# On The Controlled Generation and Detailed Observation of the Onset of Detonation

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### **Summary**

The detailed observation of deflagration to detonation transition (DDT) is inherently difficult due to the stochastic nature of the flame acceleration processes that lead to shock formation which in turn gives rise to the conditions required for detonation to start. The present paper describes how shock tube techniques have been used to generate the conditions required for the onset of detonation in a more direct manner.

### Introduction

An evaluation of the extent of possible flame acceleration and shock formation in accidental releases of flammable vapours is an important activity in relation to practical explosion



Figure 1. Flame propagation following ignition downstream of a grid.  $\Delta t$  50  $\mu$ s. Tube (H) 76 mm (W) 38 mm.  $C_2H_4+3.O_2+50\%N_2 M_s$  1.37  $P_o$  0.52 bar. Vertical bars: left, grid; right, igniter array of 5 sparks hazard scenarios. The problem when observing explosions and transition to detonation in their 'natural' environment is that the turbulence processes involved are stochastic and it is almost impossible to observe at the exact position and time at which the onset of detonation occurs. More importantly, this also makes it impossible to observe the conditions that are the immediate pre-cursors to the onset of detonation. The present work is directed at identifying more precisely the conditions at which detonations will form within a larger DDT event by means of controlled experiments under laboratory conditions.

### **Previous experimental work**

Unlike flame acceleration processes, laboratory based shock wave techniques provide a controlled means of heating and compressing a gas. Shock tubes are widely used in the study of chemical kinetics but studies of the subsequent flame propagation are far less common. Bambrey (1993) used a shock flow to study flame front growth following the deliberate ignition of turbulent gas that had passed over a grid, work continued by Jones et al. (1998). The aim of these exploratory studies was to observe flame propagation as a function of the turbulence intensity and mixture reactivity. An example of the later stages of development is

however of interest for other related reasons. Typical schlieren images are reproduced in Fig 1. Observing the gas between the igniter and the grid, a rapid intensification of the flame

front is seen as the flame front burns back towards the grid. Further, as the flame front passes upstream over the grid, clear pressure fronts are seen to develop ahead of the flame front. These features continued to move upstream and eventually led to a transition to detonation. These initial studies thus indicated that controlled generation of DDT in a shock tube might be possible if regions of sufficiently intense turbulent combustion could be achieved. However the grid configuration did not give sufficient local acceleration for transition to be observed within the test section window and the initial geometry was complicated. Later work utilised existing knowledge that a spherical flame perturbed by a shock could lead to rapid increases in local turbulent burning velocity.

Markstein (1964) was the first to demonstrate how local combustion wave enhancement could result if a shock wave perturbed a flame. Scaricni et al. (1993) extended this work, using a line of five flame bubbles, and attempted to quantify the extent of the local increase in combustion rates. This was modelled by Khokhlov et al. (1999) who demonstrated the importance of multidimensional interactions, which permitted substantial increases in flame area and local energy release rates the pre-cursors to the onset of detonation.

Thomas et al. (2000) have reported an extension to this work, using a single flame bubble. Their work, using stoichiometric ethylene-oxygen diluted with 50% nitrogen, was conducted with initial test gas pressures of 0.13 bar and a range of incident shock strengths. The initial evolution of the flame front is shown in Fig. 2,





Figure 3. Reflected shock (moving right to left) emerging following multiple-shock flame interaction. Original incident shock M<sub>s</sub> 1.7, P<sub>0</sub> 0.053 bar. Δt 50 us. Frame 2 missing

obtained in a shock tube cross section 76mm high by 38 mm wide.

As the reflected shock emerged from the highly



Figure 2. Initial distortion of two spherical flame bubbles by an incident shock (from the left).  $\Delta t \ 100 \ \mu s$ , image height 76 mm.  $M_s \ 1.7, \ P_0$  $0.0.52 \ bar.$ 

convoluted flame bubble the shock and flame were closely coupled in many instances. Recently Gamezo et al. (2001) conducted extremely detailed CFD simulations of these events and showed that preferential flame propagation in the turbulent boundary layer can explain images such as those in Fig. 3. In some instance the coupling between the combustion near the wall greatly enhance the strength of the bifurcated shock although, under other circumstances, it is also seen to de-couple as in the last frame of Fig. 3. In this case the flame separates rapidly from the lead shock once it has



Figure 4. Original incident shock  $M_s 2.2 P_0$ 0.26 bar,  $\Delta t 10 \ \mu s$ . Shock and flame decouple but detonation arises due to oblique shock reflection at the top wall.

enhancement. Their studies showed was that detonation could be initiated in a controlled manner, with initial conditions that are sufficiently well defined to allow successful CFD simulation. Nonetheless, the experiments still gave rise to extremely complex and highly nonsteady and non-linear events. At least one further significant experimental refinement has been possible, observed during investigations of changes in global activation energy of autoignition delay times at temperatures of 750-1100K.

## **Onset Of Detonation Following Non-Ideal Ignition Behind A Reflected Shock**

The results of separate investigations, see Cadman et al. (2000) and Goy et al. (2001), had indicated that the ignition mechanisms of propane and methane auto-ignition changed significantly at temperatures below ca. 1200 K. Other circumstantial evidence from pressure histories at various positions near the end wall had also suggested that the ignition point moved away from the end wall. For ideal gasdynamic

passed the igniter rod. Detonation was only observed when the incident shock Mach number was increased to 2.2. In this case the intensity of combustion is much greater and the film in the open shutter camera was fogged due to the emission. In Fig. 4 an initially closely coupled and highly non-steady shock and flame regimes is again formed. These separate after passing the location of the igniter rod after. Detonation first appears at the upper wall, probably due to oblique shock reflection at that position. After transition has occurred, there is evidence of preferential flame growth in the boundary layer along the bottom wall. The complete series of experiment reported by Thomas et al (2000) included results which showed that any object that left a turbulent wake could lead to local flame velocity



Figure 5.Non-ideal ignition in a reflected shock leading to detonation.  $\Delta t$  50 µs,  $P_0$  - 0.52 bar.  $T_{ref}$ 1065±20 K,  $P_{ref}$  1.27±0.5 bar. Mixture  $C_2H_4$  +  $3O_2$  + 12Ar.



Figure 6. Non-ideal ignition leading to detonation in reflected shock gas.  $\Delta t$  20 µs,  $P_0$  - 0.53 bar.  $T_{ref}$  981K,  $P_{ref}$  1.14 bar Mixture,  $C_2H_4$  + 3 $O_2$  + 12Ar.

conditions ignition would be expected to occur first close to the reflecting wall, as the gas there has the longest residence time at the desired temperature and pressure. This non-ideal ignition had been observed earlier by several investigators and in a transition to detonation context classified as mild or spotty ignition.

A series of experiments were thus conducted to investigate this non-ideal auto-ignition phenomenon in greater detail. The mixture used for this series was stoichiometric ethylene-oxygen, but now diluted with 75% argon. A series of schlieren images of a mild ignition is shown in Fig. 5 The flame front is formed several milliseconds after the reflect shock had left the test section. The final two frames show that a compression formed leading front to a rapid combustion of the remaining gas between the flame and the real wall (on the right hand side of Fig. 5). The theoretical reflected gas temperature and pressure in this test was  $1065\pm20$ K. The reaction front in this case is highly reminiscent of a turbulent flame bubble in quiescent flow. Some visual evidence that the surrounding flow is turbulent is also evident from these and other images.

Better resolved images of the onset of detonation were obtained with a reflected gas temperature of 981 K, pressure 1.14

bar, reproduced in Fig. 6. In this case the evolution of a pre-cursor compression wave is easily discerned. However, unlike the event shown in Fig. 1, the formation of the compression front is not the result of some obvious external perturbation of the bulk flow but must arise from internal perturbations. Differences in fundamental laminar burning velocities between the two mixtures at the prevailing temperatures and pressures must also play a role. Images from a similar event at a slightly faster imaging rate and reproduced at greater magnification are shown in Fig. 7 where two pre-cursor compression fronts are observed.

The present new images capture the evolution of non-linear chemistry coupling with the local turbulent flow field and where the subsequent onset of detonation appears to arise spontaneously near the moving flame front. Figure 7 and similar observations represent the best controlled experimental conditions yet developed for the study of the onset of



detonation. Even so, the final onset is still highly unpredictably. It is also necessary to consider the contributions from flame propagation phenomena up to the very last instant. This must also be closely coupled to the pre-exothermic autoignition reactions developing in the surrounding gas.

More detailed analyses will be presented in the full paper. The paper will also consider some further optimisation of the spatial and temporal localisation of the onset of detonation.

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Figure 7. Emergence of detonation from a turbulent flame brush following auto-ignition of nominally quiescent gas behind a reflected shock. Mixture,  $C_2H_4 + 3O_2 + 12Ar$ .  $\Delta t \ 15 \ \mu s \ P_0 - 0.52 \ bar$ .  $T_{ref} \ 970 \ K$ ,  $P_{ref} \ 1.12 \ bar$ .