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ON THE TRANSITION FROM DEFLAGRATION TO DETONATION

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ABSTRACT

An introduction is given to the problem and principal research themes of the deflagration-to-detonation transition phenomenon. The key ideas of flame acceleration and detonation initiation are briefly discussed. Recent research is described with an emphasis on photographic studies of the propagation mechanisms of quasi-detonations. Theoretical notions about the spontaneous development of detonation are reviewed. Relationships between hotspots, reaction waves, and shock wave amplification are emphasized.

1 Introduction

Generally speaking, an explosive mixture can support two modes of combustion; deflagration and detonation. A detonation wave can be generated "instantaneously" if a sufficiently powerful igniter is used. This is referred to as direct initiation. If a weak igniter is used, a deflagration wave is obtained. Under the appropriate conditions, a deflagration will accelerate rapidly and undergo an "abrupt" transition to a detonation wave. There are many conditions in which this transition can occur, one common example is within a tube with very rough walls. This mode of initiation is referred to as deflagration to detonation transition or DDT.

The problem of DDT is one of the more difficult in combustion. Experimental studies have provided great insight but continue to demonstrate variety in the phenomenon rather than pointing toward simple criteria for DDT. Numerical studies are difficult since

DDT prediction requires the computation of unsteady and turbulent, multi-dimensional, compressible reacting flow. No satisfactory model is presently available and many gaps still exist in our basic knowledge of this phenomenon. There is great interest in improving our understanding since detonations represent the most severe form of explosive hazard and DDT is the least understood and most likely means of obtaining detonation initiation in an accidental explosion.

This paper discusses the DDT problem, summarizing what is known experimentally and what are the basic problems that need to be resolved. A previous review paper [1] has already dealt with all the different fundamental aspects of the DDT problem. Hence this paper emphasizes the more recent results and the changes of viewpoint as a consequence of these more recent findings.

2 Some Basic Considerations

In a transition from deflagration to detonation, we are more concerned with a change or transition in the mechanism of propagation than in the change of wave speed. Thus it is important to briefly review these mechanisms of deflagration and detonation to see what is required for a transition to take place.

2.1 Flames

A flame or deflagration is a subsonic combustion wave in which the pressure and density decrease across the wave. The microscopic mechanism of propagation is via the molecular transport of energy and free radicals from the reaction zone to the unburned mixture ahead of it. Flames are very sensitive to disturbances in the surrounding flow and the macroscopic motion of flames is dominated by the convecting and distorting action of the gas flow the flame moves into, flow that is often produced by the flame itself. Local straining motions in the fluid, particularly those associated with the vortical structures of turbulent flow, cause compression or stretching of the reaction zone, which results in changes in the local combustion rate. In extreme cases, the flame can be extinguished altogether by strong strain fields.

The propagation velocity of a deflagration depends strongly on the composition and initial thermodynamic state of the mixture. For a given upstream state, there is a unique intrinsic laminar flame velocity which is determined by the balance of convection, diffusion

and reaction within the flame. Laminar burning velocities S_u have a maximum value of about 0.5 m/s for typical hydrocarbon fuels in air.

Propagating flames rarely have a smooth or laminar appearance. The many natural instability mechanisms (thermal-diffusive, hydrodynamic, Rayleigh-Taylor, etc. [2]) and interactions with upstream flow disturbances cause the flame surface to become highly distorted and we speak of a "turbulent" flame. For a flame propagating in a duct, the increase in the flame area leads to an increase in the burning rate per unit area of the duct and thus an increased "effective" burning velocity of the flame. This effect is usually described in terms of a "turbulent" burning velocity S_T which is much larger than the laminar value. Up to moderate turbulent intensities, the apparent turbulent burning velocity is directly proportional to the level of velocity fluctuations u'.

It should be noted that the *burning velocity* S_u is defined as the wave speed relative to the unburned gas ahead of the front, while the *flame speed* U_f is generally relative to a fixed observer. The motion of the unburned gas motion ahead of the flame front depends on the boundary condition behind the wave. For a closed–end tube, in which the burned gas velocity relative to a fixed observer is zero, the unburned gas velocity U_u is typically the specific volume ratio v_b/v_u across the flame times the burning velocity S_u itself. For a planar laminar flame, the flame velocity relative to the tube is then $S_f = (v_b/v_u - 1)S_u$. The specific volume ratio can be computed from the ideal gas law as $v_b/v_u = N_u T_u/N_b T_b$, since the pressure change across the wave is negligible for typical flame velocities. For many hydrocarbon fuels in air, this ratio has a value of approximately 7, resulting in a idealized flame propagation velocity of 6 times the laminar burning velocity.

2.2 Flame Acceleration

An even more significant effect associated with the displacing action of the volume expansion is the motion produced in the unburned gas ahead of the flame. The natural instability of high Reynolds number flows (in a smooth tube) or the separation (rotational flow) associated with flow over obstructions, openings, or bends upstream of the flame will ultimately result in the production of unsteady and turbulent regions upstream of the flame. When the flame reaches these disturbed portions of the flow, stretching and folding of the

flame by vortical fluid will result in a considerable distortion of the flame.

The appearance and dynamics of the distorted flame will depend strongly on the nature of the fluid dynamic disturbances, *i.e.*, the length scales and intensity of the turbulence in the upstream flow. This complex problem has been considered by a number of researchers in the last decade and at least 5 distinct regimes of combustion have been identified [3-5]. Since the typical thickness of a hydrocarbon-air flame at atmospheric pressure is ℓ_f = 500-1000 μm, the flame appears as a discontinuity surface or sharp front on the scale of the typical DDT experiment, 0.1 to 1 m. However, since a continuous spectrum of length scales exists in a turbulent flow, from the integral scale L down to the Kolmogorov microscale η, it is possible that the flame may to comparable or even intermediate in size to these scales of fluid motion. In addition, the fluctuating strain rates (equivalent to vorticity fluctuations) may be sufficiently large that the flame is extinguished by the flow. Clearly, predicting flame behavior under these conditions is a daunting problem, particularly since the turbulence is generated by the previous motion of the flame!

The flow velocities and turbulence intensities are time dependent during flame acceleration and a wide range of values can be expected during the course of the event. In the initial stage of flame propagation, velocity fluctuations are small $u' < S_u$, and have relatively large length scales ℓ compared to the flame thickness. In this case, the velocity field will gently distort the flame sheet and small variations in the local burning velocity will result from the effects of strain in the flowfield. This is the *wrinkled laminar flame regime*; a situation that only exists for a short initial period. As the flame accelerates, the mean flow and turbulent intensity increases, resulting in a decrease in smallest flow length scales. The flame becomes increasingly disturbed by the flow and passes through the *corrugated flame* regime in which the effects of strain are important but the flame still forms discernible sheets or flamelets.

Finally, during the latter stages of flame acceleration, both mean and fluctuating velocities are quite high ($U \sim$ 100 - 1000 m/s, $u'/U \sim$ 0.1 - 0.2). The flame front becomes extensively distorted, forming a complex and convoluted surface, a flame "brush". In this stage, the flame surface is fragmented into disconnected portions and broadened by interacting with the turbulent flow. This regime of *distributed reaction zone* or *microvolume combustion* is characterized by very strong straining motion and large amplitude temperature and species

concentration fluctuations at the flame length scale level. Very little is known about combustion under these conditions; this situation is quite far removed from slightly wrinkled laminar flames of ordinary experience.

An appreciation for the relative flow scales in this extreme situation can be obtained by considering a simple example of a hypothetical large-scale experiment with an integral scale of $L = 1$ m, a mean flow velocity of 100 m/s and a turbulent intensity $u'/U = 0.1$. The length scale at which most of the dissipation occurs is the Taylor microscale $\lambda = 400$ μm; this is comparable to the flame thickness. The smallest turbulent scale is the Kolmogorov microscale $\eta = 8$ μm; much smaller than the flame thickness $\ell_f \sim 1$ mm. If we are considering a typical light hydrocarbon fuel burning in air, a representative laminar flame speed is $S_u = 0.5$ m/s. We conclude that the length scales are ordered as $L >> \ell_f >> \eta$ and that relative velocity scaling is $u'/S_u = 20$. Even more significant is the magnitude of the fluctuating strain rate $\omega' = u'/\lambda = 2.5 \times 10^4$ s^{-1}! This is a factor of fifty larger than the characteristic strain $S_u/\ell_f = 500$ s^{-1} needed for extinction by stretching and several times the maximum strain experimentally observed [6] to be required to quench flames in turbulent flows. It is these simple estimates that lead us to the conclusion that a highly unusual regime of combustion exists in the high-speed flame propagation just prior to transition to detonation.

Most significant for the DDT problem is the substantial increase in total burning rate associated with the flame-upstream flow interaction. In the earlier stages of the process, strain rate effects on the laminar burning velocity can probably be neglected and the burning rate increase associated exclusively with the increase in the flame area. As the flame accelerates, both strain rate effects and fluctuations in temperature and concentration will play an increasingly significant role in limiting the simple linear amplification in burning rate provided by flame area increase alone. The amplification of the burning rate by the flame is unstable. An increase in the burning rate in a closed-end tube results in a greater effective flame propagation velocity and velocity of the displaced unburned fluid. Larger velocities in the upstream fluid will increase the turbulence intensity and vorticity in separated regions that the flame will encounter subsequently. In this fashion a feedback process is set up that will accelerate the flame to high velocities (up to 1000 m/s) and ultimately, can set the stage for the transition to detonation. This process is indicated schematically in Fig. 1.

The process of positive feedback between a flame and it's induced flow is one of the principal and recurring themes in deflagration to detonation transition studies. Determination of the dominant processes involved in the flame-flow feedback mechanism has served to define the problem of flame acceleration in many recent studies. Two types of major feedback mechanisms have been considered: fluid dynamic and gasdynamic. It is possible to construct simple models with either mechanism which exhibit a runaway growth in the burning rate for confined flames.

A typical fluid-dynamic feedback mechanism considered to be responsible for flame acceleration is the growth in flame area due to either turbulence or unsteady flow generated upstream by the flame motion. Batchelor's estimate [7] of exponential growth of a material surface immersed within "isotropic turbulence" suggests the potential effectiveness of the area amplification process. The paradigm of these area amplification processes is the interaction of a flame with an isolated vortex. Experimental [8–10] and numerical [11–14] studies have been carried out on line and ring vortex structures. Comparison of the results of the 2-D vortex dynamics numerical simulations and several experiments shows that up to moderate flame velocities, flame-vortex interactions can be explained as the stretching and folding of essentially passive flame fronts, which serve as moving source terms for incompressible and inviscid flow in both products and reactants.

Consider the interaction of a flame with a typical vortical structure, the fundamental elements of turbulent shear flows. As shown in Fig. 2, the flame will be entrained in the vortex and form a layered structure resembling a jelly roll with alternating layers of products and reactants separated by strained laminar flames. Recently this problem was considered theoretically by Peters and Williams [15], who suggest that the normal burning motion of the flames may produce a central core of burned material which grows radially as $t^{2/3}$ *if* the strain effect is not too strong (near–unity Lewis number). However, they also note that strain effects may extinguish the flames in the interior, resulting in a central unburned region. Subsequent diffusion of energy and radicals into the unburned gas layers in the vortex may lead to reignition of the entire structure after some delay time. This picture of flame interaction with vortex structures suggests a simple physical interpretation of the combustion process in the distributed reaction zone regime mentioned above: the flame brush is composed of volumetrically-exploding eddies distributed in

size and frequency of occurrence.

Experimentally, these exploding eddies are observed to produce intense local pressure fluctuations. The schlieren photographs of Urtiew and Oppenheim [16] and Meyer *et al.* [17] clearly demonstrate the presence of these intense pressure waves in the neighborhood of the turbulent flame brush. Coalescence of these pressure waves results in weak shock waves ahead of the flame. These waves are too weak to trigger detonation directly (the induction times are too long and the acoustic and reaction waves are uncoupled) [17] and the increase in burning rate due to the temperature rise is modest since $S_u \sim T^{1.5}$ [18]. However, due to the extreme temperature sensitivity of combustion processes, the mild temperature increases caused by these waves will initiate a slow reaction process. This partially-reacted fluid becomes progressively more unstable as the pressure-wave effects accumulate, and as discussed below in the Detonation Onset section, can serve as an amplifying medium for pressure and reaction waves.

Pressure waves also play an important role in creating further vorticity either via shock reflections (i.e. Mach stems and shear layers) or via Rayleigh-Taylor instability as these shocks traverse the various density interfaces. Rudinger and Somers [19], Haas and Sturtevant [20] and the numerical work of Picone and Boris [21] have demonstrated the vortex formation due to a shock wave traversing a bubble of a different density. In a confined tube, the tube walls provide reflecting surfaces and these transverse pressure waves can also amplify according to the Rayleigh criterion. This suggests yet another way in which the propagation mechanisms of intense turbulent deflagration differs drastically from the diffusive-convective mechanism of the weak turbulent flame.

The appearance of pressure waves ahead of high–speed flames also suggests a gasdynamic feedback mechanism of flame acceleration. Such mechanisms depend on the temperature increase across the weak leading shock and the temperature dependence of the flame speed. Numerical [22] and analytical models [23] of this process in a closed-end tube demonstrate that a runaway growth in flame speed will occur if burning velocity temperature dependence of either the form $S_u \sim T^m$, $m > 0$, or $S_u \sim \exp(-E/RT)$ is used. This process is indicated schematically in Fig. 3. Recent experimental observations on acceleration indicate that acceleration due to the flame folding mechanism is a much more generic and faster acting mechanism. Clearly there is a role for both gasdynamic and flame folding effects

in any acceleration process. It is significant to note that the actual event of transition to detonation is distinct from flame acceleration and cannot be predicted by either model.

The onset of detonation requires that the mode of combustion propagation must finally switch over to a coupled shock wave-reaction zone system. The traditional view is that unlike the flame mode of propagation, diffusive processes are too slow to play a role in detonation propagation. A strong shock (Mach number 4-6) results in the explosion of the reactants close behind the shock and the energy released by the explosion drives the shock waves. In order to set up this special relationship and have it become self-sustaining, certain conditions must be achieved. These conditions are still imperfectly understood, but as discussed in the last section of this paper, involve hotspots, reaction waves, and the amplification of weak shock waves through regions of gradients within the flow.

2.3 Detonations

A detonation is a supersonic combustion wave across which the pressure and density increase. The wave speed is typically 1800 m/s for hydrocarbon fuel-air mixtures. An idealized model of detonation structure (the classical ZND model) is a planar shock followed by a laminar, adiabatic chemical reaction zone, shown in Fig. 4a. Reactions are initiated thermally in the high-temperature ($\sim$1500 K) gases produced by the adiabatic compression at the shock front. The reaction zone terminates with a rapid excursion in temperature associated with the exothermic character of the combination of radical species to form products. In the context of the simplest models of reaction kinetics, this excursion is simply a convected thermal explosion. The laminar version of detonation structure is unstable and all self-sustaining gaseous detonations exhibit quasi-periodic transverse wave instabilities that result in the formation of the characteristic cellular pattern produced by the triple point trajectories. The characteristic pattern size or "cell size" is between 10 and 100 times the idealized reaction zone length, and determines the apparent thickness of the detonation wave. For example, in stoichiometric H_2-air initially at standard conditions, the idealized reaction zone length is about 0.25 mm and the measured cell width is about 15 mm.

A key issue in detonation propagation is the role of the transverse waves. Are transverse waves necessary for self-sustaining detonations? Experiments [24], as well as recent numerical simulations

[25] have conclusively demonstrated the necessity for the presence of transverse waves for detonations to propagate. A detonation wave fails when its transverse waves are attenuated by the acoustic absorbing wall of the tube. Why are transverse waves necessary? Transverse waves are a necessary consequence of the nonlinear shock interactions associated with the detonation instability. The collision of transverse waves also provides a mechanism for producing *hotspots* or explosion centers. Thus it appears that in the absence of solid boundaries for normal shock reflections, instability creates Mach reflections to achieve the high local temperatures required for ignition and rapid energy release.

A less obvious role of the transverse waves is that accompanying each triple shock configuration is a shear layer which eventually breaks down into turbulence via Kelvin-Helmholtz instability. Hence the Mach configuration is an alternate means of generating shear layers for energy dissipation via shock interactions. Again this is achieved without solid boundaries. Furthermore, a shock traversing a density field also leads to vorticity generation. This suggests that the propagation mechanism of detonation is similar to that of an intense turbulent flame where compressibility effects dominate. The regularity of the transverse wave patterns in a detonation is a consequence of a resonant coupling between the chemical energy release rate and the pressure fluctuation field itself.

Finally, the wavelength of the transverse wave instability serves to define a characteristic length scale (the cell size) that can be used determine the geometric propagation limits of detonations [26] and possibly, the geometric limits for transition to detonation [27]. Calculations of the idealized ZND reaction zone length using detailed chemical reaction mechanisms [28] have demonstrated that the cell size is approximately [29, 30] proportional to the reaction zone length. Using the cell size as a scaling length therefore incorporates the chemical sensitivity of the mixtures in a very natural fashion. Insensitive mixtures have very long reaction zones, large cell sizes and as a direct consequence, require extremely large geometric scale for experimental demonstrations of DDT. The influence of geometric scale on DDT in insensitive mixtures has been dramatically confirmed by large-scale experiments in the last decade. However, rigorous prediction of geometric limits for DDT as a function of mixture sensitivity are not yet possible.

In contrast to subsonic deflagration waves, a supersonic detonation wave does not produce or influence the flow in front of the wave.

In addition, detonation velocities are so large that even substantial upstream turbulent fluctuations have a small influence on detonation propagation. Finally, the most significant feature of detonations is that unlike flames, which have a wide range of possible propagation speeds depending on the spectrum of turbulent fluctuations in the flow ahead of the flame, a self-sustaining detonation wave has a unique propagation velocity. This unique detonation velocity is known as the Chapman-Jouguet (C-J) velocity and is proportional to the square root of the total chemical energy release. The C-J velocity is fixed by requiring that gas leaving the reaction zone moves with a velocity (relative to the wave) equal to the sound speed in the product gas immediately behind the reaction zone. This velocity is determined by thermochemistry alone and does not depend on the chemical reaction or transport rates. Experimental values for the detonation velocity are in general quite close (within 5-10%) to the C-J values in spite of the three-dimensional transient nature of the wave structure itself.

As discussed above, deflagrations and detonations are very seldom one-dimensional structures. However, if one draws a control volume between two planes in front of, and sufficiently far behind the reaction zone where equilibrium conditions can be achieved, then the steady flow one-dimensional conservation equations may be valid when applied to the direction of propagation (provided the curvature of the wave is negligible). This implies that the radius of curvature be large compared to the thickness of the zone itself and the flow be quasi-steady. If the one-dimensional steady flow equations are valid, then the locus of the equilibrium states behind the reaction front (for a given initial state) are represented by the Hugoniot curve in a p-v diagram (Fig. 4b). A straight line drawn from the initial state $(p,v)_o$ to the Hugoniot satisfies the conservation of mass and momentum and is known as the Rayleigh line. Tangency of the Rayleigh line to the Hugoniot curve defines the upper and lower C-J points giving the minimum detonation velocity and the maximum deflagration speed. The vertical line drawn up from the initial state $(p,v)_o$ to the Hugoniot curve defines the state achieved in a constant volume explosion ($v = v_o$), while the horizontal line from $(p,v)_o$ to the Hugoniot defines the constant pressure combustion state ($p = p_o$). The constant volume and constant pressure combustion states divides the Hugoniot into the upper detonation branch and the lower deflagration branch. No real solutions exist between the constant volume and constant pressure states in the Hugoniot curve because

the wave speed is imaginary.

Since the wave speed corresponding to the detonation branch of the Hugoniot is supersonic, the initial state $(p, v)_o$ is not perturbed. So for a given mixture at a a specified initial state $(p, v)_o$, the upper branch of the Hugoniot does represent the locus of states for various detonation speeds. However, deflagration waves are subsonic and the initial state $(p, v)_o$ may be perturbed depending on the back boundary conditions. For fast deflagrations, precursor shock waves are generated ahead of the deflagration which leads to a different initial state prior to combustion. A separate deflagration Hugoniot must be constructed for each such initial state.

3 Experimental Research in the 1980s

Research in the 1980s was driven by the need to understand the detonability of vapor clouds produced in accidental explosions. This still remains a major concern and source of industrial hazards. Great progress has been made but many unresolved issues remain. Two outstanding problems are: scaling up experiments done in the laboratory, and developing numerical predictions of DDT that can be used for hazard assessment. Recognition of difficulties in both scaling and prediction led to a number of frontal assaults on hazard assessment; large–scale experiments were very important.

A significant effort has been made in the last decade to understand the interaction of flames with obstacles and the role of complex geometries in promoting DDT. Two factors contributed to this emphasis. First, experiments on unconfined flames (spherical or hemispherical clouds with central ignition) demonstrated that transition to detonation is exceedingly difficult for completely unconfined configurations. Only with the addition of grids or screens in the path of the flame was DDT produced in sensitive fuel-oxygen mixtures [31]. Even with large-scale (10 m diameter) clouds, merely low speed (20-50 m/s) flames were produced in completely unconfined fuel-air mixtures [32]. There appear to be two significant factors contributing to the ineffectiveness of flame acceleration for completely unconfined flames. First, the natural instability mechanisms of flames only cause a moderate growth in the flame surface area. Second, the lack of confinement results in a substantial decoupling between the upstream fluid motion and the flame motion. This corresponds to rapid decay $(1/r^2)$ of the velocity and pressure fields in spherical source flows.

Second was the realization that the addition of obstacles to confined flames produced dramatic accelerations (flame speeds up to 400 m/s) within a short distance for both tubes [33] and cylindrical (pancake) geometries [34, 35]. The acceleration mechanism was presented in the Flame Acceleration discussion above and is shown in Fig. 5. The flame-generated flow pulls the flame through the narrow region (throat) at the obstacle locations and the flame is then wrapped up in the vortices shed from the downstream side of the obstacle. The flame shoots out ahead since it is pushed from behind as the pockets of reactants between the obstacles are burned out.

While initial studies were with sensitive fuel-oxygen mixtures in small-scale, large-scale experiments [36] demonstrated that similar effects could be obtained with insensitive fuel-air mixtures if the scale was increased sufficiently. Using periodic obstacles (orifice plates) or spirals within a tube, Lee *et al.* [37] were able to obtain sufficient flame acceleration to produce DDT in H_2-air and C_2H_2-air mixtures and flame speeds of up to 800 m/s in methane-air mixtures within 5-10 tube diameters of the igniter. Further studies on these configurations [38, 39] demonstrated that several propagation regimes exist for a flame in a very rough (highly obstructed) tube. Both the mode of propagation and the onset of DDT were found to be correlated with the sensitivity of the mixture and the minimum size of the orifices within the tube.

Propagation regimes within a rough tube depend on both the reaction and transport rates in the mixture and the tube and obstacle geometry. The following parameters are found to be important: i) the laminar flame propagation velocity; ii) detonation cell size (reaction zone thickness; iii) obstructed area ratio; iv) minimum transverse dimension of the obstacles or tube. In order of increasing propagation velocity (or increasing mixture sensitivity) the mode of propagation varies from: a) quenched, b) turbulent flame, c) choked turbulent flame, d) quasi-detonations, and e) detonations. An example of the variation of propagation velocity with fuel concentration is shown in Fig. 6.

In the quenching regime, the flame propagation occurs by sequential ignition of each chamber (formed by the obstacles) due to jetting of hot combustion products from the previously burned chamber. If the jet mixing is rapid compared to chemical reaction, complete extinction of the flame may occur [40]. If the flame is not quenched, it will accelerate until an equilibrium is reached between the positive effects of flame folding and the negative effects of tube and obstacle

flow resistance. Ultimately, the flame may accelerate up to a velocity comparable to the sound speed and gasdynamic *choking* will occur. Unless transition to detonation takes place, more sensitive mixtures will be limited to velocities (500-1000 m/s) resulting in choked flow within the product gases. This was the case for the methane, propane and ethylene mixtures shown in Fig. 6.

Transition to detonation is found [39,41] to be possible if the detonation cell size λ is less than the minimum transverse dimension in the system D_m. For a tube with orifice plate blockages, this dimension is the diameter of the orifice; for smooth tubes, it is the tube diameter itself. The transition process corresponds to the jump in velocity shown in Fig. 6. After transition, the velocity is intermediate between the choked flame velocity and the CJ detonation velocity; this is the *quasi-detonation regime*. The velocity deficit $(V_{CJ} - V)$ is due to the losses caused by continuous diffraction of the detonation through the obstacle field. If the obstacle field is terminated or the mixture made more sensitive (by increasing the ratio of D_m/λ) the propagation velocity will approach that of a CJ detonation. The mechanisms of quasi-detonation propagation have been the subject of several recent investigations [41-44] and are discussed in more detail in the section below.

A distinction should be made between DDT in rough tubes and smooth tubes since the wall roughness plays a very strong role on both the propagation of deflagration and detonation. In smooth tubes, the onset of detonation is marked by an abrupt change in the propagation speeds. Typically, pre-detonation flame velocity is less than 1000 m/s and the C-J detonation speed is over 2000 m/s. A very strong local explosion always occurs at the onset of detonation so that the detonation wave formed is highly overdriven initially and decays subsequently to its C-J value. High-resolution schlieren photography of the onset of detonation processes [16] revealed that the local explosion usually occurs at the turbulent flame brush.

For very rough tubes, the flame acceleration is much more rapid. Transition to detonation is also not so clearly marked by an abrupt change in the propagation speed. Quite often, an almost continuous acceleration to the final steady–state propagation speed is observed. The presence of very rough walls (or obstacles) permits steady-state flame speeds over the entire range from slow deflagration to C-J detonation. The wall roughness controls the propagation of the wave by creating a) large-amplitude unsteady and turbulent flow b) shock reflection, diffraction, and other complex wave interaction processes,

c) high temperatures behind shock reflections (normal and Mach) which result in localized explosions. These mechanisms all represent ways in which mean flow can be used to generate either large-scale turbulent motions for flame folding or large temperature fluctuations for spontaneous ignition and detonation initiation.

Due to the wide spectrum of possible combustion wave speeds in tubes with very rough walls, the distinction between deflagration and detonation becomes blurred. Accordingly, the onset of detonation is quite often quite obscure, since the final steady state propagation mode itself is strongly dependent on boundary conditions. In these cases, no well-defined transition point can be identified and the notion of DDT is no longer useful.

Another theme of recent research efforts has been the initiation of detonation by high-speed turbulent flame-jets or combustion product jets. The first demonstration [45] of this important mechanism for shockless initiation of detonation was in small scale with sensitive fuel-oxygen mixtures. Later studies [46-49] have concentrated on the initiation of less sensitive fuel-air mixtures at large (1-10 m) scales. These experiments have demonstrated that transition to detonation can be induced in essentially unconfined fuel-air mixtures of moderate sensitivity (H_2 and C_2H_2). Such tests are a dramatic confirmation of the modern notions that the absolute dimensions and method of ignition play a key role in determining the ability to initiate detonations. Even though detonation was not produced in less sensitive fuel-air mixtures such as ethylene and propane, substantial overpressures (1-6 bar) were produced by these explosions. This indicates the hazardous nature of flame-jet ignition, a common scenario in industrial accident analysis. Criteria for jet initiation of detonations are less clear but the absolute velocity [49] of the jet and the jet turbulence parameters [45] appear to be the most important factors.

Finally, there have been a number of experiments on flame acceleration and DDT in complex geometries combining partial confinement and obstructions. Partial confinement or venting is important in mitigating the effects of vessel explosions, particularly in the case of large vessels containing obstructions [50, 51], for which the standard venting guidelines may be inadequate. Partially confined and obstructed configurations are prototypical of most industrial accidents involving fuel-air explosions. Work in small-scale by Chan *et al.* [52] and Urtiew *et al.* [53] reinforced the significance of confinement for producing substantial accelerations and also showed the significance of the flame-vortex interactions. Experiments have also

been performed with pancaked-shaped fuel-air mixtures at various scales through "forests" of obstacles [54]. Ultimate flame velocities were increased by a factor of up to 8 by confining the flame to a cylindrical channel but only moderate terminal velocities (50 m/s) were achieved. Those experiments demonstrated that the early stages of flame acceleration in hydrocarbon-air mixtures could be scaled on the basis of a single parameter, the laminar flame speed, this is consistent with the modeling approach taken by Barr [11-14].

Later work at large scale showed the possibility of acceleration leading to DDT for H_2-air mixtures in partially-obstructed and vented channels [55-57]. These tests demonstrate that venting can have both a negative and positive effect on flame acceleration. With a small amount of venting from the top of a channel confined on the remaining three sides, the flows induced by venting contributed to flame acceleration. Increasing the venting (percentage of open area) results in the eventual reduction of the flame acceleration and inhibits transition to detonation completely if the venting is large enough. Moen *et al.*. [58] demonstrated DDT in C_2H_2-air mixtures in a channel, vented on the top and filled with an array of pipe obstructions. The flame speed just prior to transition was $\sim$ 400 m/s. Flame speeds up to 200 m/s were observed in propane-air mixtures and a quasi-steady-state propagation rate was achieved within several meters of the ignition source.

Numerical modeling of DDT has been directed at understanding the flame acceleration portion of the process. No method has been developed yet that is capable of accurately predicting a complete flame acceleration and transition to detonation event. Hazard assessment for DDT events therefore proceeds by a combination of experiment, partial numerical modeling, and judgement. Two principal types of numerical models have been applied to this problem: inviscid, incompressible vortex dynamics and flame front tracking [11-14]; finite–difference, compressible flow with k-ϵ turbulence models and mixing-rate limited chemistry [59-61]. Each scheme has its peculiar merits and deficiencies. Comparisons with experiments indicate that the initial stages of flame acceleration can be predicted successfully by either model. Details of the flame-vortex interaction process are well resolved by the vortex dynamics technique. The compressible flow models are successful in predicting the pressure waves produced by high-speed flames in partially confined and obstructed tubes. However, the actual onset of detonation can not be treated by the present models. This problem is due in large mea-

sure to the practical limitations on spatial and temporal resolution in multidimensional computations. However, in current models, a key difficulty also lies in the combustion submodel: it is simply not possible to simulate details of reaction zones (needed for detonation onset modeling) with the current subgrid-scale models of turbulent combustion.

To summarize: at least some degree of confinement, partial obstruction of the flow paths, or a high-speed jet ignition source is required to produce DDT. The less sensitive the explosive (the larger the detonation cell size), the larger the scale and the greater the degree of confinement or obstruction is required to produce DDT. If turbulent flame-jet ignition is used, the velocity and geometric scales must be appropriately large to obtain DDT. Both confinement and obstructions provide a means of feedback between the flame-produced mean flow and the flame itself. Production of vorticity and the reflection of pressure waves are the physical mechanisms by which the feedback occurs. With very rough-walled tubes, the obstacles provide an extremely efficient means of converting the mean flow to large-scale turbulence motions and reflecting pressure waves created by exploding vortical structures. DDT can readily be observed, but the two modes of deflagration and detonation are now no longer sharply defined and DDT becomes less meaningful and the quasi-detonation mode of propagation more significant.

Furthermore, the DDT phenomenon can be divided into two separate problems, i) the flame acceleration leading to the conditions for the onset of detonation and ii) the actual formation of the detonation wave itself. Flame acceleration processes are particular to the specific initial and boundary conditions of a problem. However, the actual formation of the detonation appears to be a universal phenomenon.

4 Some Recent Experimental Results

We shall briefly review some recent experimental results obtained at McGill University. Experiments have been carried out in rectangular channels with two transparent walls and low-pressure fuel-oxygen mixtures in order to visualize the physical phenomena. A high-speed framing camera has been used to photograph sequences of schlieren images to form a cinematic impression of the behavior of flames and detonations in rough tubes.

First we shall demonstrate that transverse waves are essential to

the propagation of a detonation. Figure 7 presents schlieren photographs of a detonation wave, with visible cellular structures, propagating from a channel with solid walls into a section in which the bottom wall is replaced by a fiberglass layer. Upon reflection from the fiberglass layer, the transverse shock waves are damped, thus reducing the total number of transverse waves across the channel and increasing the cell size. The progressive decoupling of the reaction zone from the leading shock front is clearly evident as the transverse waves are eliminated. Eventually, the transverse waves are all attenuated and a planar shock followed by a reaction front results. This complex propagates at about one-half the initial C-J velocity. Whether the decoupled shock and reaction front transits back to a regular cellular detonation afterwards will depend on the wall roughness of the tube downstream of the damping section. A wide range of acoustic damping materials (e.g. foam, layers of close mesh screens, porous metal, etc.) all give similar results and the attenuated decoupled shock-reaction zone complex always seems to travel at one-half the C-J velocity when the transverse waves are eliminated.

In Fig. 8, the sequence of schlieren photographs show the transition process in a very rough-walled channel. Note that the turbulent flame brush takes on a V-shape with the leading edges at the wall where intense turbulence is generated by the wall roughness. Continuous generation of pressure waves in the violent burning zone is observed and eventually a detonation is formed which then propagates at a velocity slightly below the normal C-J velocity of the mixture (Fig. 9). Figure 10 shows the same mixture with the same obstacle configuration. However, layers of fine wire mesh are put on the walls beneath the obstacles to damp the transverse pressure waves. Transitions to detonation were never observed in these experiments. Furthermore, the deflagration flame speed is of the order of 100 m/s as compared to the case without the screens of about 1000 m/s just prior to DDT. The importance of the transverse waves even in the deflagration regime is evident. It can be concluded therefore that DDT requires the formation of a set of transverse waves on the front. These waves are required both to accelerate the flame and to sustain detonation.

Figures 11 and 12 show the role of the obstacles and tube walls in causing DDT when the precursor shocks are reflected from them. In Fig. 11, the precursor shock diffracts around the obstacle and reflects off the bottom wall. At first the reflection is regular since the incident shock angle to the wall is small. Later the regular reflec-

tion changes to a Mach reflection and the temperature behind the Mach stem is sufficiently high to cause ignition and subsequent local initiation of the detonation. In Fig. 12, the sequence of schlieren photographs shows the ignition and local initiation when the precursor shock reflects from the forward face of the obstacle. Subsequently, the wave fails when it diffracts over the obstacle. After passing over the obstacle, the diffracted wave reflects from the top of the channel and produces a Mach stem that results in local reinitiation of the detonation.

These sequences of photographs clearly demonstrate the role of the obstacles in inducing wave reflections to give local hot spots and detonation initiation. The obstacles can also cause the detonation to fail by diffraction. It is this periodic initiation and failure that accounts for the low averaged velocity of the detonation giving rise to the so-called quasi-detonation regime [44].

In Fig. 13, the sequence of schlieren photographs shows the fast deflagration mode in rough (obstacle-filled) tubes. Here the precursor shock is not strong enough for prompt ignition via normal or Mach reflections. Interaction of the precursor shocks with the obstacles produce a complex system of periodic waves associated with the flame front. This is an example of coupled compressible and vortical motions. Shock diffraction over the obstacles produces vorticity which greatly augments the combustion rate, providing the volumetric energy sources that power the precursor shock wave system.

In this mode, these complex turbulent deflagrations can propagate at supersonic velocities close to 1000 m/s, about one-half the normal C-J value. In a smooth tube where only the shear at the wall provides the means for turbulence generation, the deflagration speeds are typically an order of magnitude less. There is a striking resemblance of these artificially-generated wave trains to the natural instability systems of detonation transverse waves. We see that there are great similarities in the propagation mechanisms of detonations and high speed deflagrations in rough tubes. A continuous spectrum of behavior emerges and distinctions between propagation mechanisms become blurred as compressibility, vorticity and distributed reaction zones appear significant in all modes.

5 Detonation Onset

As mentioned in the Introduction above, detonations can be generated *directly*, *i.e.*, without a precursor deflagration wave, if a large amount of energy is quickly added to an explosive mixture [62]. This energy source is usually a detonator and high-explosive booster, or in the case of more sensitive mixtures, an exploding wire or spark. For a given mixture and initial conditions, a critical amount of energy[a] is required to initiate a detonation. For a spherical geometry, the critical energy is found to be proportional to the cube of the reaction zone length (or cell size) and ranges from mere joules for acetylene-oxygen mixtures to tens of megajoules (tens of kilograms of explosive) for methane-air mixtures [62, 26]. Experimental observations and physical models [63] indicate that the dynamics of the *reaction wave* induced by the blast is the key to understanding direct initiation.

The rapid deposition of energy in the mixture creates a high-pressure region which, upon expanding, sets up a strong blast (shock) wave which decays as it propagates away from the source region. Some reaction will occur in the gas adjacent to the energy source due to thermal diffusion (or mixing at contact surfaces), however the influence of this region is quite limited compared to that of fluid processed by the supersonic shock wave. Adiabatic compression of the gas by the shock wave increases the temperature sufficiently that vigorous chemical reactions occur immediately behind the shock wave. For most fuel-air or fuel-oxygen systems, these reactions are initially thermally-neutral (or endothermic) and after an *induction delay* time, exothermic reactions result in a substantial temperature rise and volume expansion in the flow.[b]

The spatial location of exothermic reaction changes with time as the first (oldest) fluid elements processed by the shock have exploded and the most recently processed (youngest) ones age. The explosion therefore appears to move as a *reaction wave* or *fast flame* [64]. Reaction waves are a convected explosion in which the key processes

[a] The general requirement is that both a critical energy and power is required for initiation[62]. However, if the power is above a certain minimum level, only the total energy is significant.

[b] Note that in all realistic chemical systems, the processes in the induction phase and in the energy release phase have substantially different state sensitivities and energetics, unlike the simple irreversible one-step reaction models which are often assumed in mathematical models. The exact character of the energy release profile depends on the details of the chemistry and initial conditions.

are reaction, convection and compressibility; unlike ordinary flames, diffusion plays no role. However, if the process is quasi-steady, then it can be visualized as a deflagration-type discontinuity across which pressure decreases, temperature and specific volume increase. Reaction zones in the idealized ZND model of detonations (Fig. 4) are steady reaction waves that convect at exactly the same speed (in the lab frame) as the leading shock. It is this special coupling of reaction and shock waves that gives a detonation it's unique character.

The wave or explosion trajectory is a consequence of the induction time that elapses between when a fluid element is shocked and when the explosion occurs. Induction time is determined by the thermodynamic history of the fluid element and includes the effect of the shock and the influence the flow processes in the rarefaction following a blast wave. In initiation by decaying blast waves (as in spherical geometries), the induction time rapidly increases for fluid elements at increasing initial distance from the source of energy *unless* the chemical energy release substantially contributes to determining the shock motion. Three cases, shown in Fig. 14, can be distinguished [63] on the basis of the amount of energy supplied: subcritical, failure to initiate detonation; supercritical, prompt detonation initiation; critical, creation of a quasi-steady reaction zone followed by an explosion within the reaction zone.

In the subcritical case (Fig. 14a), the chemical energy release never contributes substantially to the shock and the blast wave continuously decays. This leads to a reaction wave trajectory that lags behind the shock, the separation increasing with time. The shock wave finally becomes too weak to set up the needed induction time and the reaction wave decouples and transforms into an ordinary diffusively-controlled flame. In the supercritical case (Fig. 14c), the blast and reaction wave are coupled from the very outset of the process and a spherical detonation wave (complete with transverse instabilities) travels outward at a velocity close to the CJ value. The critical case (Fig. 14b) represents the marginal condition for initiation and is the most interesting.

The reaction wave initially decouples from the shock but later reaches a parallel trajectory, with a wide quasi-steady reaction zone between. The shock-reaction wave complex travels at a sub-CJ velocity, a situation for which no truly steady solutions exists. This situation is unstable, as manifested by an eventual explosion within the reacting gas between the shock and the reaction wave. This explosion triggers the development (3-dimensional) of a spherical det-

onation moving close to the CJ velocity. Lee [62] has suggested that the explosion within the reaction zone is of the type associated with *hotspots* observed in weak ignition by planar shocks. Instability appears inevitable in this case since mass must be accumulating between the shock and reaction wave as the complex moves outward at a constant speed. Since the accumulating gas is all reacting, and the residence time within the layer is continually increasing, a point will be reached where at least one fluid element will explode before it reaches the end of the reaction zone.

Reaction waves play a similar important role in planar shock initiation, either by incident [65] or reflected [66-68] waves. Experimental observations and numerical simulation [67, 69] indicate that reaction begins at the contact surface (or wall) and proceeds outward as a subsonic, accelerating wave. The displacement effect of the reaction wave produces a secondary shock wave moving ahead. Under conditions of *strong* ignition, all three waves merge to form a overdriven detonation in a one-dimensional fashion. Under conditions of *mild* ignition, fluctuations in the region between the reaction wave and the shock result in the creation of a number of discrete *hotspots* or *exothermic centers* resulting in a multidimensional, spatially-distributed ignition [70, 66]. The reaction and pressure waves generated by this process ultimately merge to form a detonation.

The photographic observations [16, 17] of DDT in smooth tubes indicate that reaction waves and hotspots also play a key role there. The detonation waves that finally emerge from the flame acceleration process in a smooth tube appear to originate from a localized explosion (hotspot) near a flame brush. However, these waves are initially too weak [17] and the reaction wave must undergo further acceleration to ultimately result in a CJ velocity detonation. The acceleration or *amplification* process is crucial and is discussed further below. Both features (hotspots and reaction waves) have been demonstrated to be the consequences of gasdynamics and simple reaction models in recent numerical simulations [71-73] of shock initiation in one space dimension.

Detailed models of individual hotspots have also been developed (see [74] for examples) which demonstrate the generation of pressure waves in the surrounding gas. However, many of these previous studies on hotspots have only considered the generation of pressure waves in inert surroundings and have ignored the question of amplification. Only recently [75] has the full problem of hotspots embedded in a reactive medium begun to be explored. The results are found

to be sensitive to both the assumptions regarding the coupling between chemistry and flow (*i.e.*, the equation of state) and the reaction mechanism model. For a simple, one-step irreversible reaction, asymptotic analysis [76] of planar shock initiation reveals that a *supersonic, decelerating* reaction wave emerges from the hotspot at the contact surface. If a multistep mechanism is used that separates induction and energy release processes, then a subsonic accelerating wave is produced [77], in accord with the observations [66-68] mentioned above.

How can detonations be formed in the absence of strong energy sources and associated blast waves? The key idea for shockless initiation of detonation is that critical reaction wave trajectories can be set up by reactant and temperature gradients alone. The flame-vortex interaction situation with partial flame quenching in the vortex core is an example of how this can occur. The region between an accelerated flame and a precursor shock appears to be another. Finally, the general situation appears to be a sensitized volume of partially-reacted gas surrounding an incipient hotspot. The reaction waves generated in these processes will (if they are subsonic) generate shock or acoustic waves. If these pressure disturbances and the reaction waves move synchronously, the amplitude of the pressure disturbance can be amplified *while* the reaction wave remains closely coupled, spontaneously forming a detonation.

Central to the process of wave amplification is the unstable response of a reactive material to small–amplitude pressure waves. This instability is a special instance of the general instability of reactive flows [78, 64] and could be considered a microscopic version of the gasdynamic feedback process proposed for flame acceleration. In the present case, the feedback is between acoustic disturbances (weak shock waves) and the reaction waves created by the special conditions (mixing, weak shocks, etc.) of the flow.

Lee *et al.* [79] first proposed and demonstrated the shockless initiation (SWACER) process by using photochemical excitation of H_2-Cl_2 mixtures. These experiments and associated computations by Thibault and Yoshikawa [80, 1] and more recently by Zel'dovich *et al.* [81] clearly show that an optimum trajectory for the reaction wave is required for successful detonation initiation. The reaction wave trajectory can be visualized as being a direct consequence of the sensitizing process that produces the nonuniform initial state of the mixture. A distribution in radical concentration or temperature will result in an associated reaction wave trajectory, as shown in Fig.

15a. The actual trajectory will differ due to the gas motion induced by the exothermic nature of the reaction wave.

Existence of an optimum gradient is readily demonstrated. If a volume is nearly uniformly sensitized, producing an highly supersonic reaction wave (Fig. 15b, case a), the reaction wave is totally decoupled from the pressure waves and only a constant volume explosion is created. If too narrow a region is sensitized, a very low–speed reaction wave is produced (Fig. 15b, case c), which is also decoupled from the pressure waves and a constant-pressure, flame-like process results. Between these two extremes, an optimum sensitization process (Fig. 15b, case b) results in a coupled system similar to the quasi-steady reaction zone stage of shock initiation. Numerical simulation by Zel'dovich *et al.* indicates that the subsequent development strongly depends on the initial conditions. Two possibilities are: continuous acceleration to detonation or a gradual decoupling followed by a reinitiation from a hotspot within the unsteady region between shock and reaction wave.

We close with an example of a spontaneous reaction wave formation and shock amplification appropriate to DDT. Figure 16 shows the results of a numerical computations by Thibault and Hassam [82] of the spontaneous generation and amplification of a pressure wave within a nonuniform region. The region consists of a mixture of products and reactants from stoichiometric H_2-air combustion; the product fraction varies linearly between 0 and 1 over a 30 cm distance. Both the detailed chemical reaction kinetics of the H_2 oxidation and the gasdynamics of the motion are treated by an extension of Yoshikawa's [80] Lagrangean McCormack-FCT method. This situation modeled resembles the nonuniform regions created within vortices produced by impulsive flame-jet ignition of fuel-air clouds. Gradients in temperature, radical concentrations and reactants all contribute to the reaction wave formation and shock amplification. While the present case did not result in transition to detonation, a pressure wave with a maximum amplitude of 10 bar was generated before it began to decay, compare this with a maximum amplitude of $\sim$ 1.2–1.8 bar for an exploding hotspot in an inert medium [74]. Computations with larger mixing regions are in progress and indicate that DDT is possible.

A picture of detonation onset emerges as the interplay between shock amplification, reaction wave propagation, and hotspot evolution. Weak shock waves and the violently unsteady combustion and mixing processes occurring in DDT prepare the mixture to support

reaction waves with near-optimal trajectories. Reaction waves are created within hotspots and drive pressure waves out into the surrounding medium. The pressure waves are amplified as the reaction waves accelerate synchronously from behind. If the reaction-shock coupling is strong enough, a detonation wave emerges. Research into the complex situations representative of actual DDT events is just beginning. Mathematical analysis, numerical simulation and physical mechanisms must be successfully integrated to give a clearer picture of the phenomenon. Only the surface has been scratched up to now. Understanding and categorizing the various regimes and phases in shockless initiation is a challenging task for the future.

6 Concluding Remarks

Deflagration to detonation transition is portrayed as a fundamental change in propagation mechanism. Flame propagation via the diffusive and turbulent mixing processes of low-speed flow are replaced in detonation propagation by the process of convected explosions or reaction waves coupled to initiating shock waves. The process of transformation can be separated into flame acceleration and onset of detonation. In the flame acceleration process, unsteady (turbulent) motion induced by the flame itself causes a rapid multiplication of the effective flame surface. A very large range of length scales is relevant in the high Reynolds number flows of interest in industrial explosions. The large straining motions created by these unsteady flows result in partial extinction of the flame and the creation of a distributed reaction zone.

Confinement and partial blockage of the flow path appears to play a key role in promoting DDT. It is exceedingly difficult to obtain DDT in completely unconfined mixtures due to the weak feedback mechanisms between flame and flowfield in this case. Energetic ignition sources such as turbulent flame-jets can cause DDT in large fuel-air clouds of more sensitive mixtures. The extraordinary effectiveness of obstructions and confinement in promoting flame acceleration and DDT can be explained in terms of the enhanced feedback mechanisms. Reflection of pressure waves and the generation of vorticity are the key agents of feedback. Propagation speeds over a wide range are possible in very rough tubes. The most rapid modes of propagation are the choked flame ($\sim$ 1000 m/s) and the quasi-detonation (1000-2000 m/s). Natural and artificial pressure waves

play a key role in quasi-detonation propagation, which proceeds as sequence of initiation, diffraction, failure, and reinitiation processes. The traditional concept of DDT appears meaningless in that situation.

Onset of detonation is characterized by the emergence of reaction waves from hotspots, driving shock waves ahead into sensitized (partially reacted) gas. Given an optimal trajectory for the reaction wave, the shock amplitude will be increased until a coupled reaction wave-shock complex (a detonation) created. Optimal trajectories are associated with regions of the flow that contain gradients of temperature, reactants, radical species, etc. Entrainment of flames into the vortical structures within boundary layers or in wakes and the subsequent quenching of the flame is a generic mechanism for creating such regions. Shock waves can appear spontaneously and be readily amplified to become detonations within such a structure.

Both the deflagration structure just prior to the onset of detonation as well as the structure of the detonation itself is three dimensional. A enormous range in space and temporal scales exists in both the chemical and fluid dynamic aspects of these flows. Compressibility, unsteadiness, vorticity, and strong gradients are essential features. Clearly, numerical simulation of the complete flame acceleration and detonation onset process is extremely greedy of computing resources and not really practical at present. Studies of individual aspects have been very successful and several areas are now ripe for exploitation. Current examples are the analytical and numerical studies of: flame-vortex interaction; hotspot evolution; spontaneous shock generation and amplification; the relationship between detonation initiation and reaction wave trajectories. Valuable insight into the DDT phenomenon can be obtained by synthesizing these studies with the knowledge of physical processes obtained over the last four decades of experimentation.

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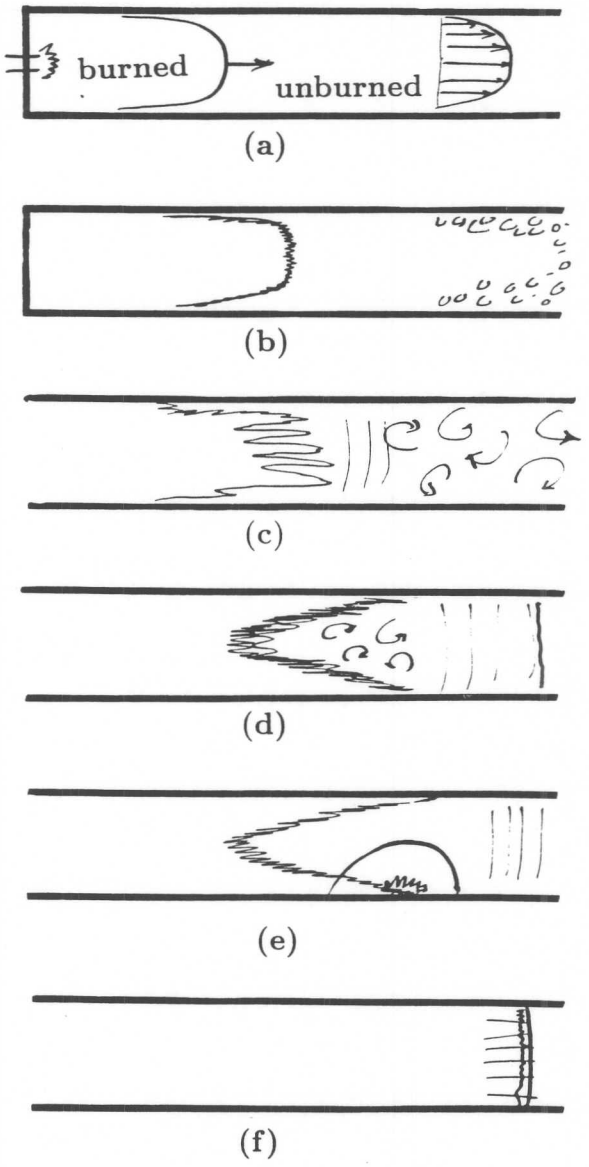


Figure 1. Progress of a DDT event in a smooth tube with a closed end. a) the initial configuration showing a smooth flame and the laminar flow ahead. b) first wrinkling of flame and instability of the upstream flow. c) breakdown into turbulent flow and a corrugated flame. d) production of pressure waves ahead of the turbulent flame e) local explosion of a vortical structure within the flame f) transition to detonation.

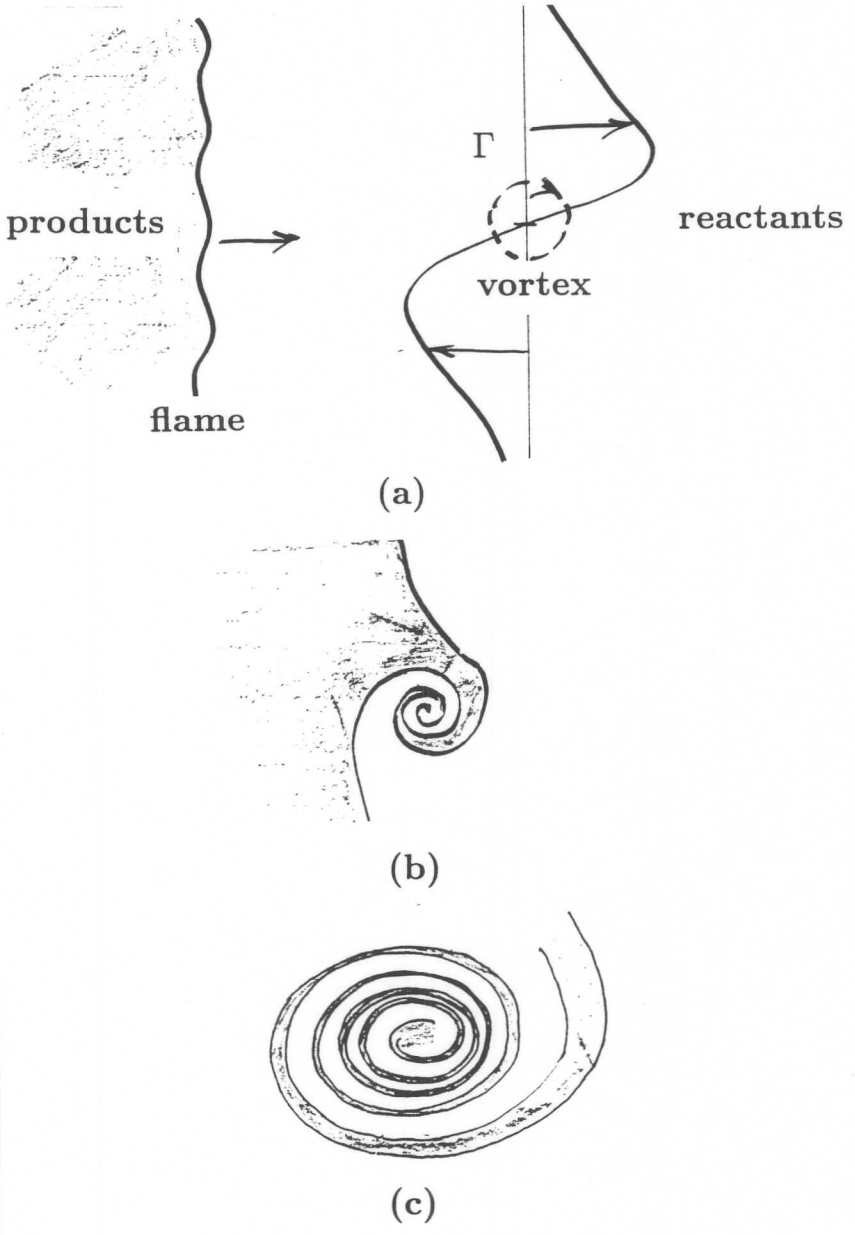


Figure 2. Flame-vortex interaction at large Reynolds number $\Gamma/\nu \gg 1$ illustrating the a) the initial configuration; b) entrainment of the flame into the vortex; c) formation of the "jelly-roll"structure of alternating layers of product and reactant separated by flame sheets.

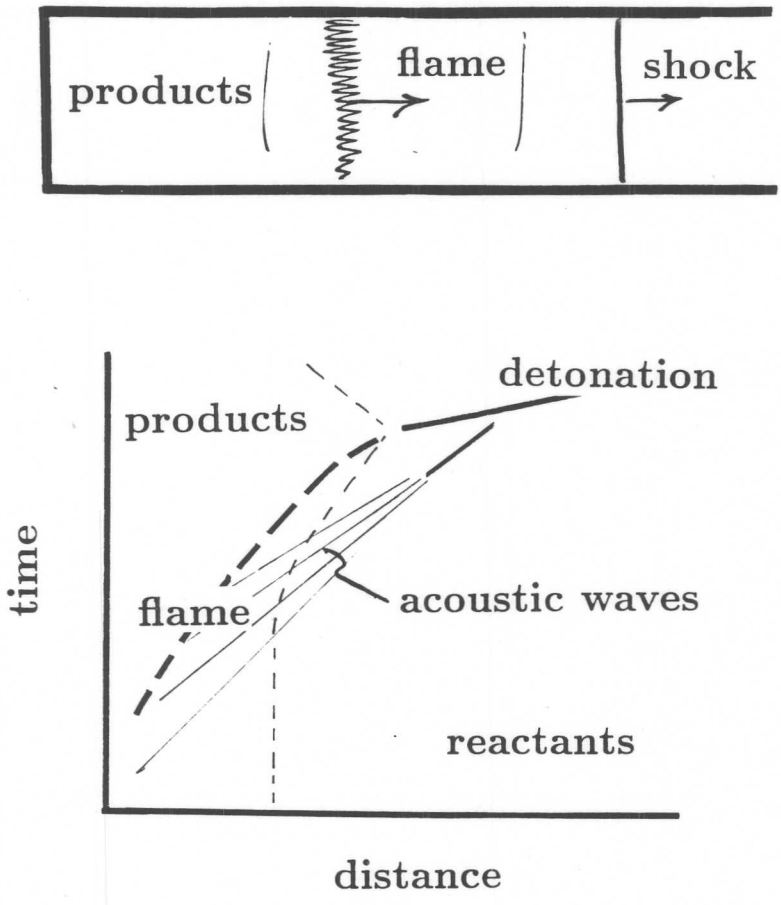


Figure 3. Gasdynamic feedback mechanism model of flame acceleration. The accelerating flame produces adiabatic compression of the fluid ahead, increasing it's temperature and therefore increasing the flame speed at a later time when the heated fluid is burned. After Kurylo *et al.* [22].

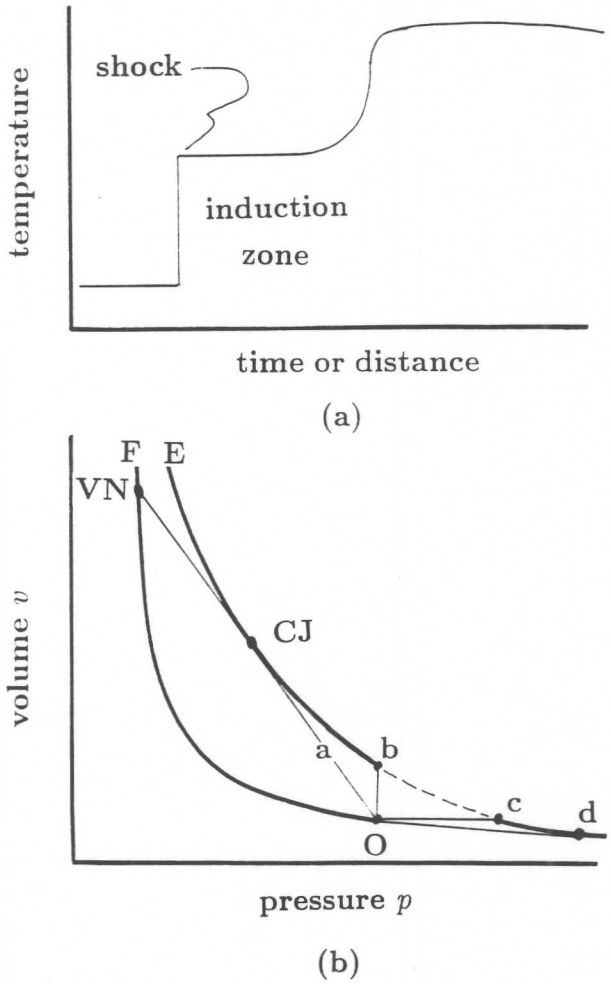
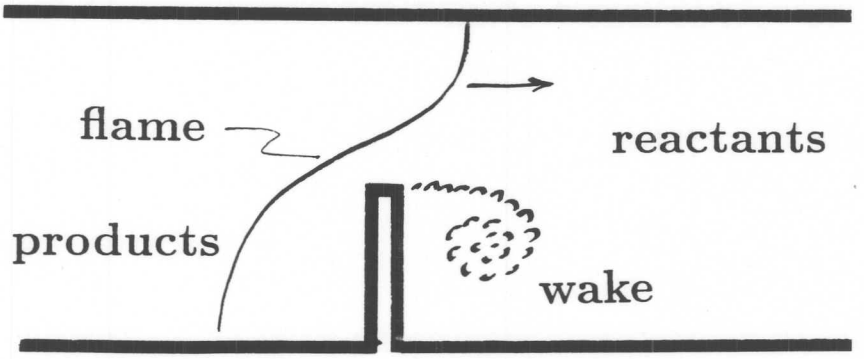
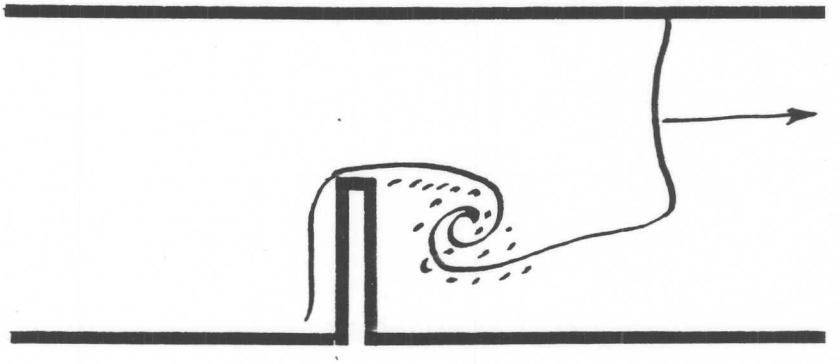


Figure 4. a) Temperature profile in the reaction zone of an idealized ZND model of detonation structure. b) Pressure-volume (P, v) diagram showing the initial state and the locus of possible final states (the Hugoniot or shock adiabat) for a steady wave in a reacting gas. E - equilibrium states, deflagration ($p < p_o$) or detonation ($v < v_o$); F - frozen (nonreactive) states, VN is the post shock state in the ZND structure. Rayleigh lines (a-d) are shown drawn from the initial state O to four possible final states: a - CJ detonation; b - constant volume explosion; c- constant pressure explosion; d - deflagration.



(a)



(b)

Figure 5. Flame propagation through an obstructed tube. a) Prior to reaching the obstacle, the flame is accelerated by the convergence as the flow passes through the area minimum at the obstacle location. b) After reaching the obstacle the flame is wrapped up in the vorticity shed from the downstream side. The leading edge of the flame races ahead as the vortical fluid between the obstacles is burned out.

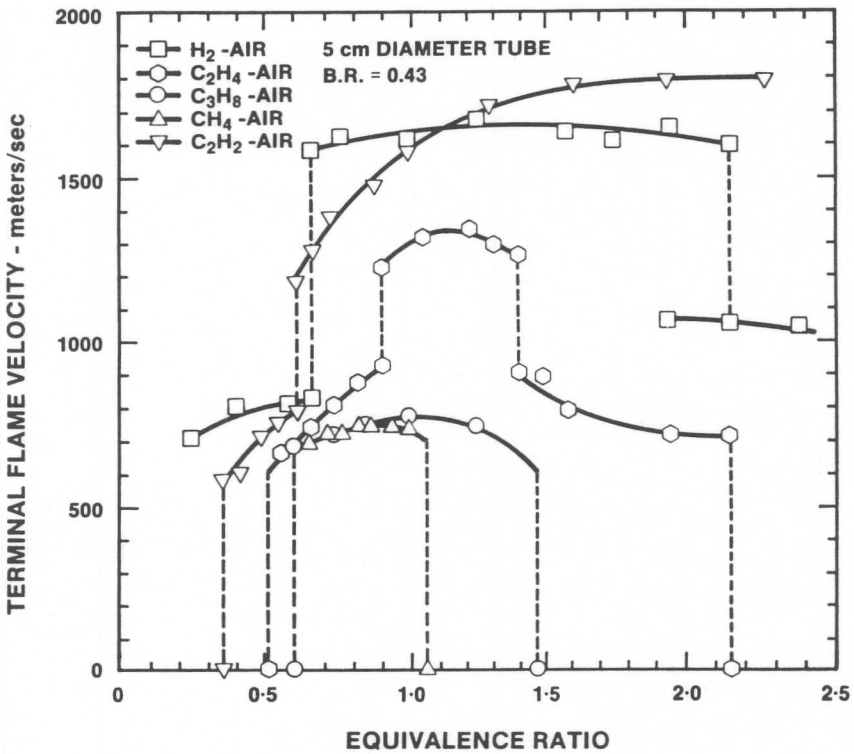


Figure 6. Wave speeds for flame and detonation propagation in very rough tubes. Tube diameter, 50 mm; orifice inner diameter 37.4 mm; ratio of obstructed area to tube cross section area = 0.43. Fuel–air mixtures initially at nominal ambient conditions: 1 atm and 298 K. DDT observed for H_2-air and C_2H_2-air systems.

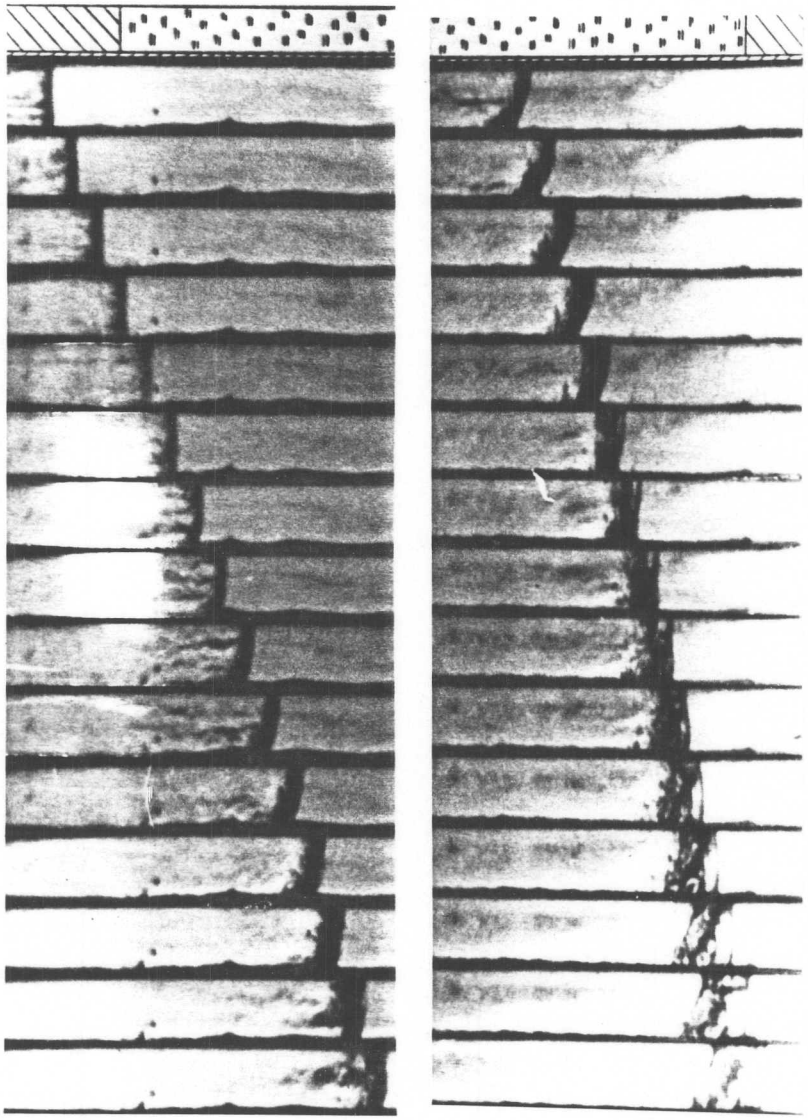


Figure 7. Time sequence of schlieren photographs illustrating the damping of transverse waves by an acoustically absorbing wall. Note the decoupling of the reaction zone and main shock front in the last few frames. Stoichiometric H_2-O_2 mixture at 120 torr; nominal cell width is 11.4 mm. Channel height is 65 mm, width is 65 mm; absorbing material is only present on bottom wall. The time interval between frames is approximately 3.3 μs.

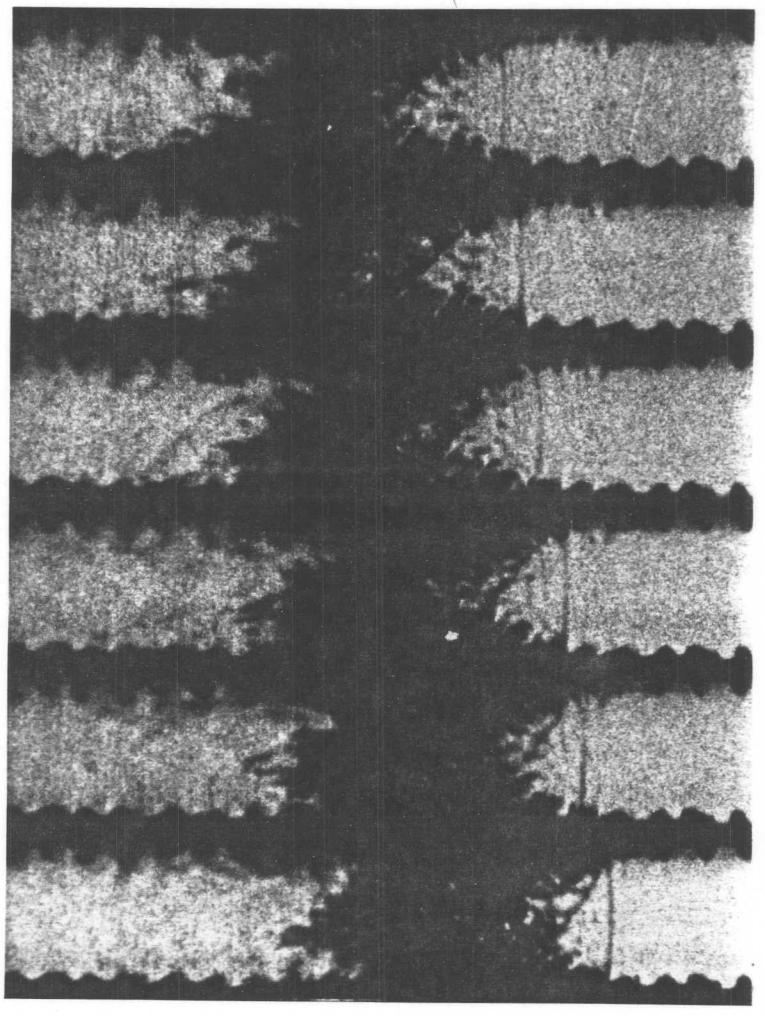


Figure 8. Time sequence of schlieren photographs illustrating the process of rapid deflagration in a channel with rough top and bottom walls. Flame has propagated approximately .38 m from the igniter and has an average velocity of 1070 m/s at this point. Stoichiometric H_2-O_2 at 150 torr; nominal cell width is 9 mm for unimpeded detonation; channel height is 37 mm, width 65 mm. The roughness elements are spaced 5 mm apart and are 2.5 mm high. Note the generation of pressure waves by the flame brush and their coalescence to form a curved leading shock wave preceding the flame.

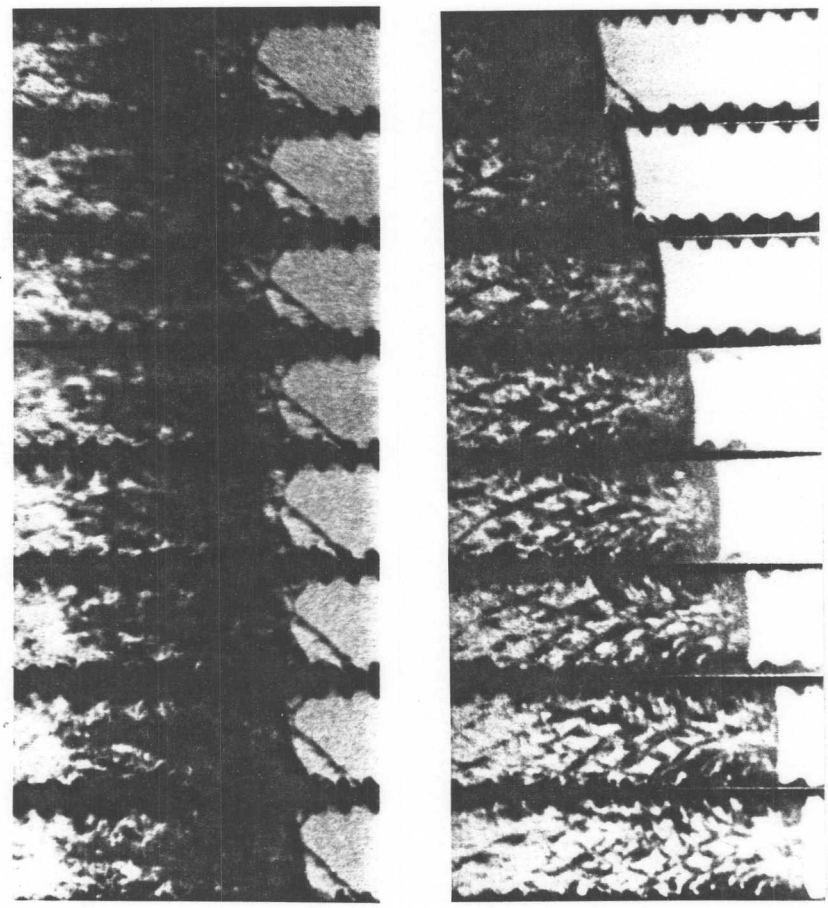


Figure 9. Same experiment as in previous figure, but a little later in time after ignition. The flame has propagated .42 m from the igniter and the flame and shock merge (near frame 11) to form a detonation. Note the substantial transverse pressure waves that can be observed in the products. These are generated by the detonation diffracting over the roughness elements. The detonation mean velocity after transition is 2760 m/s, comparable to the computed CJ velocity of 2751 m/s.

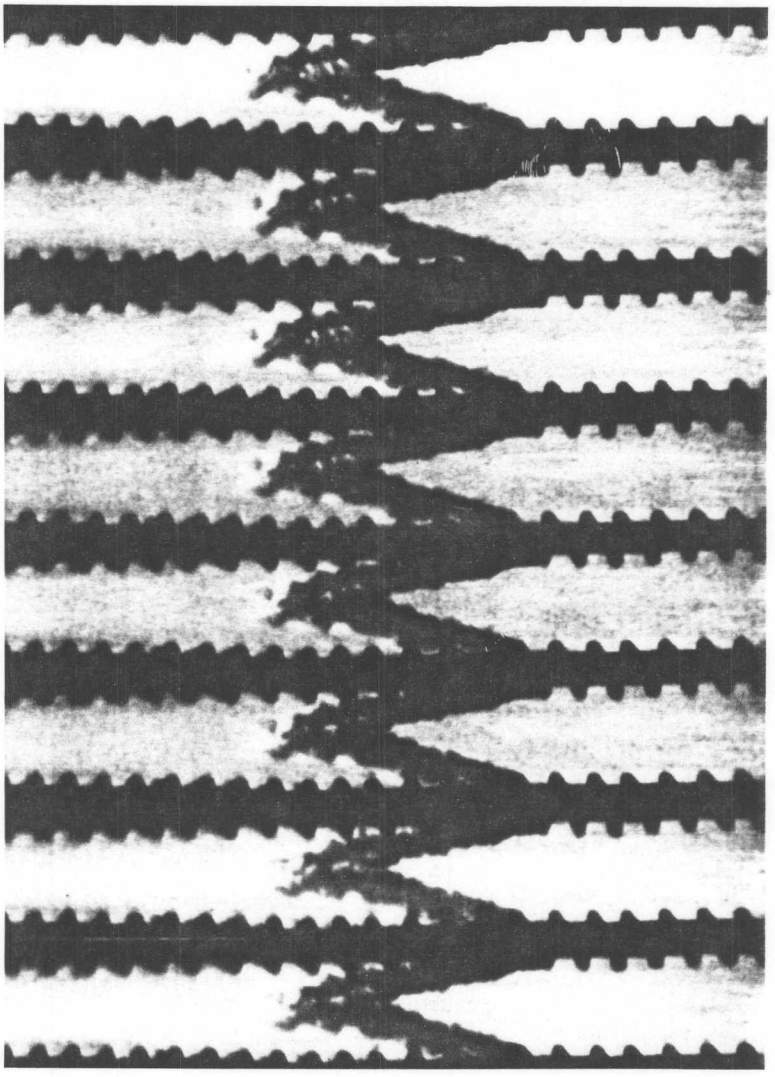


Figure 10. Experiments similar to those illustrated in Figures 8 and 9 but with acoustic absorbing screen layer under the roughness elements. Mixture and dimensions identical to Fig. 9 except that the channel height is reduced to 30 mm. The presence of the fine wire mesh screens dramatically reduces the flame speed (to about 100 m/s) and prevents transition to detonation from ever occurring. Note the characteristic V or "tulip" shape of the flame.

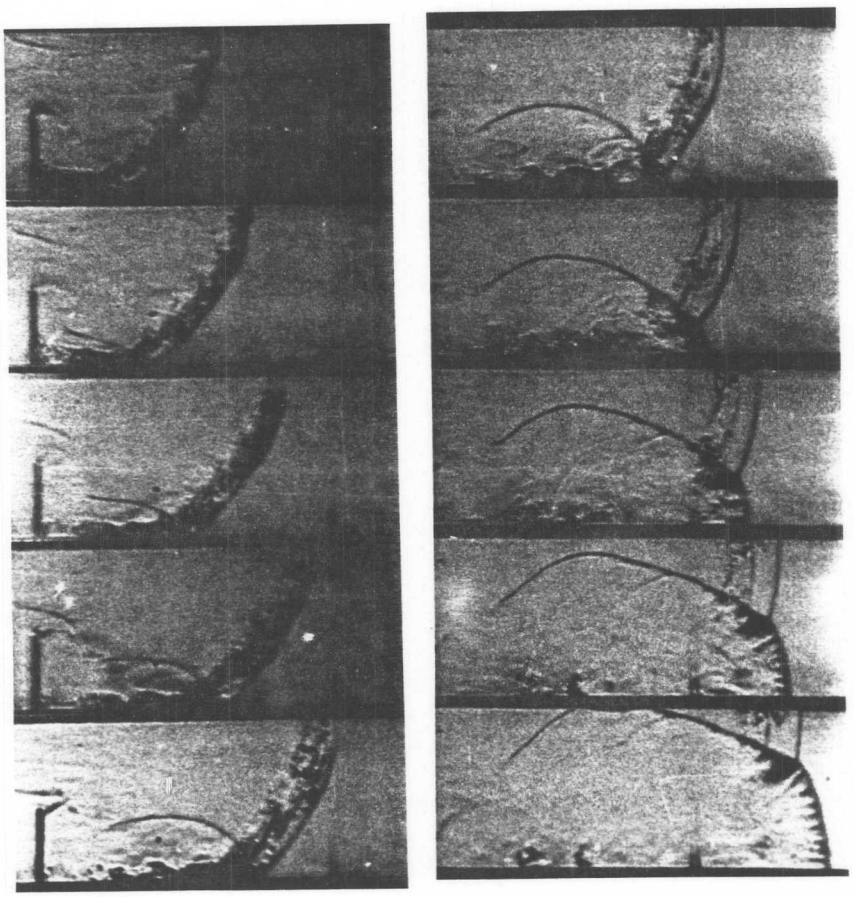


Figure 11. Sequence of schlieren photographs illustrating decoupling of the reaction zone (failure), and reinitiation processes after the detonation diffraction over a single obstacle [44]. Detonation is reinitiated by the Mach stem formed (between frames 6 and 7) during the oblique reflection of shock wave from the bottom of the duct. Stoichiometric H_2-O_2 mixture at 140 torr initial pressure. The channel is 16 mm wide, 76 mm high and 1.5 m long; the obstacles are plates mounted normal to the channel axis, 25.4 mm high and 1.6 mm thick and span the width of the channel. Time between frames in Figs. 7-12 is approximately 6 μs.

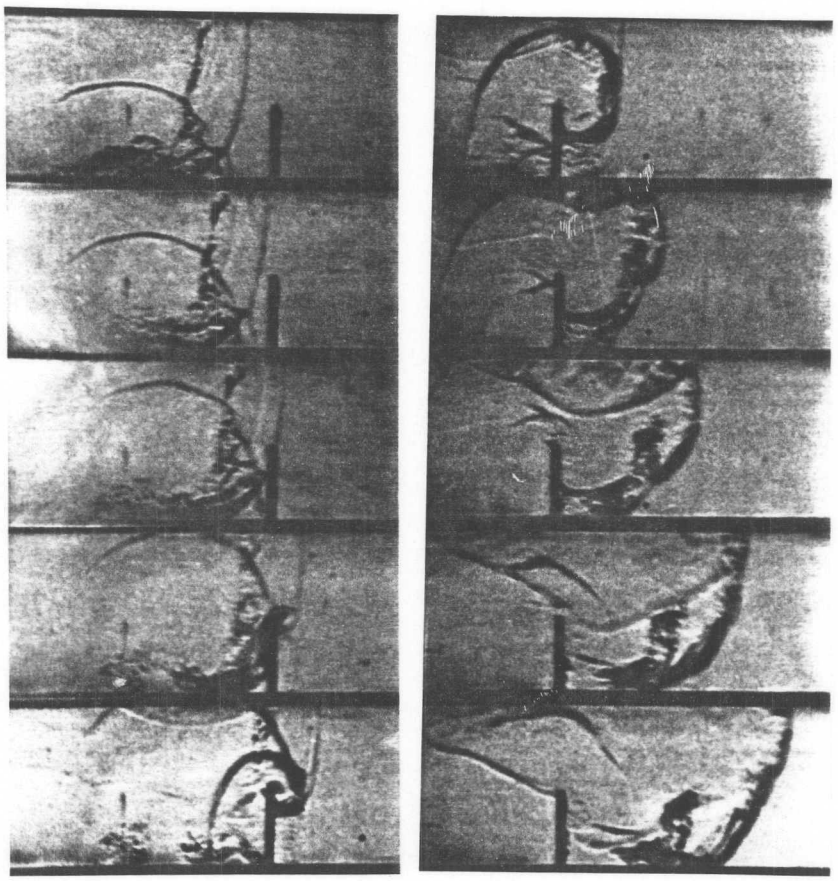


Figure 12. Experiment identical to that described in Fig. 11, but with quasi–detonation propagation over periodic obstacles spaced 100 mm apart. The leading shock is weaker than in the previous case of Fig. 11 and reflection fails to reinitiate detonation. A decoupled reaction zone can be observed trailing the shock in frames 1 and 2. Normal reflection of the Mach stem from the front of the obstacle causes a wave of detonation reinitiation which sweeps upward and diffracts over the obstacle. The wave fails again during the diffraction process but is reinitiated by the Mach reflection from the upper wall. Configuration similar to that described in Fig. 11 but at an initial pressure of 120 torr. Mean propagation velocity of 2250 m/s *vs* CJ velocity of 2700 m/s.

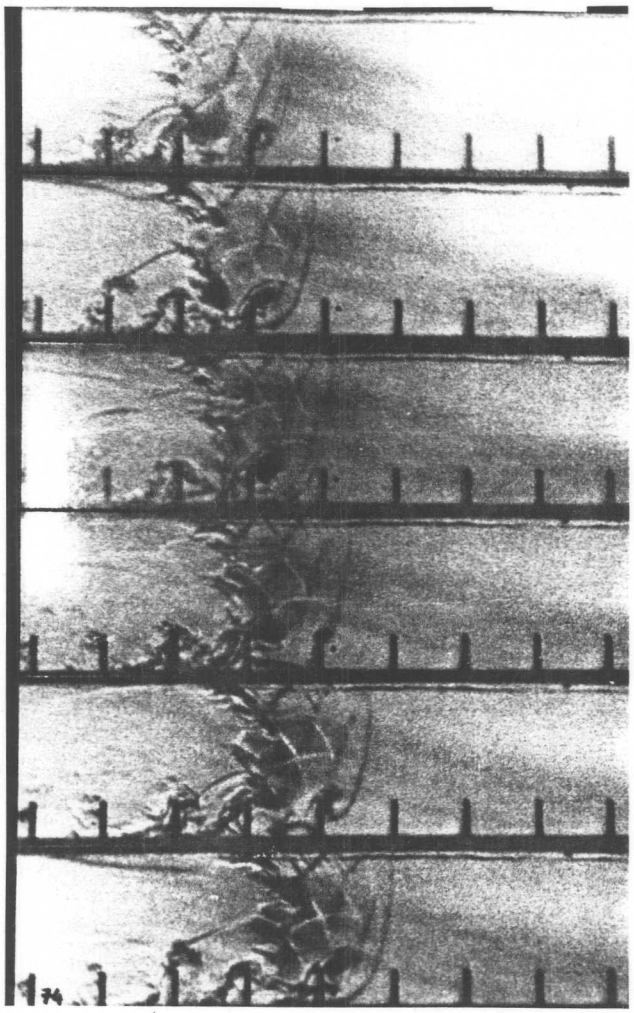


Figure 13. Experiment similar to that described in Fig. 12 but at a lower initial pressure (100 torr) and with a closer obstacle spacing (50 mm). In this case, wave reflections are too weak to initiate detonation so that only the fast deflagration (mean velocity of 800 m/s) mode of propagation results. Note the periodic train of shock reflections produced by shock diffraction over the obstacles and the broad region of combustion trailing behind the shock and in the region between the obstacles.

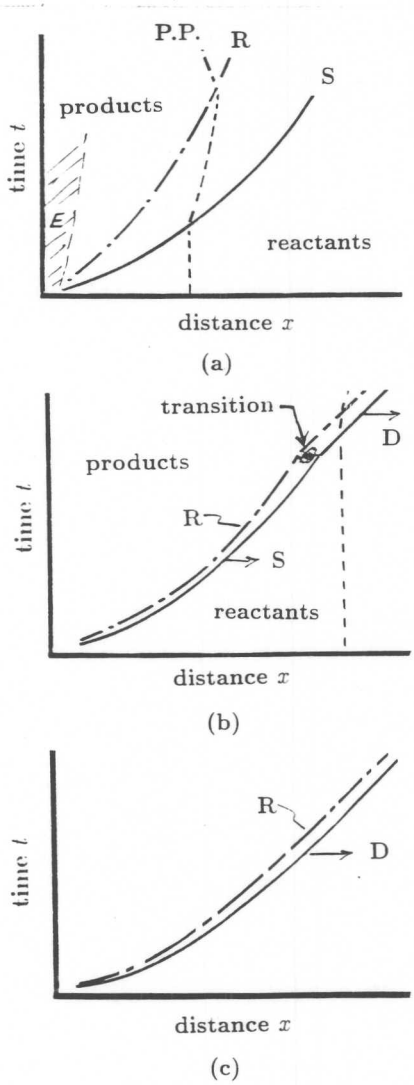


Figure 14. Space-time diagram for shock initiation showing the decaying blast wave S, the resulting reaction wave R, particle path PP, and detonation D generated by the initial energy deposition in region E. a) subcritical case, reaction wave decouples from the shock and no detonation initiation occurs. b) critical case, reaction wave trails shock wave in a quasi-steady configuration which is terminated by an explosion (labeled Transition) within the reaction zone. c) supercritical case, coupled reaction wave-shock wave structure formed promptly.

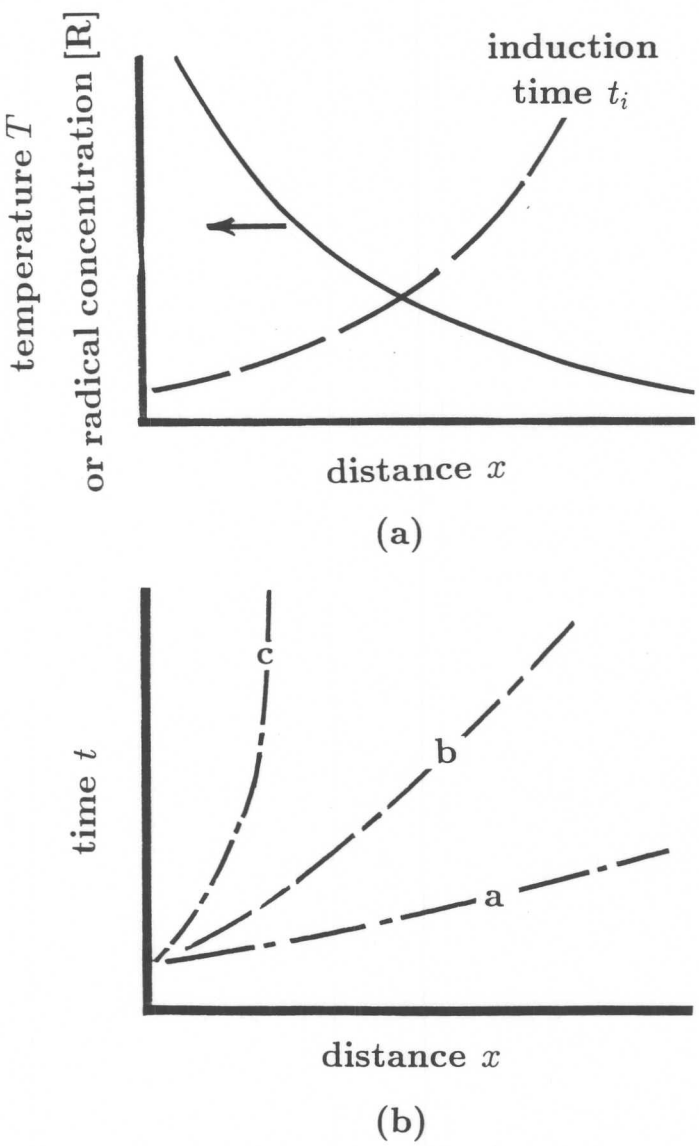


Figure 15. a) Temperature or radical distribution and the corresponding reaction wave trajectory. b) Three reaction wave trajectories corresponding to the three extreme cases of: a – constant-volume explosion; b – constant-speed (CJ) or accelerating trajectory leading to detonation; c – decelerating trajectory leading to a low-speed flame.

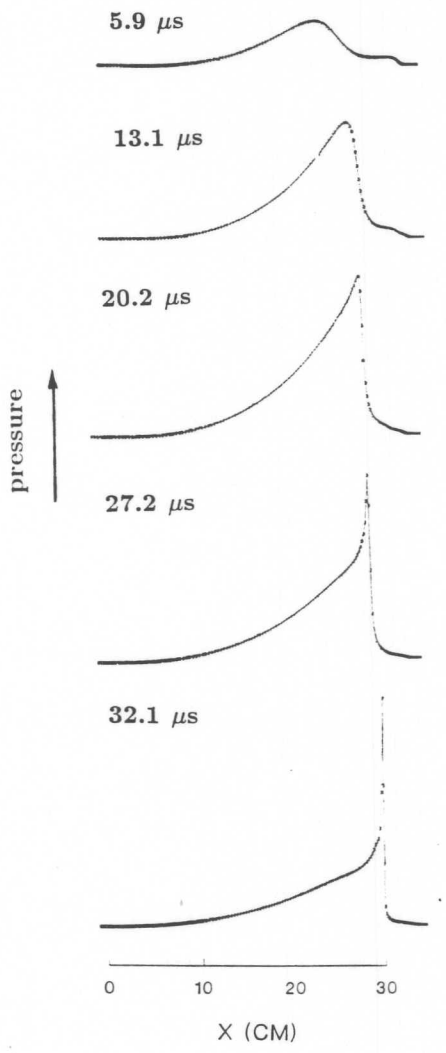


Figure 16. Numerical simulation of spontaneous generation of pressure waves within a mixing region consisting of stoichiometric H_2-air reactants and products. Reactant region (at 300 K) is on the right, product region (at 2400 K) is on the left, the entire region is initially at 1 atm pressure. Pressure scales have been changed for each time to make the details clearer. Thibault and Hassam 1990.