. Note that the focusing effect of regular shaped obstacles in the tube on shock wave propagation in reactive media has not hitherto been studied, although the phenomenon of shock wave focusing in straight tubes after reflection from a nonflat end wall has long been known [3].

Problem Formulation

Among different shapes of obstacles, orifice plates and combinations of parabolas were chosen for consideration in this study. Regular orifice plates were taken as an example of obstacles used in the majority of available DDT studies. Their performance as DDT enhancing elements was compared with the performance of regular obstacles shaped as shown in Fig. 1.

The obstacles of Fig. 1 are composed of two parabolas x_1 and x_2 with the identical focal point F lying at the symmetry plane of the

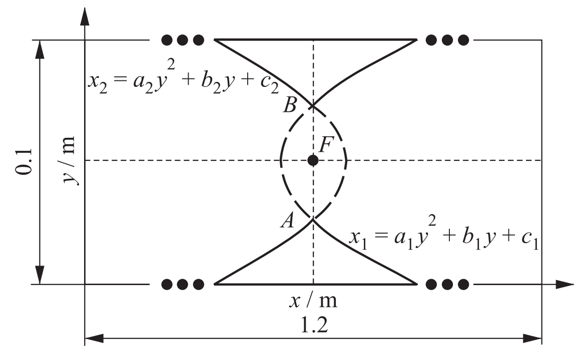

Figure 1 Schematic of shaped parabolic obstacles in the 2D channel

two-dimensional (2D) channel of height H. The obstacle contours are depicted by solid curves, so that points A and B correspond to obstacle vertices. Obstacle height is denoted as h. In general, coefficients a_1, b_1, and c_1 can differ from coefficients a_2, b_2, and c_2, and the focal points of parabolas x_1 and x_2 do not coincide. Similar obstacles are positioned in the channel at a distance between vertices $\delta = x_1(0) - x_2(0)$ thus forming a regular array of shaped obstacles. The total length of the channel section with regular obstacles is L. To the left and to the right of the obstructed section, a provision is made for smooth initiation and outlet channel sections of height H and lengths L_- and L_+. For the sake of comparison, regular obstacles in the form of orifice plates are used. In this case, the height h and the total cross-section area of the obstacles in the x–y plane are kept similar to the corresponding case with the shaped obstacles.

It is assumed that initially the channel is filled with a quiescent, premixed, explosive gas at temperature T_0 and pressure p_0. A planar shock wave of initial Mach number M and compression phase duration τ is generated in the initiation section and, propagating from left to right, enters the obstructed section of the channel. In the obstructed section, ignition of the explosive gas caused by shock wave reflections from the obstacles and interactions between various wave systems can occur. After ignition, two scenarios of the postshock flow evolution leading to SDT can be considered. In the first, turbulent flame kernels develop in the channel, giving rise to combustion-generated compression waves catching up with the lead shock wave. In the long run, the "explosion in the explosion" phenomenon can occur in the region between the turbulent flame brush and the lead shock wave [4]. In the second, the stage of turbulent flame development and propagation is of minor importance as compared to fast energy deposition in the spontaneous ignition fronts propagating in the portions of explosive gas preconditioned by multiple shock compression. This study is focused on the second scenario.

Mathematical Model

The mathematical model used was based on the full 2D Navier–Stokes equations supplemented by the equation of energy conservation, equation of chemical kinetics, and the ideal gas equation of state. The explosive gas was the stoichiometric propane–air mixture at normal initial conditions ($T_0 = 298$ K and $p_0 = 0.1$ MPa). The chemical transformation in the mixture was modeled by a single-step chemical reaction [5]:

$$C_3H_8 + 5O_2 = 3CO_2 + 4H_2O + Q$$

with the reaction rate determined as

$$\dot{\omega} = k[C_3H_8][O_2]$$

$$k = 7 \cdot 10^{14} p^{-0.2264} \exp\left(-\frac{E}{RT}\right) \ \text{cm}^3/(\text{mol} \cdot \text{s})$$

$$E = 190.3 \ \text{kJ/mol}$$

where p is the pressure in atm and T is the temperature in K. The reaction heat was taken equal to $Q = 46.6$ kJ/g. This value provides the adequate Chapman–Jouguet detonation velocity in the propane–air mixture (about 1800 m/s). Since the primary focus of this study is the fast SDT due to spontaneous ignitions governed by shock reflections, no turbulence and turbulent combustion models were involved.

The geometrical dimensions of the channel were: $L_- = 0.25$ m, $L = 0.76$ m, $L_+ = 0.19$ m, and $H = 0.1$ m. The initial parameters of the shock wave were: $\mathrm{M} = 3$ and $\tau \approx 800$ μs. The shock wave was generated by a high-pressure domain L_- filled initially with air at $T_- = 1159$ K and $P_- = 6.06$ MPa. The only parameters varied in this study were the parameters determining the obstacle shape.

Numerical Procedure

The numerical procedure was similar to that reported in [6]. It was based on the finite volume approach and Godunov flux approximation and was implemented for parallel computing. The problem was solved for the lower part of the channel of Fig. 1 with the symmetry boundary conditions at the symmetry plane. A fine (structured) computational grid with 200 000 cells was used. The spatial resolution was about 100 μm and the maximal time step was 10 ns.

Results and Discussion

The optimal obstacle shape for the conditions outline above was obtained in the course of the special optimization study. The parabolic obstacle height was $h = 0.025$ m. The coordinate of obstacle focus was $x = 0.065$ m, $y = 0.05$ m, $c_1 = 0.08$ m, and $c_2 = 0$ m. The total number of obstacles at length L was 9.

Figure 2 shows the predicted snapshots of the temperature field in the channel with regular parabolic obstacles. At about 490 μs (snapshot 5 from above), spontaneous ignition occurs above the fifth obstacle in the vicinity to the focal point, which gives rise to a detonation. The detonation wave passes the obstructed section of the channel and propagates steadily in the smooth outlet section.

Similar calculations for the channel with 9 orifice plates of the same height $h = 0.025$ m and pitch $\delta = 0.08$ m did not result in the detonation onset. Figure 3 shows the corresponding predicted snapshots of the temperature field in the channel with regular orifice plates. Despite earlier ignition as compared to Fig. 2, the orifice plates do not promote fast SDT.

For better understanding of the SDT phenomenon in the channel with regular parabolic obstacles, consider Figs. 4 and 5. Figure 4 shows in more detail the evolution of the temperature field after gas autoignition around the focal point above the fifth obstacle. One can see very fast spontaneous flame propagation in the gas preconditioned by multiple shock reflections followed by detonation formation at the last snapshot (590 μs). Figure 5 shows the temperature isolines in the vicinity of the exothermic center where ignition occurs at 490 μs. The

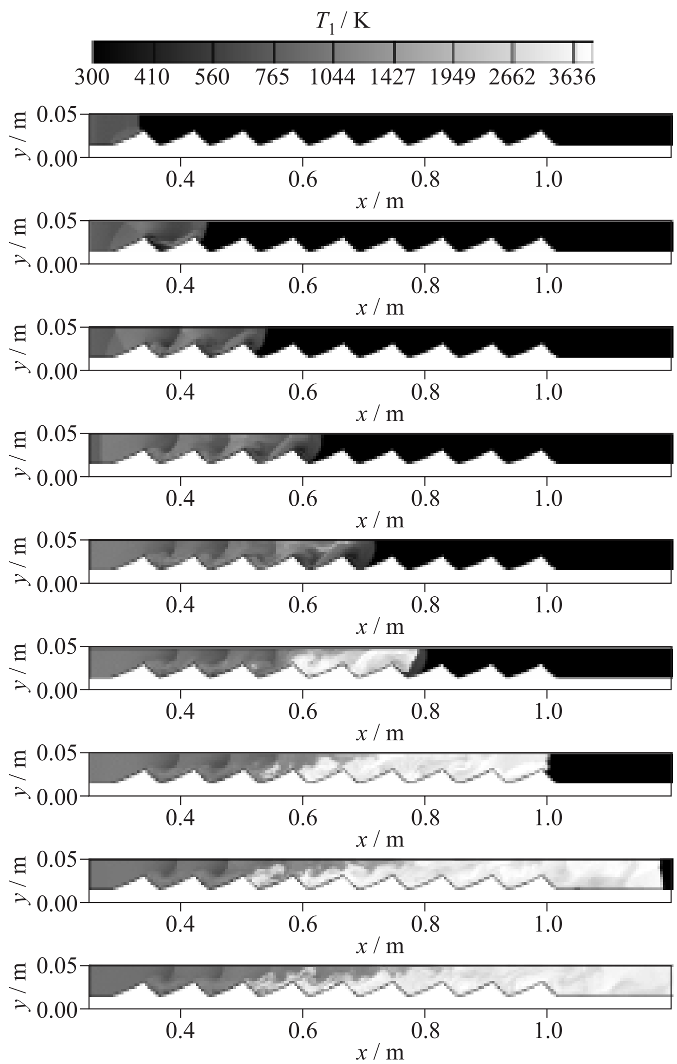

Figure 2 Snapshots of temperature fields at SDT in the channel with regular parabolic obstacles. The upper snapshot corresponds to time instants of 80 μs. All other snapshots are plotted with time interval of 100 μs

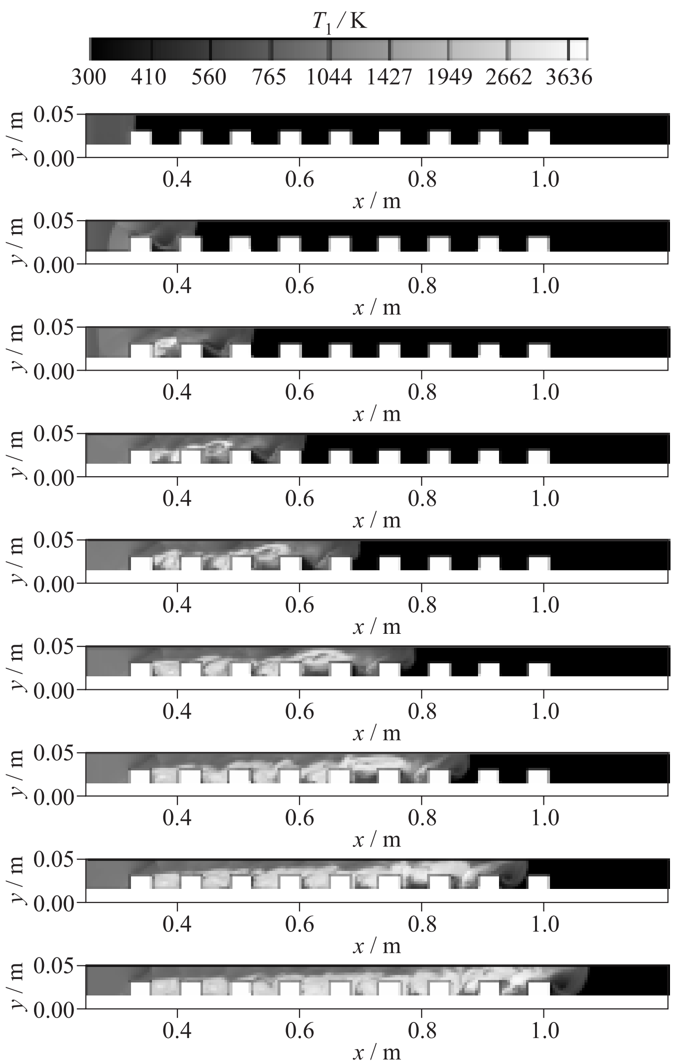

Figure 3 Snapshots of temperature fields in the channel with regular orifice plates. The upper snapshot corresponds to a time instant of 80 μs. All other snapshots are plotted with time interval of 100 μs

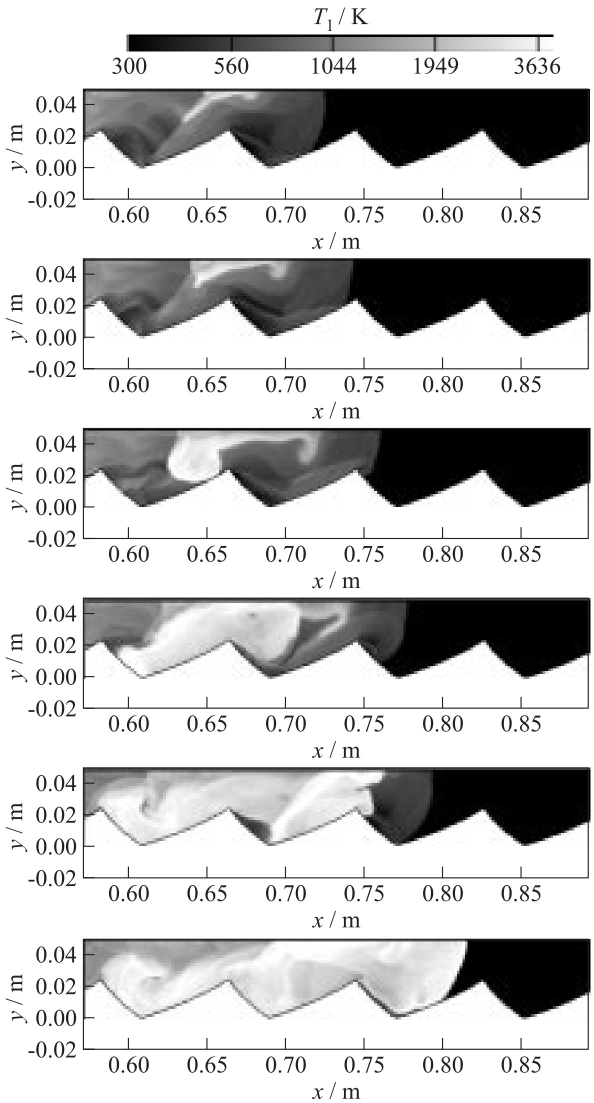

Figure 4 Evolution of temperature field after gas autoignition above the fifth parabolic obstacle. The upper snapshot corresponds to the time instant of 590 μs. All other snapshots are plotted with time interval of 20 μs

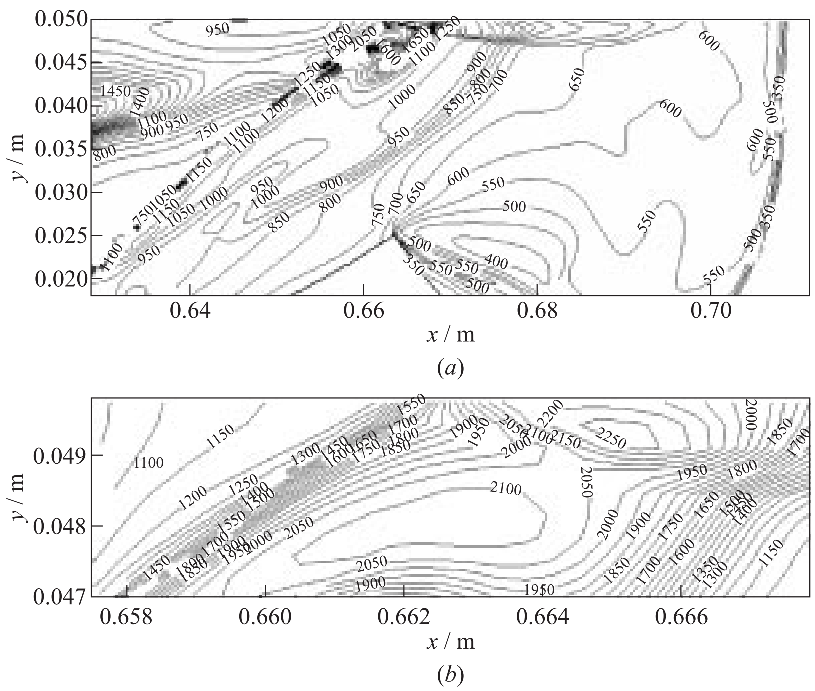

Figure 5 Predicted temperature isolines in the vicinity of the exothermic center where ignition occurs at 490 μs. The isolines correspond to a time instant of 470 μs: (a) complete temperature field, and (b) explosive view of the temperature field near the exothermic center

isolines are plotted for the time instant shortly prior to ignition (470 μs). It is seen that there exists a large mixture volume (about 10 mm long and 3 mm wide) with the temperature exceeding 2000 K. The temperature distribution in this volume is not homogeneous: there are two islands with the maximal temperatures of 2250 and 2100 K separated with a narrow "strait" with the temperature of 2050 K. The islands are oriented streamwise but are shifted both horizontally and vertically with respect to each other. Analyzing simultaneously Figs. 4 and 5, one observes that the reaction front propagates exactly along this preconditioned volume, giving rise to a strong secondary blast wave. After reflection of this blast wave from the obstacle, a detonation bubble forms (see snapshot 3 in Fig. 4). These observations testify that the detonation forms due to spontaneous generation of a strong blast wave in the exothermic center. The mechanism of blast wave formation due to propagation of fast spontaneous flames in the compressible medium was studied elsewhere [7].

Concluding Remarks

The results of numerical simulation of SDT in the channel with regular obstacles indicate that proper obstacle shaping can be used for a considerable reduction of the SDT distance and time for PDE applications. In the example considered, the SDT distance and time for the stoichiometric propane–air mixture was about 0.55 m and 590 μs, respectively. The physical mechanism governing fast SDT is closely connected with explosive gas preconditioning by multiple shock compression in the vicinity to the focal points of the parabolic obstacles. The use of regular "unshaped" obstacles did not result in the SDT, other conditions being equal.

Acknowledgments

This work was supported by the Russian Foundation for Basic Research (grant 05-08-50115a) and International Science and Technology Center project 2740. Dr. I. Semenov also acknowledges the support of "Russian Science Support Foundation."

References

1. Frolov, S. M. 2005. Initiation of strong reactive shocks and detonation by traveling ignition pulses. *J. Loss Prevention* 19/2–3:238–44.
2. Shchelkin, K. I. 1949. *Fast combustion and spinning detonation of gases.* Moscow: Voenizdat. 44–73.
3. Sturtervant, B., and V. A. Kulkarny. 1976. The focusing of weak shock waves. *J. Fluid Mechanics* 73:651–71.
4. Oppenheim, A. K. 1972. *Introduction to gasdynamics of explosions*. Wien – N.Y.: Springer-Verlag.

5. Frolov, S. M., V. S. Aksenov, and I. O. Shamshin. 2005. Detonation propagation through U-bends. In: *Nonequilibrium processes. Volume 1: Combustion and detonation*. Eds. G. Roy, S. Frolov, and A. Starik. Moscow: TORUS PRESS. 348–64.
6. Korobeinikov, V. P., I. V. Semenov, I. S. Men'shov, R. Klemens, P. Wolanski, and P. Kosinski. 2002. Modelling of flow and combustion behind shock waves propagating along dust layers in long ducts. *J. Physics (IV France)* 12:Pr7-113–Pr7-119.
7. Frolov, S. M. 1992. Nonideal effects at explosion origin and propagation. D.Sc. Thesis. Moscow: N. N. Semenov Institute of Chemical Physiccs.