On the Mechanism of Transition of Self-Sustained Detonation from a Tube to a Half-Space Through an Annular Orifice with Central Obstacle

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Abstract. Experimental and numerical studies of critical conditions of detonation transition from a tube to a half-space through an annular orifice with central obstacle shows that the mechanism of transition to detonation is more complicated than it was thought before. Comparison of experimental and numerical soot traces displays that in a wide range of initial pressures the interaction of diffracted shocks on the axes of symmetry does not result in re-initiation of detonation. However, the implosion generates a super-detonation wave propagating along a thin layer separating the diverging curved shock and the front of associated decoupled flame. Curvature radius of this layer and its thickness are initially too small to re-initiate detonation in the fresh mixture during the super-detonation wave travel from the implosion point towards the basement wall and the flame again separates from the shock. During this travel the size of the bubble of reaction products escaping from the shock tube significantly grows. Reflection of the primary super-detonation from the basement wall initiates secondary super-detonation wave, which successfully ignites the fresh mixture and marks the layer between the shock and flame by very fine cells. Thus, the transition to self-sustained detonation is due to the interaction of the super-detonation with the basement wall.

Introduction

The mechanism of transition of gaseous detonations from a tube to an unconfined volume is important for safety considerations and evaluation of critical energy of detonation initiation. Moen et al. [1] compared critical conditions for transmission of detonation from an open tube and through an annular orifice and concluded that central blockage of the tube can enhance detonation transition. As cited in [1], Thibault et al. [2] attribute the mechanism of this detonation transmission to implosion of the shock wave diffracted through the orifice. Murray et al. [3] recently provided additional numerical evidence to this mechanism.

However, the proposed study on the critical conditions of detonation transition to a half-space through annular orifice with central obstacle shows that the aforementioned implosion directly reinitiates detonation only when ambient pressure is well above the critical pressure corresponding to a given orifice geometry. Soot histories of the transition process show that in a wide range of ambient pressures the mechanism of transition to detonation in presence of obstacles is significantly more complicated. To provide better understanding of this mechanism we also performed numerical analysis but in contrast to [3] we resolved fine detonation structure during detonation transition.

Experimental Study

The experiments were performed with the C_2H_2+2.5O_2 mixture at different initial pressures P_o and room temperature with a set-up displayed on Fig. 1. A 4-m long and 52 mm i.d. detonation tube was connected to a 500-mm long 380-mm i.d. chamber.

The diameter of the tube in its outlet section is progressively reduced from 52 mm to 26 mm forming a conical shape with a half-angle of 15°. To enhance detonation transmission a central conical obstacle with a half angle of 15° was mounted at the outlet section of the detonation tube. Its base diameter is 18.4 mm. All the events related with detonation transmission from the tube to the chamber were recorded on a smoked foil. Detonation velocity before the outlet section of the tube was close to the CJ velocity within 1% as measured by ionisation probes and pressure gauges.

Figure 2 presents self-signature of detonation wave left inside the tube at P_o=31 mbar (one can see that cell width of self-sustained detonation before entering the converging end of detonation tube is about 5-6 mm). Figure 3 shows typical soot history of detonation transition at P_o=33 mbar which is about 2 mbar higher than the critical pressure for detonation transmission for the given orifice. Figure 4 shows magnified part of primary super-detonation wave seen inside the white frame on Fig. 3. An example of failure of this detonation at P_o=28 mbar is shown in Fig. 5. At significantly higher initial pressures we observed the same flow pattern as described in [1-3].

Analysis of critical detonation diffraction shows that detonation transition proceeds through a few stages of successful detonation onset and propagation but at first only in local thin layers of shocked fresh mixture behind the expanding curved shock. These layers manifest themselves by very fine detonation cells at the periphery of the bubble of detonation products. Inside the bubble there are practically no traces left by detonation since the expansion rate dominates the heat release rate. The detailed description of the transition mechanism is given below along with results of numerical modelling.

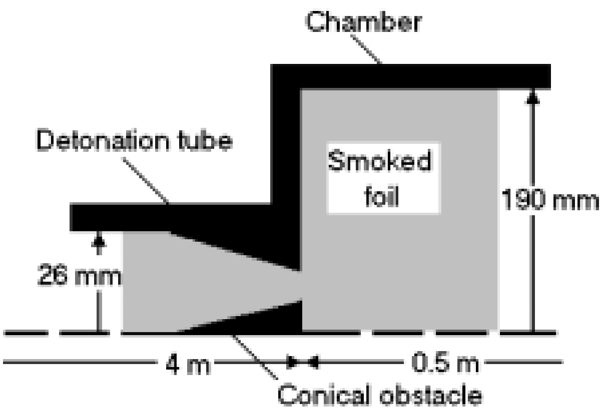

Fig.1. Scheme of experimental set-up.

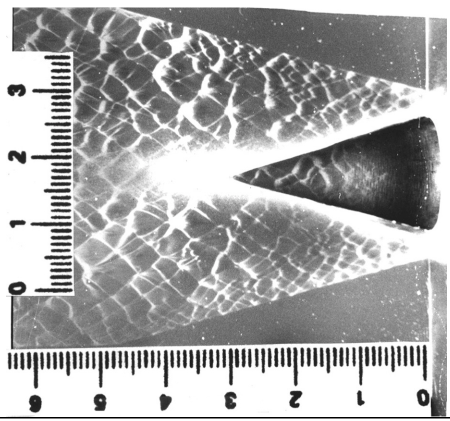

Fig.2. Soot traces inside tube at P_o=31 mbar

Numerical Study

To provide clear interpretation of the observed detonation transmission we solved the gasdynamic unsteady conservation equations for inviscid reactive gas using the Flux-Corrected Transport (FCT) technique [4]. One-step Arrhenius reaction was used along with perfect gas equation of state with constant molecular mass and γ. Best-fitting value of the pre-exponential factor was found via comparison of calculated and numerical cell width for self-sustained detonation in C_2H_2+2.5O_2 mixture. At P_o=33 mbar the detonation CJ pressure and velocity are 0.88 bar and 2118 m/s respectively.

First, calculations were performed for a 3.6-m long tube with a constant 26-mm radius using adaptation technique along longitudinal *x*-axes. Detonation was initiated at the left closed end of the tube (*x*=0) using pressure jump. During first half of the tube the evolution of detonation wave was described in plane 1D approximation. Then 1D profiles of flow parameters were used as initial conditions for 2D cylindrical problem. Mesh size along longitudinal *x*-axes was smoothly decreased from that at the left wall to *dx*=0.05 mm in the leading zone of detonation wave. We used constant number of meshes N_x=800 along x, hence, longitudinal size of the leftmost meshes at x=0 increases with time. The supersonic character of detonation propagation is favourable for this kind of adaptation. The mesh size in radial direction is dr=0.05 mm (N_r=520 cells). Calculations were performed at Courant number 0.5.

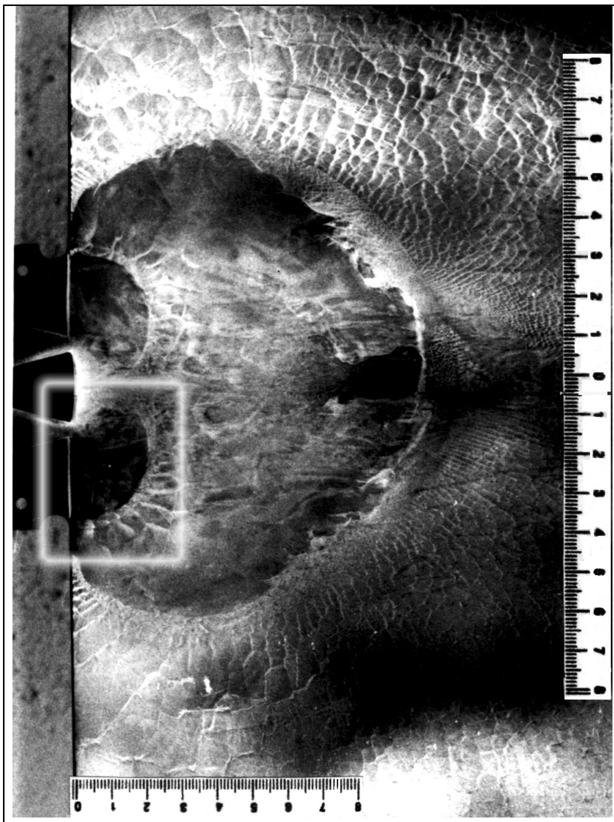

Fig.3. Detonation transition at P_o=33 mbar (the ruler unit is 1 cm)

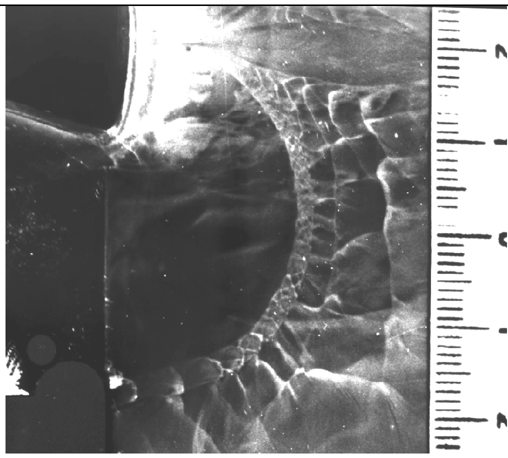

Fig.4. Magnified traces of primary super-detonation from Fig.3

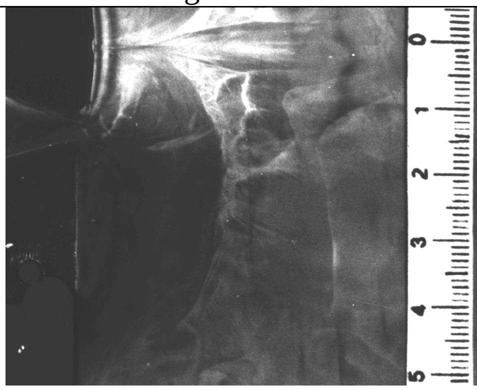

Fig.5. Detonation quenching at P_o=28 mbar

Calculation Results and Discussion

Initially uniform flow along radial direction after a few thousands time steps becomes significantly nonuniform due to formation of triple points. Figure 6 shows traces of triple points near the end of the tube at t=1.754 ms (27700 time steps, i.e. mean time step is 6.3 ns). The cell pattern prior to tube contraction, in spite of long propagation distance of detonation and its quasi-steadiness, is quite irregular because $E/RT_{ZND}\approx 10.5$ is large (here T_{ZND} is the temperature behind a shock front of steady detonation). In reasonable agreement with experiment there are about 10-12 cells across the tube diameter. Thus, both theoretical and experimental diameter for detonation transition is below the critical one corresponding to an open tube diameter of ≈13λ. Decrease of detonation cell size λ induced by detonation interaction with the contracted section of the tube reasonably corresponds to Fig.2.

To simulate detonation transition to the half-space we connected to the aforementioned tube a large cylindrical volume with a radius of 80 mm and length of about 150 mm. All boundaries of this cylindrical region except for the rigid basement are treated as continuous ones. Numerical resolution in this region is uniform with dx=dr=0.05 mm. Longitudinal size of meshes inside the tube gradually increases from dx=0.05 mm near the tube exit to about 140 mm at x=0. Maximum number of meshes along x- and r-axes is 4000 and 1600 respectively. Time needed to solve this problem on 1 MHz PC is about 1 week. Without obstacle at the outlet section the detonation transition did not take place both in experiment and calculations.

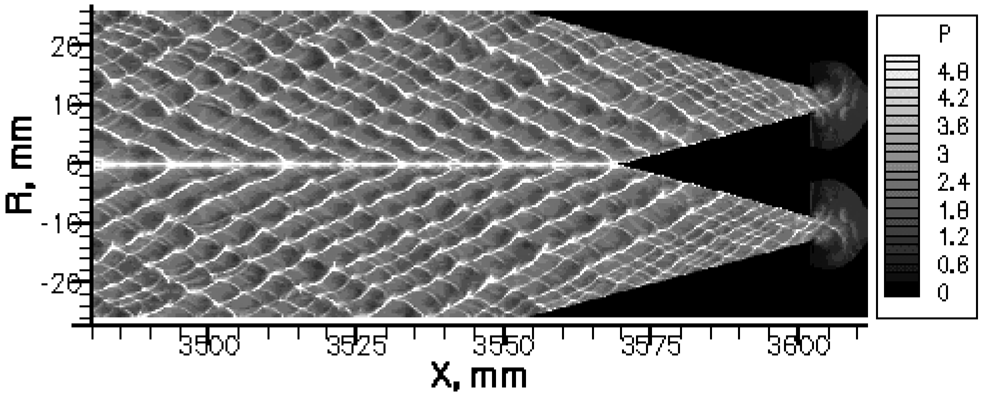

Figure 6. Calculated maximum pressure traces near the end of the tube at *t*=1.754 ms.

Figure 7 displays traces of maximum pressure. Comparison with Fig.3 shows that numerical simulation reproduces reasonably well the most important features of successful detonation transition through the annular orifice to the half-space. Calculated sizes of characteristic domains and especially size of first dark zone reasonably agree with the experimental ones. Based on profiles of flow parameters at different instants of time the mechanism of detonation transition can thus be interpreted in the following way:

1) At first, the shock rapidly expanding from the annular orifice fails to ignite the fresh mixture and the detonation is quenched by the rapid expansion. Hence, thickness of the layer between the shock and flame front increases with time. It is important that this layer contains shocked fresh mixture and that detonation velocity depends only slightly on ambient pressure, while cell size is practically inversely proportional to density of the mixture [5]. Though implosion of diffracted shock waves initiates detonation in some conical region in agreement with [2,3], the expansion waves rapidly quench this detonation since diameter of cone basement is smaller than 13λ.

2) The implosion also initiates super-detonation wave, which propagates tangentially to the direction of the flow of expanding detonation products through the aforementioned layer of shocked fresh mixture printing narrow trace with fine cells inside (this trace encircles the first dark zone near the orifice). At this stage of the process the expansion rate apparently is higher than reaction rate (curvature radius is too small) and super-detonation fails to initiate detonation in the surrounding fresh mixture.

3) While super-detonation runs toward the confining basement of the half-space the size of the bubble of detonation products escaping from the tube gradually increases.

4) Then super-detonation impacts the basement wall. It is this event that initiates detonation in the fresh mixture near the wall (the larger reaction rate, the faster detonation grows from the impact point). In addition, the secondary super-detonation is initiated in the layer of shocked fresh mixture surrounding the bubble. This secondary super-detonation propagates again tangentially to the direction of the flow of expanding gases. Both detonations grow up but super-detonation propagates in a shocked gas and therefore produces much finer cells than that in the fresh mixture as explained above. One can see that surface of flame front is much less smooth than that of the shock front.

5) Finally, implosion of converging super-detonation waves takes place at the axes of symmetry (numerical resolution above the implosion point becomes insufficient to resolve most fine cells in this area).

Figure 8 shows detonation quenching calculated at 40% smaller value of preexponential factor at P_o=0.033 bar. Resulting pattern is quite similar to the experimental one shown in Fig.5. Thus, at lower ambient pressure (and reaction rate) the primary super-detonation can be rapidly quenched by rarefaction waves. It is interesting that comparison of Fig.7 and 8 (as well as of experiments in Fig.3 and 5) shows that size of the first dark zone is controlled by tube and obstacle geometry rather than by chemical kinetics.

Thus, experimental and numerical studies of critical conditions for detonation transmission from a tube through an annular orifice with central obstacle to a half-space show that basement wall of the half-space can be responsible for detonation re-initiation in a wide range of governing parameters. The soot history of transition clearly shows that implosion of diffracted shocks hardly can be considered as the only reason of detonation re-initiation.

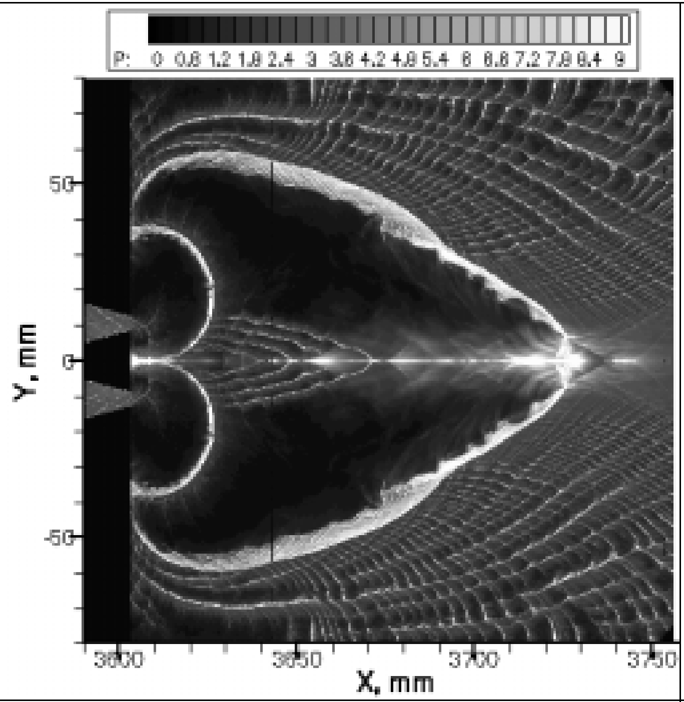

Fig. 7. Calculated traces of maximum pressure under conditions of Fig.3 at t=1.8807 ms.

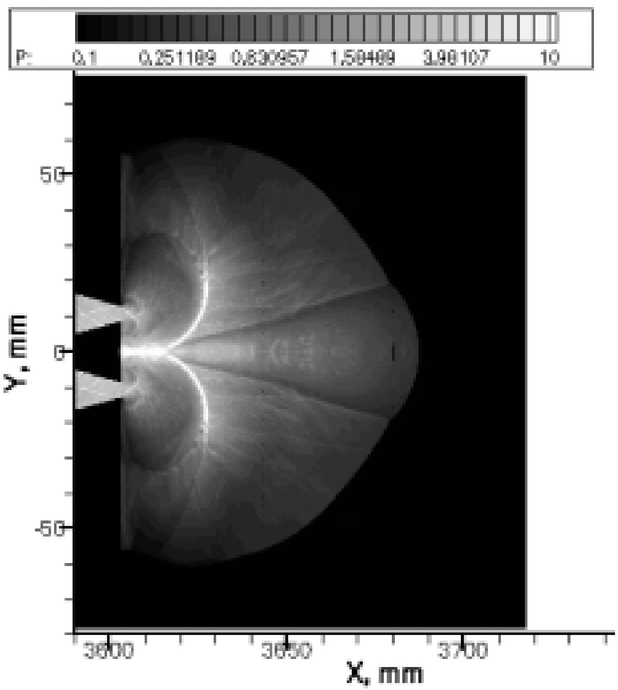

Fig. 8. Pressure traces at t=1.832 ms and smaller reaction rate than in Fig.7.

References

[1] Moen I.O., Sulmistras A., Thomas G.O., Bjerketvedt D., Thibault P.A., Influence of Cell Regularity on the Behaviour of Gaseous Detonations. 10th ICDERS, Berkeley, California, August 4-9 (1985) 220-243.

[2] Thibault P.A., Bjerketvedt D., Thomas G.O., et al., The role of energy distribution on the transmission of gaseous detonations into the unconfined. Paper presented at the 10th ICDERS, Berkeley, California, August 4-9 (1985)

[3] Murray S.B., Thibault P.A., Zhang F. et al., The Role of Energy Distribution on the Transmission of Detonation. International Colloquium on Control of Detonation Processes, Moscow, Russia, July 4-7, 2000.

[4] Oran E.S., Boris J.P., Numerical Simulation of Reactive Flow. Elsevier Science Publishing Co., Inc. (1987)

[5] Auffrey Y., Desbordes D., Presles H.N., Detonation structure and detonability of C_2H_2-O_2 mixtures at elevated initial temperature. Accepted for publication in Shock Waves (2001).