On Critical Conditions For Detonation Initiation By Shock Reflection From Rectangular Obstacles

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Summary

A series of numerical simulations supported by experiments are reported on the interaction between a planar incident shock and a single rectangular obstacle. The dynamics of the interaction are described, particularly the reflection of the incident shock and the onset or otherwise of detonation. The test mixtures used were stoichiometric hydrogen and oxygen diluted with either argon or nitrogen, at an initial pressure of 5.3 kPa. The aim of the study was to determine the conditions under which a reflected detonation was generated. Predicted and observed critical conditions are compared with a simple criterion based on the auto-ignition delay time behind an ideal reflected shock and the acoustic transit time across the face of the obstacle. The physical and chemical processes that have been observed are also discussed.

INTRODUCTION

The continuing concern surrounding the potential for damaging explosions following the accidental release of large quantities of combustible volatiles has led to numerous studies of explosion development in confined and congested regions. In the limit, deflagration to detonation transition is possible. Both field and laboratory scale experiments have shown that the hazard potential of high speed deflagrations in a gaseous fuel-air mixture can be severe, particularly as the linear dimensions increase. The severity of explosion is increased when obstacles are present as they can increase the turbulent burning rate, leading to flame acceleration and, in some cases, transition to detonation. In assessing the hazard it is usually assumed that detonation will arise by a local explosion between the turbulent deflagration and the shock wave formed ahead of the deflagration. However, the potential also exists for the mixture to be ignited as the lead shock itself is reflected from obstacles ahead of the supporting deflagration. In the present paper we report the results of a preliminary computational study, with a supporting program of experimental tests, to investigate the conditions required to initiate a detonation as an incident shock reflects from obstacles of finite dimension.

NUMERICAL SIMULATIONS

The simulations performed as part of this work are conceptually identical to those performed by Kaplan and Oran (1991) in their study of shock-obstacle interaction in propane-air mixture. The simulations were performed using a code based on the FCT algorithms, see Ward (1999). A single rectangular obstacle, 38 mm x 25 mm with variable height, was located in the middle of the computational domain, which initially matched the dimensions of the experimental observation window. The gas mixtures simulated were $2H_2$+O_2+X%Ar, with X in the range 70-90%, with one case using 70% N_2. To include the effects of finite rate chemistry a full kinetic mechanism for hydrogen oxidation was used, consisting of 47 reaction, 10 species hydrogen oxidation mechanism. This was developed at the University of Leeds, and is a subset of a larger methane oxidation mechanism.

EXPERIMENTAL DETAILS

The experimental apparatus used, described in greater detail by Brown (2000), was a conventional shock tube, length 4.75 m, with an internal cross section of 38 mm x 76 mm. A special window section allowed multi-spark schlieren visualisation to be undertaken. The partially obstructing obstacle was located at the mid point of this section, which permitted a maximum observation field 76 mm high by 230 mm long.

RESULTS

Inert shocks

Initial validation calculations were undertaken for a shock in argon interacting with an obstacle 38 mm in height, one half the height of the computational domain. The inflow conditions were for a Mach 2.45 shock in argon at an initial pressure of 10 kPa. The shocked gas parameters were calculated to be, using the usual shock notation, p_2/p_1 = 7.24 T_2/T_1 = 2.72 and ρ_2 / ρ_1 = 2.67 with a corresponding fluid velocity of 493.4 ms^{-1} (shock velocity of 789.7 ms^{-1}). Fig. 1 illustrates that the shock positions observed in the experiments correspond well with those obtained from the simulations. The computational domain used for the initial simulations corresponded with the physical dimensions of the window section of the shock tube, which had 230mm by 76mm. Initial grid refinement tests were performed and acceptable convergence was found with a spatial resolution of 1 mm. This resolution provided a reasonable trade off between grid size and computation time when using a small workstation.

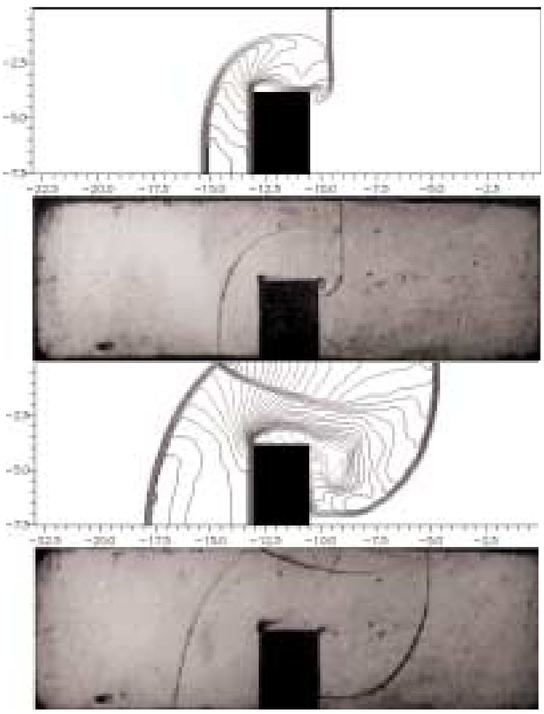

Figure 1 Experimental schlieren and computed density contour plots of shock wave reflection and diffraction in pure argon. M_s , P_0 0.1 bar

$2H_2$+O_2+70%Ar

Figure 2 show combined schlieren and simulation output. In the initial frame the curved reflected shock is clearly visible whilst the top half of the incident shock continues to propagate unhindered over the obstacle. Up to this point no exothermic chemical reaction has taken place, although elevated temperatures and pressures exist behind the reflected shock. Auto-ignition has occurred at the time of the next frame and by the third frame some burned products start to be transported over the top of the obstacle into the downstream region. The incident shock has by now started to diffract over the obstacle. From the shape of the reaction front it is apparent that the initial ignition took place at the base of the obstacle. By the final frame a self-sustaining detonation propagates away from the obstacle.

$2H_2+O_2+70\%N_2$

Tests conducted with nitrogen diluted gas mixtures yielded somewhat different

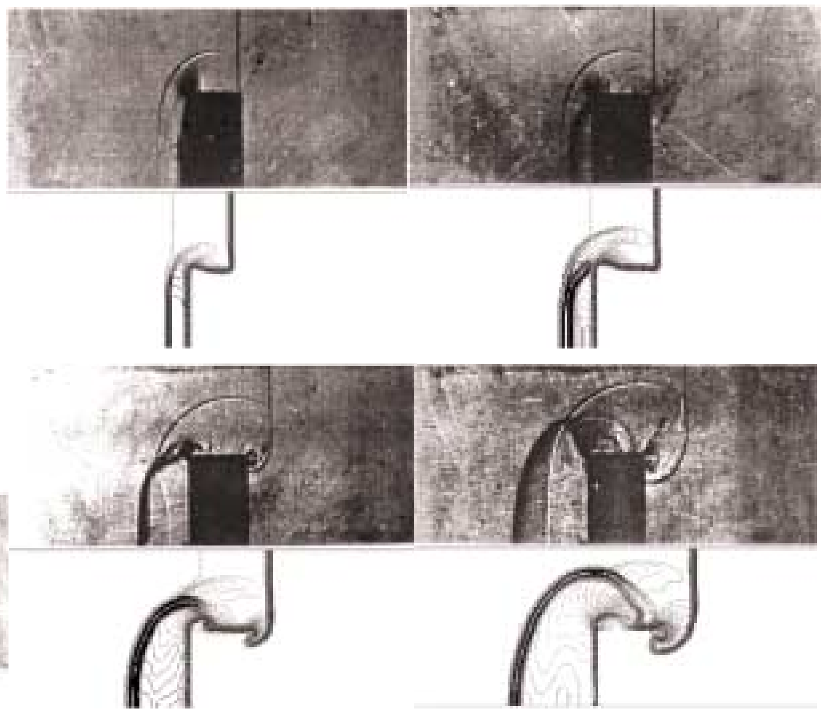

Figure 2 Experimental schlieren and computed density contour plots of shock wave reflection and detonation onset with $2H_2 + O_2 + 70\%Ar$ M_s 2.5, P_0 0.1 bar. Δt 20 µs

results to those with argon dilution.

A sequence of schlieren and simulation outputs obtained for an incident Mach number 2.5 (not shown) indicate that little exothermic reaction has taken place with the overall flow-field very similar to the non-reactive case. A study of the energy release profiles from the numerical calculations did however confirm experimental observations that some very weak emission was discernible on records obtained using a photo-multiplier set to observe the interaction. This is as expected because, for the same incident Mach number, the nitrogen diluted mixture is less likely to detonate. The primary reason is the higher reflected shock temperatures developed in monatomic argon.

When the incident Mach number was increased to 3.01 the reflected shock underwent a transition to detonation almost immediately, whilst a reaction front propagated on the downstream side of the obstacle in the wake of the incident shock. Some slight timing discrepancies between the onset of detonation in the schlieren photographs and simulations outputs can be discerned, see Fig. 3, with the computed delays found to be slightly longer than those measured in the experiment.

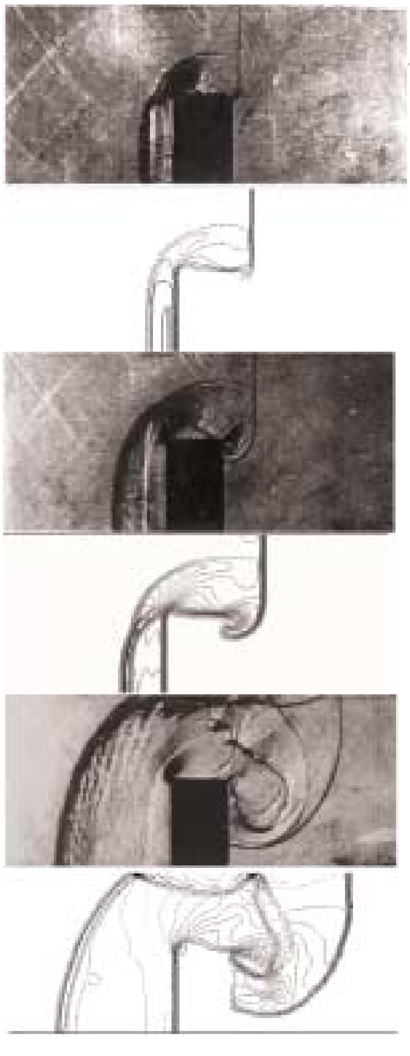

Figure 3 Experimental schlieren and computed density contour plots of shock wave reflection and detonation onset with $2H_2 + O_2 + 70\%N_2$, M_s 3.01, P_0 5.2 6kPa.

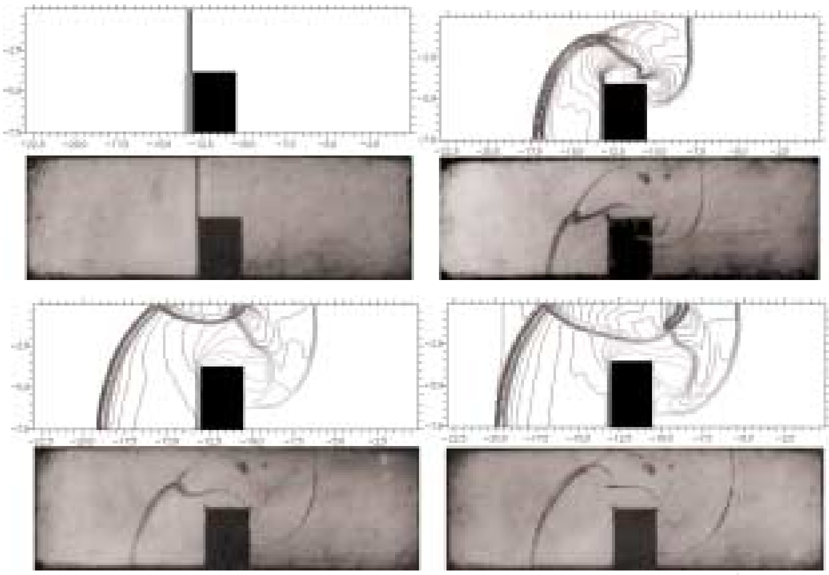

Figure 4 Shock wave reflection and detonation onset with $2H_2 + O_2 + 80\%Ar$ M_s 2.5, P_0 5.26 kPa. Δt20 μs.

$2H_2+O_2+80\%$ Ar

The sequence of schlieren images and density plots shown in Fig. 4 were obtained with an incident shock Mach number 2.5 in stoichiometric oxygen-hydrogen diluted with 80% argon. Again a rapid onset of detonation was observed and the simulation exhibited a shorter ignition delay time than that in the experiment, evidenced by the more rapid evolution of the detonation.

$2H_2+O_2+90\%$ Ar

Figure 5 shows a sequence of density plots of the evolution of combustion with 90% argon dilution for an incident shock Mach number 2.5 and initial pressure 5.26 kPa. Here a preferential growth of the combustion front at points closer to the base of the obstacle can be seen clearly. This arises as the combustion that would normally occur in the reflected shock region is inhibited by the expansion wave that propagates from the upper corner of the obstacle. There is also some indication that reacted gas is also starting to sweep forward over the obstacle, after it is ignited close to the front face.

SIMPLE CRITERION FOR THE ONSET OF DETONATION

A simple criterion for whether detonation occurs can be formed using the ratio of the chemical ignition delay time to the acoustic transit time of an expansion wave in the reflected shock gas across the obstacle face. Thus a critical condition, below which direct initiation of detonation might not occur, can be expressed as $\eta < 1$ where η is given by the expression,

$\eta = \frac{h}{a_r \tau_r}$ and h is the height of the obstacle, a_r and τ_r are the sound speed and ignition delay time in the

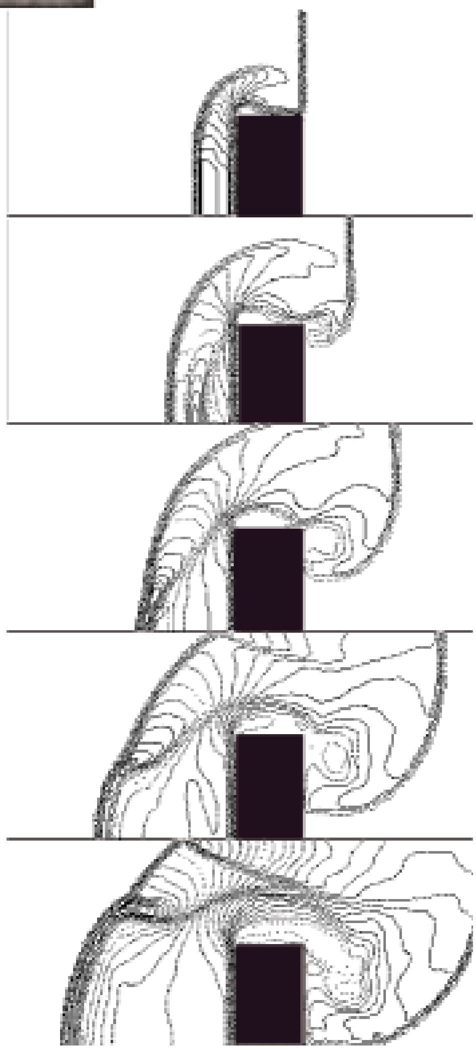

Figure 5 Density plots of shock wave reflection and detonation onset with $2H_2 + O_2 + 90\%Ar$ M_s 2.5, P_0 5.26 kPa. Δt20 μs.

undisturbed reflected shock region respectively.

A plot of values of η computed as function of incident shock Mach number are shown in Fig. 5 for oxy-hydrogen diluted with 70% argon. The ignition delay was computed using the ignition delay correlation of Strehlow and Cohen (1962). The curves are for three obstacle heights relative to the shock tube height. The critical Mach number for the 38 mm is in reasonable agreement with that found in practice.

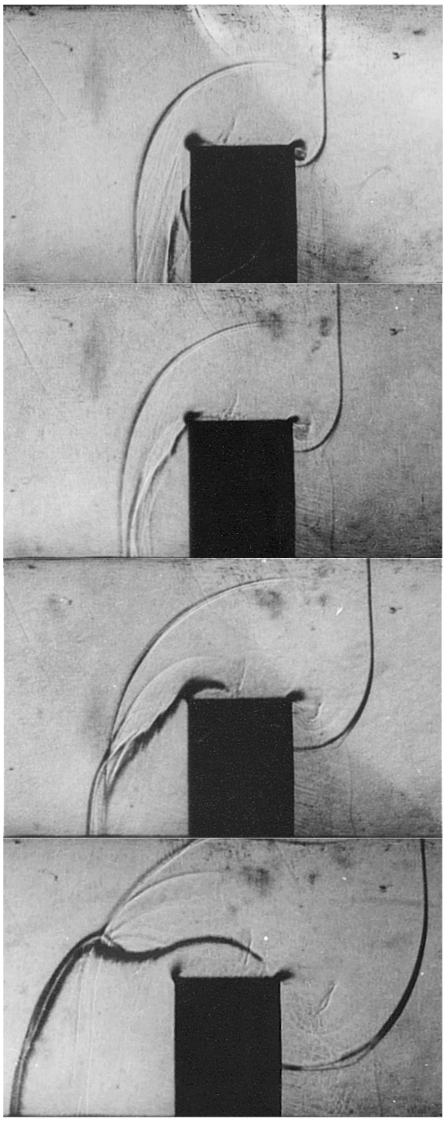

Figure 4 Sequence of schlieren images of shock wave reflection and detonation front growth with $2H_2 + O_2$ + 80%Ar. M_s 2.48,P_0 5.26 kPa Δt, 10 μs

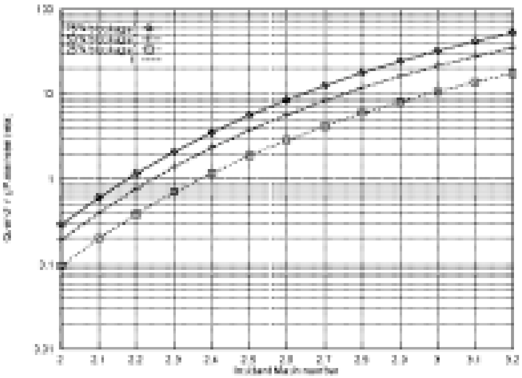

Figure 6 Variation in parameter η as a function of incident shock Mach number $2H_2 + O_2$ + 70%Ar. P_0 5.26 kPa. Obstacle height: upper 57 mm, middle 38 mm and lower 19 mm.

Figure 6 shows schlieren images from a test similar to that shown in Fig. 4, but at a faster imaging rate. Here, on the first frame, some 28.4 μs after the incident shock first contacted the obstacle, the partial onset of reaction along the bottom half of the front face can be seen, limited by the expansion. A further interesting feature is the preferential growth of the reaction front along a layer slightly displaced from the solid wall. This is most likely due to local cooling of the gas nearest the wall due to heat transfer. Also clearly visible (frame 3) is the compression wave formed ahead of that part of the reaction front that has not undergone a transition to detonation.

The full paper will present more detailed analyses and discuss the validity of the critical criterion in greater detail. Further simulations at higher grid resolutions will also be presented and the main features observed in the experiments and simulations will be described in greater detail.

REFERENCES

Brown CJ and Thomas (2000) Shock Waves J. 10:23-32

Kaplan CR and Oran ES (1991) Combust Sci. Tech. 80:185-205

Strehlow RA and Cohen A, (1962), Physics of Fluids 5:97-101

Williams R Ll (1996) The influence of chemi-acoustic interactions on detonation. PhD Thesis, University of Wales, Aberystwyth UK

Ward SM (1999) Some applications of the numerical simulations of gas-phase flows. PhD Thesis, University of Wales, Aberystwyth UK