

EFFECTS OF BOUNDARY LAYERS ON IGNITION BEHIND REFLECTED SHOCKS

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Shock-induced ignition of homogeneous reactive mixtures may occur in a variety of ways. Two limits that have been discussed by Meyer & Oppenheim (1971) are strong and weak (or mild) ignition. Strong ignition results in a detonation that is directly initiated by a strong shock produced by a violent thermal explosion of shock-compressed material. Weak ignition is characterized by the appearance of a number of small flames followed by a deflagration-to-detonation transition (DDT). The multidimensional nature of weak ignition implies nonuniformities in the flow behind the shock.

Major sources of nonuniform flow in shock-tube experiments are boundary-layer interactions. For reflected shocks, these interactions produce the types of multidimensional bifurcated structures described by Mark (1957). These structures are large compared to the thickness of the boundary layer behind the incident shock, and they generate large vortices and jets behind the reflected shock. Even though bifurcation effects are usually reduced in the reflected-shock experiments by dilution of the reactive mixture with an inert monoatomic gas, the bifurcated structures can become comparable to the channel size. For example, Vermeer and al. (1972) observed weak and strong ignition behind bifurcated reflected shocks in hydrocarbon-oxygen mixtures diluted with argon. Ignition phenomena near the reflecting wall in presence of large bifurcated shock structures were observed in two-dimensional numerical simulations by Takano (1991), who studied a hydrogen-oxygen mixture diluted with argon. In this paper, we describe numerical simulations of ignition behind reflected shocks in an undiluted ethylene-air mixture, where the bifurcated structure quickly approaches the channel size and produces intense mixing behind the reflected shock.

Two-dimensional Navier-Stokes numerical simulations were performed using an adaptive, structured mesh and an explicit, second-order, Eulerian, Godunov method. The code has been used for simulations that resolve boundary layers and flame fronts, and was tested extensively in studies of shock-flame interactions and DDT by Khokhlov & Oran (1999), Gamezo et al. (2000). We considered a shock tube filled with a stoichiometric ethylene-air mixture at the initial pressure of 100 Torr and the initial temperature $T_0 = 293$ K. The reactive system was described by the polytropic equation of state with $\gamma = 1.15$, and a one-step Arrhenius kinetics with the activation energy $30.7RT_0$ and pre-exponential factor 3.2×10^{11} m³/kg-s. The heat of chemical reaction $61.0 RT_0/M$ ($M = 29$ g/mol) corresponded to the experimental value of detonation velocity $D_{CJ} = 1870$ m/s. The complete set of parameters for the reactive system is given by Gamezo et al. (2000).

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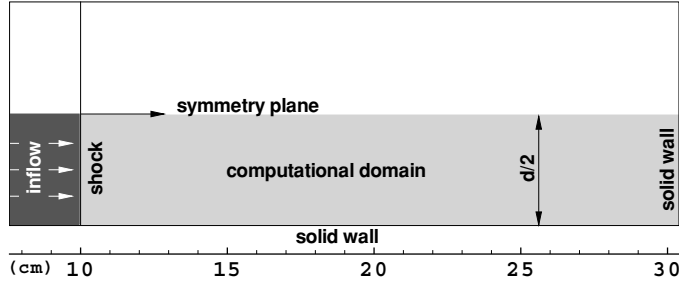


Figure 1. Schematic of the computational setup.

The computational setup is shown in Fig. 1. We model a lower half of a shock tube using the symmetry conditions at the upper boundary of the computational domain. The bottom and right boundaries are no-slip adiabatic walls. Zero-gradient inflow boundary conditions are imposed at the left. A planar incident shock is initially placed 20.4 cm from the end wall. The velocity of the gas is set to zero everywhere ahead of the shock. Between the left boundary and the shock, the flow is uniform with the post-shock parameters determined from the Rankine-Hugoniot conditions for a shock with a given Mach number, M_S .

The simulations were performed for a series of Mach numbers of the incident shock, $M_S = 2.2, 2.3, 2.4$ and 2.5 , and for two channel widths, $d/2 = 3.8$ and 0.95 cm. Before the reflection, flow behind the incident shock was almost uniform except for a thin boundary layer that developed along the bottom wall. The incident shock itself remained essentially planar as it propagated to the right towards the end wall. The flow evolution after shock reflection is shown by the sequence of temperature fields in Figs. 2 and 3.

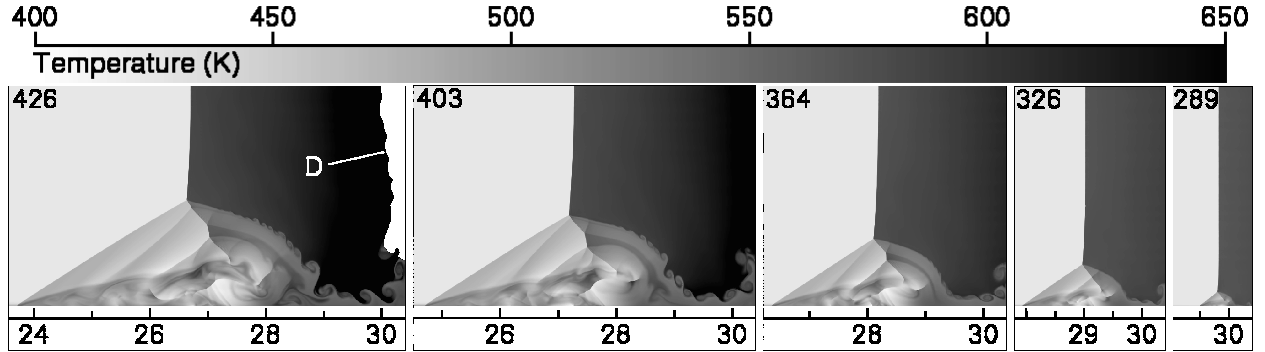


Figure 2. Sequence of temperature fields showing the evolution of the reflected shock interacting with a boundary layer in a stoichiometric ethylene-air mixture for $M_S = 2.5$ and $d/2 = 3.8$ cm. White area in the last frame contains burned material with temperature about 3000 K. **D** indicates detonation. Time (μs) is given on the left side of each frame. Scale is in centimeters.

Figure 2 shows a typical case of strong ignition for $M_S = 2.5$ and $d/2 = 3.8$ cm. The reflected shock interacted with the boundary layer and created a fast-growing bifurcated shock structure. The bifurcated shock produced a relatively cold wall jet which removed the hot material from the region around the lower corner near the end wall and destroyed

the conditions for a thermal explosion in this region. However, the most of the surface of the end wall was unaffected by the wall jet, so a thermal explosion occurred practically at the same time at all the points along the surface. The resulting shock wave was strong enough to trigger a detonation **D** that subsequently overtook the reflected shock.

Figure 3 shows a typical case of weak ignition occurring away from the end wall for $M_S = 2.4$ and $d/2 = 0.95$ cm. In this case, the wall jet removed hot material from the entire surface of the end wall before a thermal explosion occurred there. The bifurcated foot quickly reached the center of the tube and created several secondary shocks. Interactions of these shocks with vortices produced by the bifurcated shock intensified mixing in the shock-compressed material.

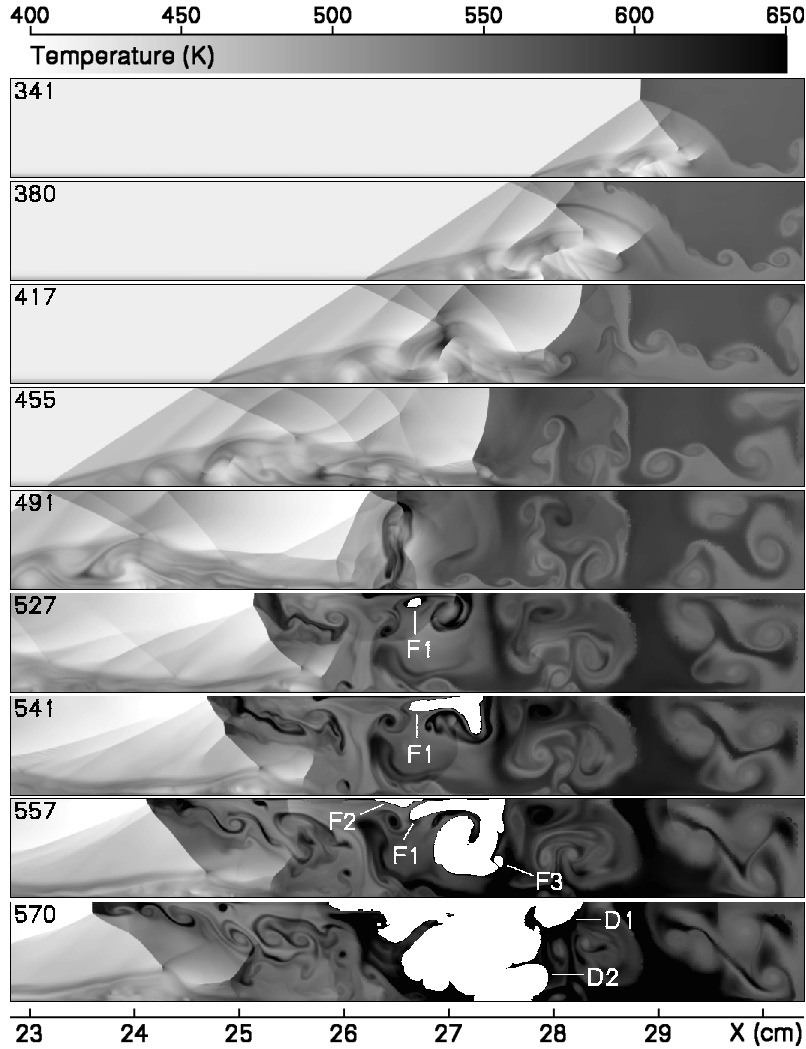


Figure 3. Sequence of temperature fields showing the evolution of the reflected shock interacting with a boundary layer in a stoichiometric ethylene-air mixture for $M_S = 2.4$ and $d/2 = 0.95$ cm. White areas in the last four frames contain burned material with temperature about 3000 K. The letters indicate flames (F1, F2, F3) and detonations (D1, D2). Time (μs) is given on the left side of each frame.

Shock-shock and shock-vortex interactions created hot spots between the reflected shocks and the end wall. Most of these hot spots disappeared because of interactions with vortices and rarefaction waves. However, one of the the hot spots survived long enough to produce a flame **F1** at 3.7 cm from the end wall. The flame developed interacting with vortical structures and generated weak compression waves that heated the surrounding material. This process created more hot spots. Two of them produced flames **F2** and **F3**, and two others eventually triggered detonations **D1** and **D2** by the gradient mechanism (Khokhlov & Oran 1999).

A comparison of ignition and DDT times in Fig. 4a shows that, for the same M_S , weak ignition producing a flame in a narrow channel occurs sooner than strong ignition at the end wall in a wider channel. The DDT time for a weak ignition in a narrow channel is almost the same as for strong ignition, even though the detonations appear at different locations as shown in Fig. 4b.

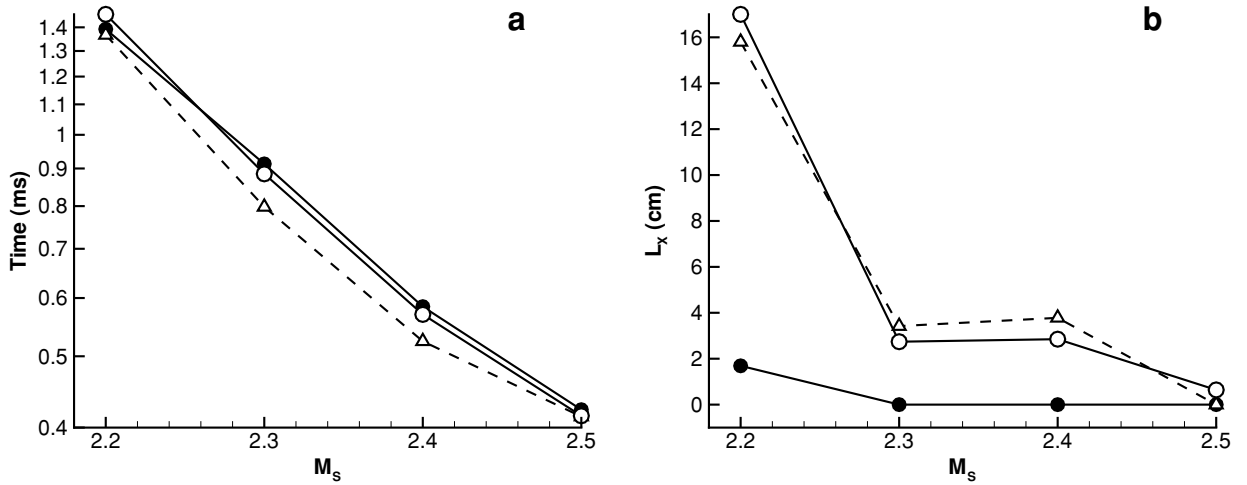


Figure 4. Ignition time (a) and distance from the ignition point to the end wall (b) as functions of Mach number of the incident shock. Circles and solid lines correspond to a first detonation triggered in the channel (black circles for $d/2 = 3.8$ cm and white circles for $d/2 = 0.95$ cm). Triangles and dashed lines correspond to a first flame that appears in the channel ($d/2 = 0.95$ cm).

Ignitions occurred closer to the end wall for stronger incident shocks and larger channels where the influence of the wall jet was less pronounced. When the wall jet was unable to remove the hot material from the end wall, or unable to mix the hot material with the cold gas soon enough, strong ignition occurred in the vicinity of the end wall. These results are consistent with experimental observations (Vermeer et al. 1972) of auto-ignition of hydrocarbon-oxygen mixtures diluted with argon behind bifurcated reflected shocks. The authors report that ignitions occurred far from the end wall for relatively weak incident shocks.

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