THE ROYAL SOCIETY

Comments on criteria for direct initiation of detonation

By J. H. S. Lee and A. J. Higgins

Department of Mechanical Engineering, McGill University, Montreal, Canada H3A 2K6

The current status of the direct initiation problem, where a powerful source drives a blast wave into an explosive gaseous mixture to generate a Chapman–Jouguet (CJ) detonation, is critically assessed. The current theories that are most successful in estimating the critical energy required for initiation are semiempirical in nature, in that they involve an experimentally determined length-scale (typically cell size) to characterize the explosive mixture. The eventual analytic theory of initiation should be based exclusively on the constitutive properties of the explosive. To date, attempts at a comprehensive theory of initiation have invoked quenching of the reaction front by curvature or unsteadiness of the blast wave. Simple analytic models of initiation as well as numerical simulations and experiments, however, all indicate that initiation near the critical regime is the result of a reacceleration of the blast wave from a sub-CJ minimum. Hence, the criterion for initiation must take into account the amplification of the blast wave due to coherent coupling with the chemical energy release. The effect of 'hot spots' is also shown to have a pronounced effect in reducing the critical energy required for initiation. These results suggest directions that future investigations can pursue toward a rigorous theory of direct initiation.

Keywords: detonation; initiation; explosion; blast wave; Chapman–Jouguet detonation; cell size

1. Introduction

Direct initiation of detonation, in contrast to the transition from deflagration to detonation, refers to the 'instantaneous' formation of a detonation in the asymptotic decay of the strong blast wave from a powerful ignition source. Since the pioneering work by Zeldovich *et al*. (1957), the problem of direct initiation has been studied extensively for the past four decades. Significant advances have been made in the understanding of the direct initiation phenomenon, but a quantitative theory that can predict the critical energy required for direct initiation from first principles (i.e. basic thermochemical and kinetic rate data of the explosive gaseous mixture) is still lacking. On the basis of recent experimental, numerical and theoretical studies, it appears worthwhile to reassess the current status of the direct initiation problem and attempt to bring into focus the key issues that remain to be resolved, thus identifying the direction future studies should take.

Direct initiation requires a strong shock of sufficient duration. This can be defined by some averaged power density of the ignition source. In the limit of the ideal instantaneous point source, however, direct initiation can be described by a single parameter, i.e. the blast energy (Knystautas & Lee 1976). Rapid electrical discharges, laser

sparks and condensed explosives have all been shown to approximate the ideal point source adequately. In the present paper, we shall focus our discussion on direct initiation by an ideal point (or equivalently, line or planar) energy source. The gas dynamic flow field associated with an ideal point source is also relatively simple. The initial decay of the strong blast is described by the self-similar solution of Sedov (1946), Taylor (1950) and von Neumann (1941, 1962). Numerous approximate solutions, e.g. perturbation (Sakurai 1953, 1954), integral (Bach & Lee 1970) and quasi-similar (Oshima 1960), are also available for the intermediate moderate-strength shock-wave regime in a non-reacting gas. Asymptotic solutions for the far-field weak-shock regime are also available (Whitham 1950). The entire propagation of the blast wave from the near field (strong shock) to the far field (weak shock) can also be accurately described numerically. For the propagation of a blast wave in an explosive mixture, the presence of chemical reactions in the wake of the decaying shock wave does not present any fundamental difficulties in the problem formulation. Thus, the numerical simulation of the direct initiation phenomenon should also be well within current computational capabilities.

2. Theories of initiation

A successful theory for direct initiation should result in an analytic expression from which the critical energy could be computed from the fundamental properties of the explosive. Either in an experiment or in a numerical simulation, the different regimes of initiation (i.e. supercritical, critical and subcritical energy) can be observed by varying the initiation or blast energy. Thus, a critical value of the blast energy at which initiation occurs can be determined. In the formulation of a theory for direct initiation, however, a criterion that defines the critical conditions for the initiation process must be specified *a priori*. In the pioneering work of Zeldovich *et al*. (1957), the criterion proposed was that the duration of the blast, until its strength had decayed to the Chapman–Jouguet (CJ) value, should be on the order of the induction period of the mixture itself. Equivalently, the criterion of Zeldovich *et al*. (1957) for direct initiation requires that the blast radius, when the shock strength has decayed to the CJ value, should be on the order of the induction zone thickness. For a strong spherical blast, the shock strength, $M_{\rm s}$, depends on the scaled radius, $R_{\rm s}/R_0$, where $R_0 = (E_0/p_0)^{1/3}$ is the explosion length. Hence, by defining a critical value of the shock strength (e.g. $M_{\rm s} = M_{\rm CJ}$) at some fixed radius (e.g. $R_{\rm s} = \ell$), where ℓ is the induction zone thickness, Zeldovich *et al.*'s (1957) criterion immediately leads to the dependence of the critical energy on the cube of the induction zone thickness (i.e. $E_0 \sim \ell^3$). This cubic dependence has been well established experimentally. Using the induction zone thickness of a ZND CJ detonation, it was shown that Zeldovich *et al.*'s (1957) criterion underestimates the critical initiation energy by about three orders of magnitude.

Subsequent improvements to Zeldovich *et al.*'s (1957) criterion generally involved modification of the critical shock strength and the critical duration (or shock radius). Selecting the CJ velocity as the critical shock strength, as done by Zeldovich *et al*. (1957), is an obvious choice since it can be determined directly from the energetics of the gaseous explosive. More recent experiments indicate that the shock strength prior to the onset of detonation, during the so-called quasi-steady period, is the more appropriate value to use (Edwards *et al*. 1978). Even for initiation energies

substantially above the critical value, the blast wave always decays below the CJ value before reaccelerating back to the CJ value at large radius. Near the critical energy, the minimum shock strength during the quasi-steady period is observed to be close to half the CJ detonation speed. The half-CJ speed corresponds to a shock strength very near the autoignition limit of a combustible mixture. Also, the half-CJ value has some physical importance in that it is very close to the CJ deflagration speed, which is the maximum speed of the shock-reaction front complex just prior to the final onset of detonation in deflagration to detonation transition (DDT) (Chue *et al*. 1998). The significance of the half-CJ speed is perhaps most convincing for experiments in which a detonation propagates into a tube with acoustic absorbing walls which dampen out the transverse wave structure, causing the CJ detonation to fail. In such cases, the speed of the decoupled planar shock-reaction front complex corresponds to about half the CJ value. Thus, the half-CJ value appears to be the critical value of shock speed prior to the onset of detonation.

The choice of the critical radius is a more difficult task. The original suggestion by Zeldovich *et al*. (1957) was to use the induction zone thickness of the detonation. Due to shock curvature and unsteady adiabatic expansion behind the shock, it is clear that a much larger reaction zone thickness should be used. The 'hydrodynamic thickness' estimated by Soloukhin (1969) is only 10 times larger and is insufficient. The cell size λ has been shown to correspond to about 30–40 times the ZND reaction zone thickness, which is still insufficient if λ is used in Zeldovich *et al.*'s (1957) criterion. Even cell length (which is about 1.5λ), while being a reasonable representative of the reaction length of cellular detonation, is still too small. It is clear that different physical considerations (even for a real cellular detonation) must be used. In the surface energy model proposed by Lee (1984), it was argued that the critical diameter represents the minimum surface area for the formation of a spherical detonation wave. As the planar detonation exits from the tube into unconfined space, expansion waves from the edges of the planar detonation will propagate towards the axis, introducing curvature into the planar wave. Maximum curvature is obtained when the expansion waves reach the axis, and, at critical conditions, reinitiation occurs at this maximum curvature. To estimate this curvature, Lee (1984) chose a detonation kernel size R_{s}^{*} to give the same surface area as the original planar wave exiting the tube, i.e. $\frac{1}{4}\pi d_{\mathrm{c}}^{2} = 4\pi R_{\mathrm{s}}^{*2}$, which leads to a kernel radius of $R_{\mathrm{s}}^{*} = \frac{1}{4}d_{\mathrm{c}}$. Using the empirical correlation of $d_{\mathrm{c}} = 13\lambda$ gives a critical kernel radius of $R_{\mathrm{s}}^{*} = 3.25\lambda$. The use of $M_{\mathrm{s}}^{*} = \frac{1}{2}M_{\mathrm{CJ}}$ and $R_{\mathrm{s}}^{*} = 3.25\lambda$ with blast wave theory results in the expression

$$E_0 = 34.3\pi\gamma p_0 M_{\mathrm{CJ}}^{2}\lambda^{3},$$

which correlates fairly well with the critical energy for a spectrum of fuel–air mixtures over a range of stoichiometry (Benedick *et al*. 1985).

A further physical argument for $R_{\mathrm{s}}^{*} = 3.25\lambda$ was also given by Lee in evoking Schelkhin's stability criterion, which states that the maximum perturbation of the reaction zone a detonation can withstand prior to failure should not exceed twice the normal reaction zone thickness (Lee 1997). This agrees with the experimental observation that the largest cells in a detonation undergoing failure from area expansion are about twice the normal cell size. Thus, if we consider the cell length 1.6λ as the representative reaction zone thickness of a cellular detonation, then 3.2λ represents the maximum thickness prior to failure according to Schelkhin's criterion.

In spite of the good agreement achieved using $M_s^* = \frac{1}{2}M_{CJ}$ and $R_s^* = 3.2\lambda$ for the initiation of spherical fuel–air detonations, it would be of interest if there exists an independent experiment of a different geometry to more rigorously verify the characteristic parameters chosen. In an effort to describe the initiation of detonation by hypervelocity projectiles, Lee (1997) applied the hypersonic blast analogy, which relates the work done by the aerodynamic drag of the projectile to the energy per unit length of a cylindrical blast wave. For the direct initiation of a cylindrical detonation, the critical energy was derived from cylindrical blast wave theory by again invoking the assumption of $M_s^* = \frac{1}{2}M_{CJ}$ and $R_s^* = 3.2\lambda$. The expression for the critical energy per unit length obtained for the cylindrical geometry was found to be

$$E_0 = 10.1\gamma p_0 M_{CJ}^2 \lambda^2,$$

and equating this to the work done by the drag force, $F = \frac{1}{2}\rho_0 \nu_\infty^2 (\frac{1}{4}\pi d^2) C_D$, where a value of the drag coefficient consistent with a blunt body is used, i.e. $C_D \approx 1$, Lee (1997) obtained

$$\frac{M_\infty}{M_{CJ}} = 5.3\frac{\lambda}{d},$$

where M_∞ is the Mach number of the projectile of diameter d, and M_{CJ} and λ are the standard properties of the explosive mixture. The agreement of this theory with the experiments of Higgins & Bruckner (1996), where spheres of different sizes were fired at the CJ velocity into a hydrogen–oxygen–argon mixture at various initial pressures, is illustrated in figure 1. In a more recent study of the initiation of a quasi-cylindrical detonation by a cord of condensed explosives, the same cylindrical initiation theory was used to predict the critical conditions for direct initiation. Again, good agreement was obtained (Higgins *et al*. 1998). Thus, it appears that current semiempirical theories that estimate the critical energy from cell size can be used to predict initiation in different geometries. These empirical models, and the experimental data they are based on, illustrate the characteristic length-scales that must be included in any formal theory of initiation.

3. Mechanism of initiation

In the original study by Zeldovich *et al*. (1957), a qualitative model was presented to show the propagation of the initiating blast wave in a detonating gas. Of particular interest, that model demonstrates that the initiating blast passes through a sub-CJ minimum before asymptotically approaching a CJ detonation at large radius. This excursion to a sub-CJ minimum before reaccelerating to a CJ detonation is also in accord with the experimental observations discussed above and is now known as the quasi-steady period before the final onset of detonation. This suggests that direct initiation is not a straightforward asymptotic decay of an overdriven detonation, but rather involves a reacceleration of the blast wave due to the increasing amount of chemical energy engulfed and released by the blast front. Thus, it appears that the key mechanism for initiation occurs during this sub-CJ regime, and to obtain the correct criterion for direct initiation, one must examine more carefully the gas dynamic processes that occur during this time. It is, therefore, of value to redevelop Zeldovich *et al.*'s (1957) qualitative model more rigorously from blast wave theory

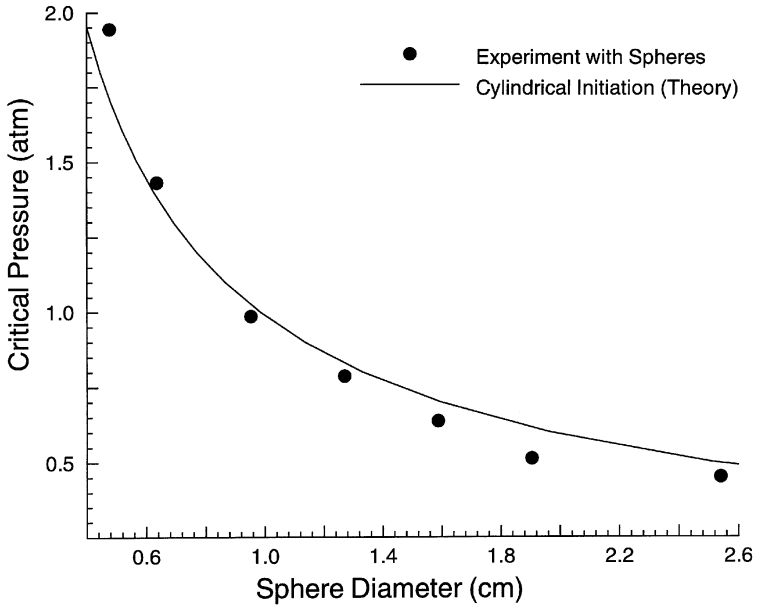

Figure 1. Results of experimental firings of supersonic projectiles into a detonable mixture of gas ($2H_2 + O_2 + 7Ar$). The velocity of the spherical projectiles was equal to the CJ speed of the hydrogen–oxygen–argon mixture used. The theory curve derives from the critical energy required to initiate a cylindrical detonation wave, which is related to projectile initiation by the hypersonic blast wave analogy.

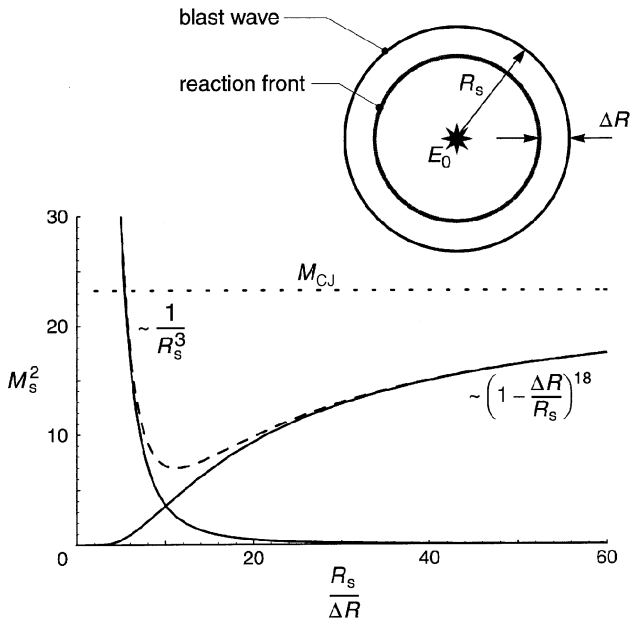

Figure 2. A simplified model for direct initiation based on energy conservation in the blast wave. For a fixed induction zone thickness ΔR, the strength of the blast wave (shown as M_s^2) is plotted as a function of distance from the initiation source, in arbitrary units of $R_s/\Delta R$.

to elucidate the mechanism that is responsible for the sub-CJ minimum and the reacceleration of the blast wave back to the CJ condition for large radius.

Conservation of total energy at any instant when the blast wave is at radius R_s gives

$$E_0 = \int_0^{R_s} (e + \tfrac{1}{2}\rho u^2) 4\pi r^2 \, \mathrm{d}r - \int_0^{R_s - \Delta R} \rho Q 4\pi r^2 \, \mathrm{d}r, \tag{3.1}$$

where E_0 is the blast energy, Q is the chemical energy per unit mass of the explosive mixture, ΔR is the induction zone thickness, and the other symbols have their usual meaning (figure 2). In this model, the combustion process is treated as a 'square wave', where the thermally neutral induction process is followed by an infinitely thin front of instantaneous heat release. Since the finite rate chemistry in most actual detonations is dominated by the induction period, this model is a fair approximation to the combustion process in a detonation. Transforming variables into blast wave coordinates, i.e.

$$\xi = \frac{r}{R_s}, \quad \psi = \frac{\rho}{\rho_0}, \quad \phi = \frac{u}{\dot{R}_s}, \quad f = \frac{p}{\rho_0 \dot{R}_s^2},$$

the above conservation equation becomes

$$E_0 = 4\pi\rho_0 R_s^3 \dot{R}_s^2 I_1 - 4\pi\rho_0 R_s^3 Q I_2, \tag{3.2}$$

where I_1 and I_2 are defined as

$$I_1 = \int_0^1 \left(\frac{f}{\gamma - 1} + \tfrac{1}{2}\psi\phi^2 \right) \xi^2 \, \mathrm{d}\xi,$$

$$I_2 = \int_0^{1 - \Delta R/R_s} \psi \xi^2 \, \mathrm{d}\xi.$$

Equation (3.2) is still exact and no approximations have been made as yet. Previous studies of blast wave decay have demonstrated that the shock strength at any instant is proportional to the averaged energy density in the blast sphere, and it is not particularly sensitive to the details of the energy distribution within the sphere itself. Following the approximation used in the previous study by Bach & Lee (1970), we assume that the density profile follows a power law distribution, i.e.

$$\frac{\rho}{\rho_0} = \frac{\rho_1}{\rho_0} \xi^q,$$

where $q = 3((\rho_1/\rho_0) - 1)$ is found from the conservation of mass and ρ_1 is the density at the shock front. With the assumed power law density profile, the particle velocity and pressure profiles can be obtained from integrating the continuity and momentum equations. With all the profiles known, the integral I_1 can be evaluated; for $\gamma = 1.4$, $I_1 = 0.423$. The integral I_2 can also be evaluated as

$$I_2 = \frac{1}{3} \left(1 - \frac{\Delta R}{R_s} \right)^{q+3},$$

where $\gamma = 1.4$, $\rho_1/\rho_0 = (\gamma + 1)/(\gamma - 1)$ and $q = 15$.

Thus equation (3.2) can now be written as

$$R_{\mathrm{s}}^2 = \frac{E_0}{Q\pi\rho_0 I_1 R_{\mathrm{s}}^3} + \frac{1}{3}\frac{Q}{I_1}\left(1 - \frac{\Delta R}{R_{\mathrm{s}}}\right)^{18},$$

and introducing the explosion length $R_0 = (E_0/p_0)^{1/3}$, the above equation can be written as

$$M_{\mathrm{s}}^2 = \frac{1}{4\pi\gamma I_1}\left(\frac{R_0}{R_{\mathrm{s}}}\right)^3 + \frac{Q}{c_0^2}\left(\frac{1}{3I_1}\right)\left(1 - \frac{\Delta R}{R_{\mathrm{s}}}\right)^{18}.$$

The above equation is qualitatively similar to the expression given by Zeldovich *et al*. (1957) which shows that, for small shock radius, the shock strength decays like the inverse cube of the shock radius, and for the large radius, the second term dominates and the shock strength approaches a constant (i.e. CJ detonation). Note that the induction zone thickness ΔR depends on the shock strength M_{s} as well as the adiabatic expansion gradient behind the shock. In fact, it is precisely this dependence that determines whether initiation is successful or not. If the reaction front decouples from the shock and propagates as a slow flame, then ΔR approaches R_{s} for large R_{s}, since the speed of the reaction front (i.e. laminar flame) is negligible compared with the shock speed. Hence, the second term vanishes and the chemical energy release fails to prevent the shock from decaying. If we assume ΔR to be constant, then detonation initiation is always possible since the second term must eventually dominate. A plot of the shock strength (M_{s}^2) versus the shock radius is shown in figure 2, where we have assumed ΔR to be a constant and the other parameters are set to arbitrary values.

The decay and reacceleration process illustrated in figure 2 is based purely on energy considerations. The existence of a sub-CJ minimum is due to the difference in the dependence of the shock strength on the blast energy term (first term) and on the chemical energy (second term). The first term dominates at small radius, leading to the 'undershoot', and M_{s}^2 recovers slowly as the second term begins to contribute to the flow field.

In reality, the induction distance ΔR is not constant; it is a function of the local shock strength when a particle first crosses the shock and is also a function of the adiabatic expansion that the particle is subjected to before the onset of reaction. Due to the exponential dependence of induction time on temperature, the increase of induction time with decreasing temperature is very rapid, particularly in the case of high activation energy. Thus, an autoignition temperature limit or critical shock strength may be defined. The induction time also depends on the adiabatic expansion that a particle undergoes upon crossing a decaying blast. The degree of adiabatic expansion depends on the curvature of the shock as well as the local rate of shock decay. Thus, the existence of a critical energy for initiation implies that under a certain shock strength, decay rate and curvature, the chemical reactions may be quenched altogether. This observation is the basis of a number of analytic theories that attempt to predict critical energy.

The use of critical curvature is implicit in the detonation kernel concept of Lee & Ramamurthi (1976) and is stated explicitly as an initiation criterion in the recent work of He & Clavin (1994*a*) and He (1996). A similar criterion for the critical tube diameter based on curvature has also been advanced by Edwards *et al*. (1979).

Apart from the shock curvature, adiabatic expansion also occurs due to the decaying strength of the shock wave. Thus, even in a planar geometry, where there is no curvature, the expansion behind the shock can be sufficient to quench reactions and cause a failure to initiate. This fact alone shows that the curvature theory of He & Clavin (1994*a*) is insufficient to predict critical energy in a planar geometry. The 'thickening' and possible quenching of the reaction front due to unsteady expansion has been investigated extensively. From a simple order of magnitude estimate, Soloukhin (1969) reported an increase in the thickness of the detonation of about 4–10 times due to unsteady effects. Bach *et al*. (1969) also computed the effect of unsteady expansion on the induction time of particles crossing a decaying blast wave. They demonstrated the interesting result that 'quenching' occurs when a particle crossing the shock at a shock radius where the blast energy is of the order of the chemical energy release. A more detailed analysis based on blast wave theory showing the influence of unsteadiness on this thickening of a detonation wave was also given by Lundstrom & Oppenheim (1969). In the recent study of Eckett *et al*. (1998), the unsteady expansion effect on the quenching of the reaction front was invoked as a formal criterion for direct initiation.

While theories of initiation based on concepts of curvature or unsteadiness are an advance over the semiempirical models discussed in § 2, they neglect a key aspect of the initiation problem. Since detonation initiation is essentially an acceleration process from a sub-CJ minimum, it is not sufficient to simply base the initiation criterion on quenching. Experiments indicate that there exists a quasi-steady regime prior to the rapid reacceleration of the shock to an overdriven detonation (or prior to blast wave decay and failure in the subcritical case). Thus, successful initiation depends on the ability of the shock to undergo rapid acceleration at the end of the quasi-steady period, and this mechanism must be addressed by the initiation criterion. The significance of shock acceleration at the end of the quasi-steady period is well elucidated in numerical simulations of direct initiation.

4. Numerical simulations of initiation

For the ideal blast initiation problem, current numerical techniques can provide more detailed information on the transient reacting flow field behind the blast wave than could be obtained experimentally. The one-dimensional reactive Euler equations, with simplified chemistry, are capable of qualitatively reproducing the phenomena observed in experiments. At the present time, this model can be efficiently solved numerically with complete confidence in the algorithm used. In the recent investigations of Mazaheri (1997), the ideal blast initiation problem was solved for planar geometry. For these simulations, the one-dimensional Euler equations with a single-step Arrhenius rate law were solved. For this simplified chemistry, there is no actual induction length. By convention, however, the characteristic chemical length-scale was taken as the half reaction length of the ZND model of a CJ detonation, defined as the distance from the leading shock at which the reaction progress variable reaches one-half of its fully reacted value. For the case of planar initiation, the blast wave strength (i.e. the post-shock pressure of the blast wave) is shown as a function of distance from the source (in units of the half reaction length) in figure 3. This result is an exact numerical solution of the complete unsteady problem, which compares with the analytic results in figure 2, where the induction-zone length was held constant.

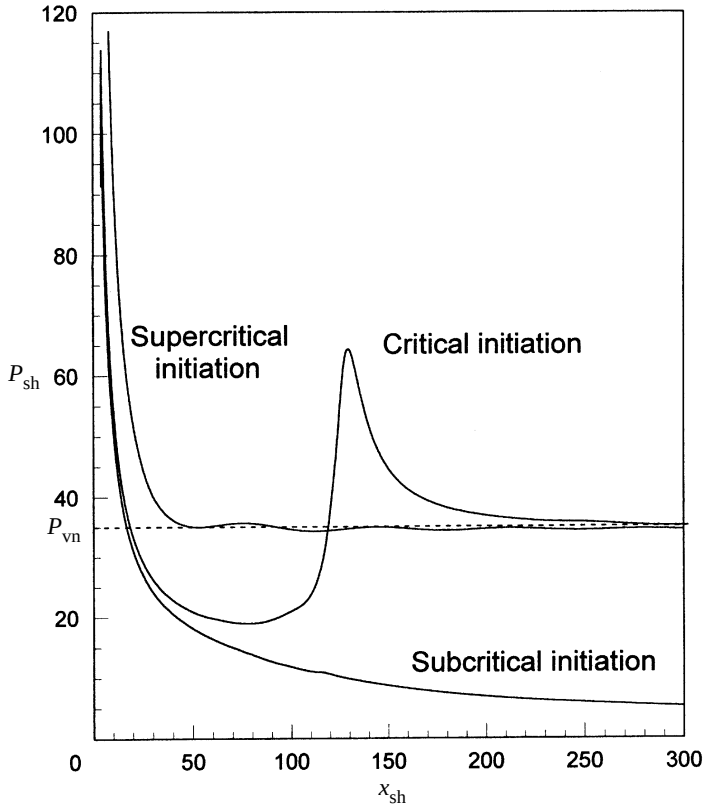

Figure 3. Numerical solution of the one-dimensional reactive Euler equations, showing the three regimes of initiation for planar blast wave initiation. Blast wave strength is shown as a function of distance from the source (in units of half reaction length). The corresponding initiation energies are $E_0/P_0 = 1615$, 1765 and 3415 for subcritical, critical and supercritical initiation, respectively. $Q/RT_0 = 50$, $\gamma = 1.2$, $E_a/RT_0 = 25$.

The results in figure 3 show the three regimes corresponding to supercritical, critical and subcritical energies. The existence of a quasi-steady period near the critical energy, where the shock propagates at a fairly constant speed of about half the CJ value prior to rapid acceleration to an overdriven detonation, is quite evident.

The temperature profiles behind the initiating blast wave for the subcritical and supercritical energy regimes are shown in figure 4. Note that in the subcritical case, the steep temperature gradient indicates that the reaction zone lags progressively behind the shock front as it decouples from the shock completely. For the supercritical case, the reaction zone is intimately coupled to the shock front throughout. For the critical case, the temperature profiles shown in figure 5 also demonstrate an initial decoupling of the reaction zone from the shock front as the blast decays. However, the temperature gradient is less steep and indicates that there is progressive chemical activity present from the shock to the final product state where the temperature is a maximum. At the end of the quasi-steady period, one notes a rapid steepening of the temperature gradient as the temperature maximum advances rapidly towards the shock front. The corresponding pressure profiles are shown in figure 6, where

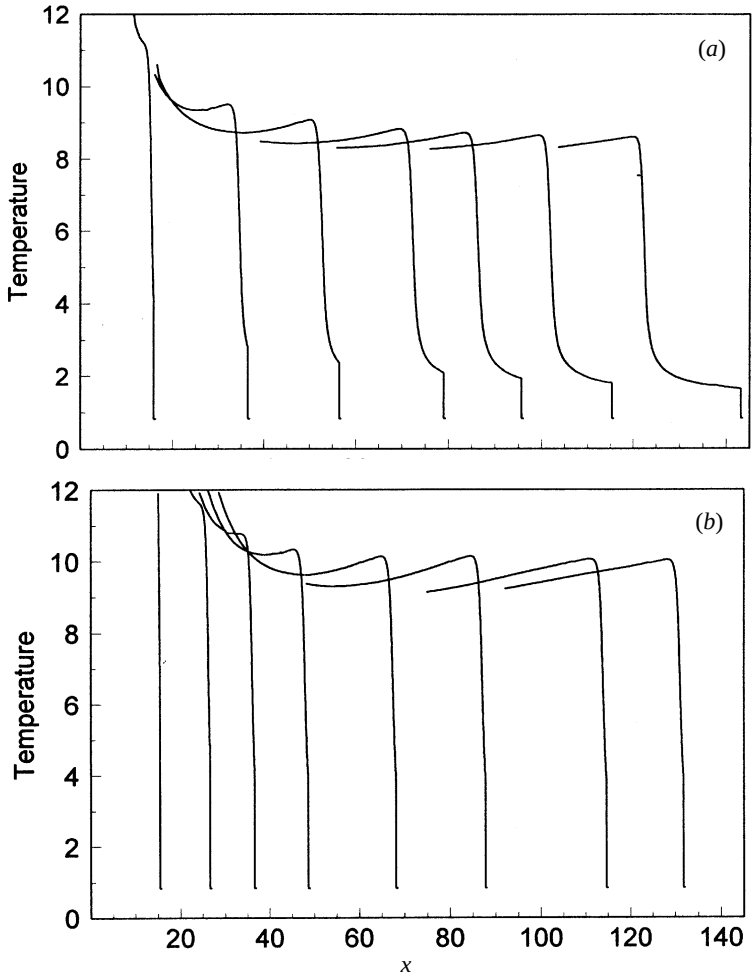

Figure 4. The temperature profiles behind the blast wave for (a) subcritical regime ($E_0/P_0 = 1615$) and (b) supercritical regime ($E_0/P_0 = 3415$).

an arrow denotes the location of the reaction front. Note that the rapid steepening of the temperature gradient behind the shock corresponds to the rapid build-up of a pressure pulse that advances towards the shock front at the end of the quasi-steady period. The coalescence of this pressure pulse with the leading shock front is responsible for the formation of an overdriven detonation that subsequently relaxes to the CJ state. This feature of the rapid build up of a pressure pulse in the gradient field of chemical activity behind the shock for the onset of detonation appears to be a universal phenomenon.

Comparing the detailed gas dynamic process for the critical regime with that of photochemical initiation where the gradient of chemical activity is obtained by photodissociation (Lee *et al.* 1978), one may conclude that the direction initiation process is due to the shock wave amplification by coherent energy release (SWACER) mechanism. The SWACER mechanism was first proposed to explain photochemical initiation, where a gradient of free radicals is generated by light absorption and

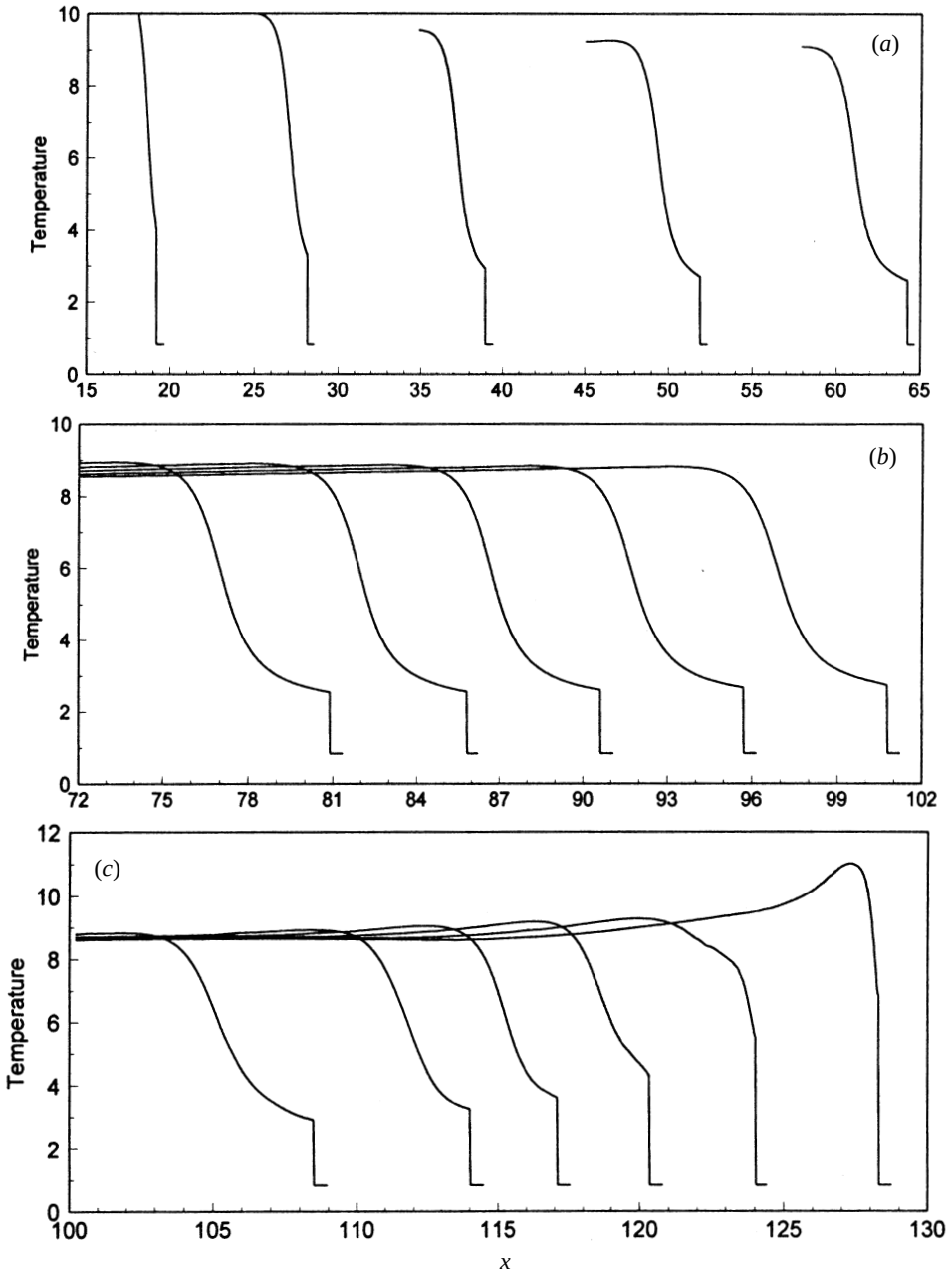

Figure 5. Temperature profiles behind the blast wave for the critical regime ($E_0/P_0 = 1765$).

photodissociation, which in turn provides a gradient of chemical reaction rate and induction time. This permits the generated pressure pulse to couple to the local chemical reaction process as it propagates into the gradient field. The result is that the shock wave accelerates to detonation more rapidly than is possible with initiation by constant volume combustion or DDT (Lee & Moen 1980). The coherence of the

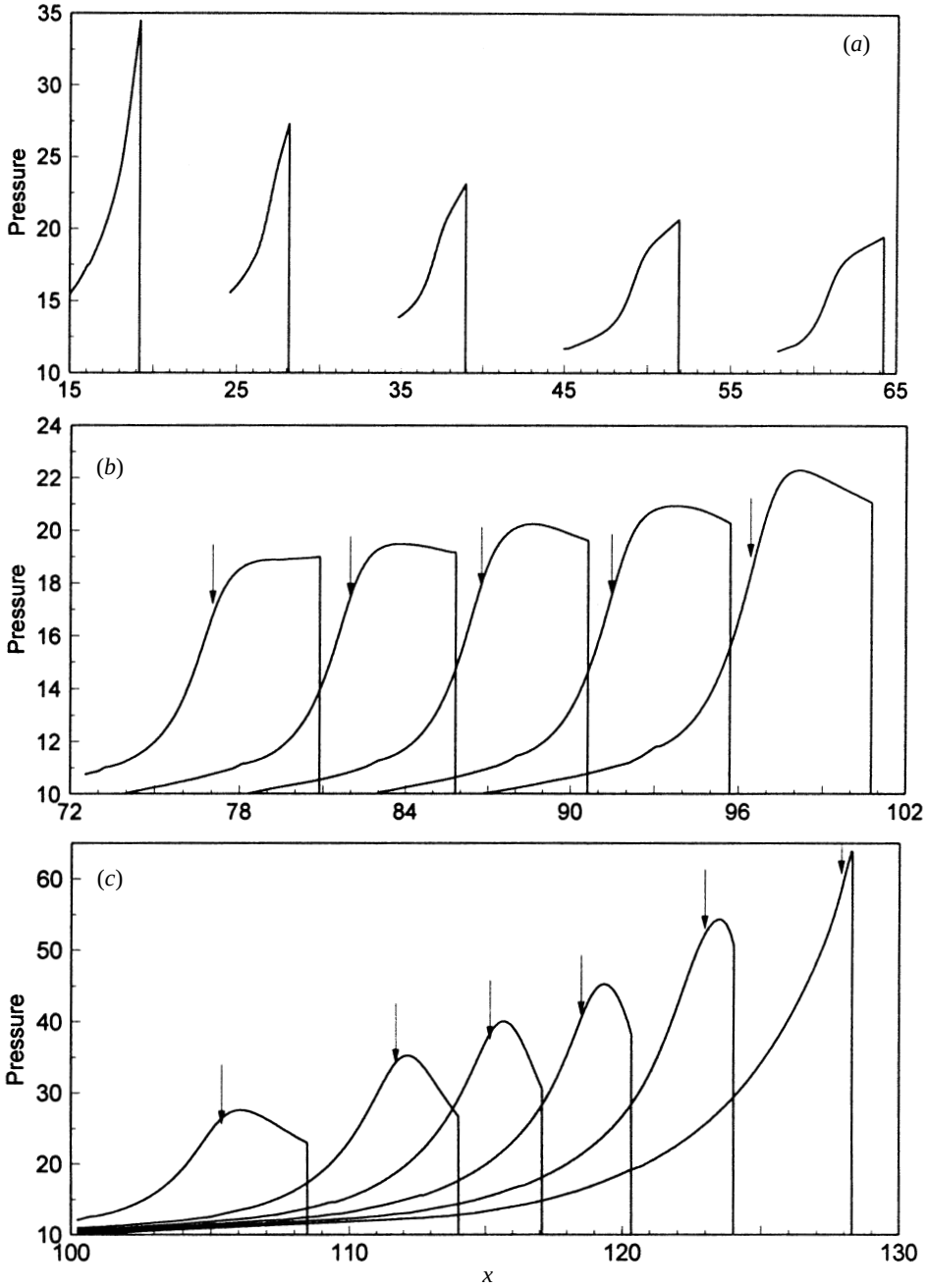

Figure 6. Pressure profiles behind the blast wave for the critical regime ($E_0/P_0 = 1765$). Arrow indicates location of reaction front.

chemical energy release with the travelling pulse is the cause of the rapid amplification, analogous to the LASER mechanism. While the SWACER mechanism has been observed in other experiments, such as turbulent jet initiation (Knystautas *et*

al. 1978) and in numerical simulations (Yoshikawa & Lee 1993; He & Clavin 1994*b*; Montgomery *et al*. 1998), no criterion has yet been formulated to define the critical conditions whereby the SWACER mechanism can occur. The results in figures 5 and 6 clearly illustrate that a SWACER-like mechanism is responsible for the reacceleration of the blast wave from the quasi-steady regime to CJ detonation. Thus, rather than focusing on a failure criterion due to curvature or unsteady expansion, the criterion for direct initiation should address the critical conditions that permit the rapid amplification of a travelling pulse in a gradient field of chemical activity.

Many of the features discussed here have been observed in other numerical simulations of detonation initiation (He & Clavin 1994*a*; He 1996; Eckett *et al*. 1998). The work of Clarke and co-workers (Clarke *et al*. 1986, 1990; Clarke & Singh 1989; Singh & Clarke 1992; Sileem *et al*. 1991), although while not addressing direct initiation per se, showed that a common so-called 'triplet' of a shock wave, unsteady reaction domain and 'fast flame' is obtained in the different means of initiation studied (heated layer of gas and piston-driven shock). This unsteady flow field is essentially identical to what was observed in experiments with detonation initiation by reflected normal shock waves in the 1960s (Urtiew & Oppenheim 1966; Gilbert & Strehlow 1966). In fact, the streak photographs of Strehlow & Gilbert (1966) show a structure strikingly similar to the 'triplet' obtained in the simulations of Clarke and co-workers. The so-called 'fast flame' has been shown, in fact, to not be a flame at all, meaning that it does not propagate by diffusion of heat or radicals. Rather, it is a shock-induced reaction front, similar to the reaction front in the Euler simulations of Mazaheri (1997) discussed above, again suggesting that the final stages of DDT and direct initiation are universal.

With these present results in mind, it is necessary to reassess the initiation criteria based on curvature or unsteadiness discussed in § 3. The numerical results of figures 5 and 6 clearly demonstrate that it is the reacceleration of the blast wave after an initial decoupling of the reaction front from the blast which is responsible for initiation in the critical regime. Any criterion based on failure due to curvature (He & Clavin 1994*a*; He 1996) or quenching due to unsteadiness (Eckett *et al*. 1998) of the initial decaying blast wave will not capture this essential mechanism of initiation in the critical case.

5. Effect of hot spots

Even for homogeneous explosive mixtures, direct initiation experiments indicate that detonation is formed from the rapid growth of reactions from localized 'hot spots' near the termination of the quasi-steady period. For a homogeneous detonable medium, the hot spots are formed from hydrodynamic fluctuations (e.g. turbulence) and instability. Due to the large temperature sensitivity of the chemical reaction rate when the activation energy is large, temperature fluctuations can result in very large changes in the reaction rate, and hence the formation of hot spots. The pressure pulse associated with the energy release of these localized hot spots subsequently propagates in an environment that is undergoing various stages of the induction process itself. This sets the stage for the SWACER mechanism to operate where the travelling pulses can couple coherently to the chemical energy release, thus resulting in the rapid amplification of these pressure pulses to form 'detonation bubbles'. Coalescence of various 'detonation bubbles' then results in the formation of a cel-

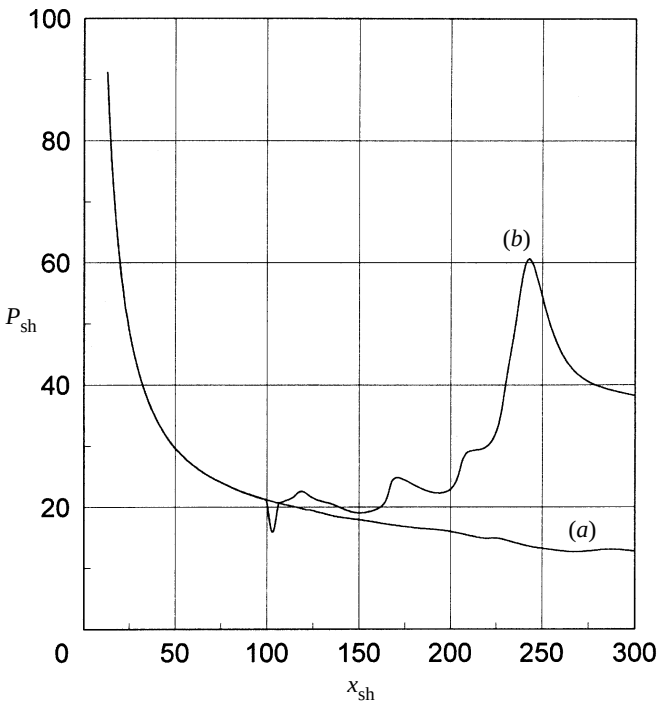

Figure 7. Effect of a temperature/density perturbation on the initiation process for equal initiation energies $E_0/P_0 = 4100$ ($Q/RT_0 = 50$, $\gamma = 1.2$, $E_a/RT_0 = 27$). Case (a) without perturbation fails to initiate. Case (b) with perturbation (located at $x = 100$) initiates detonation after a series of shock mergings.

lular detonation. Since the onset of detonation is associated with hot spots, it is natural to assume that the artificial placement of hot spots in the explosive medium can lower the initiation energy. Indeed, in condensed liquid explosives, the initiation shock pressure is found to be significantly lowered by the introduction of bubbles or glass microballoons to induce the formation of localized hot spots. The role of artificially induced hot spots in the ideal blast initiation process has been studied recently by Mazaheri (1997). The hot spot is generated via a small density perturbation in the unburned gas, and placed at some distance from the blast source within the quasi-steady period. When the initiating blast wave propagates past the density perturbation, a local temperature (hence reaction) fluctuation is effected. It is found that the artificial hot spot did assist in promoting detonation initiation. Figure 7 shows the blast wave strength versus distance from the source. For identical source energy of the blast wave, the hot-spot case leads to initiation whereas detonation initiation fails when the hot spot is not present. The location of the hot spot in the quasi-steady period is critical; studies in which the perturbation was located nearer to the source, in the region of initial blast wave decay, did not promote initiation and, in fact, resulted in a more rapid blast wave decay (Mazaheri 1997).

The mechanism of hot-spot initiation can be observed from the profiles of pressure, temperature and reaction rate shown in figure 8. At constant pressure, a density change is associated with a temperature change. Thus in figure 8*b*, the density per-

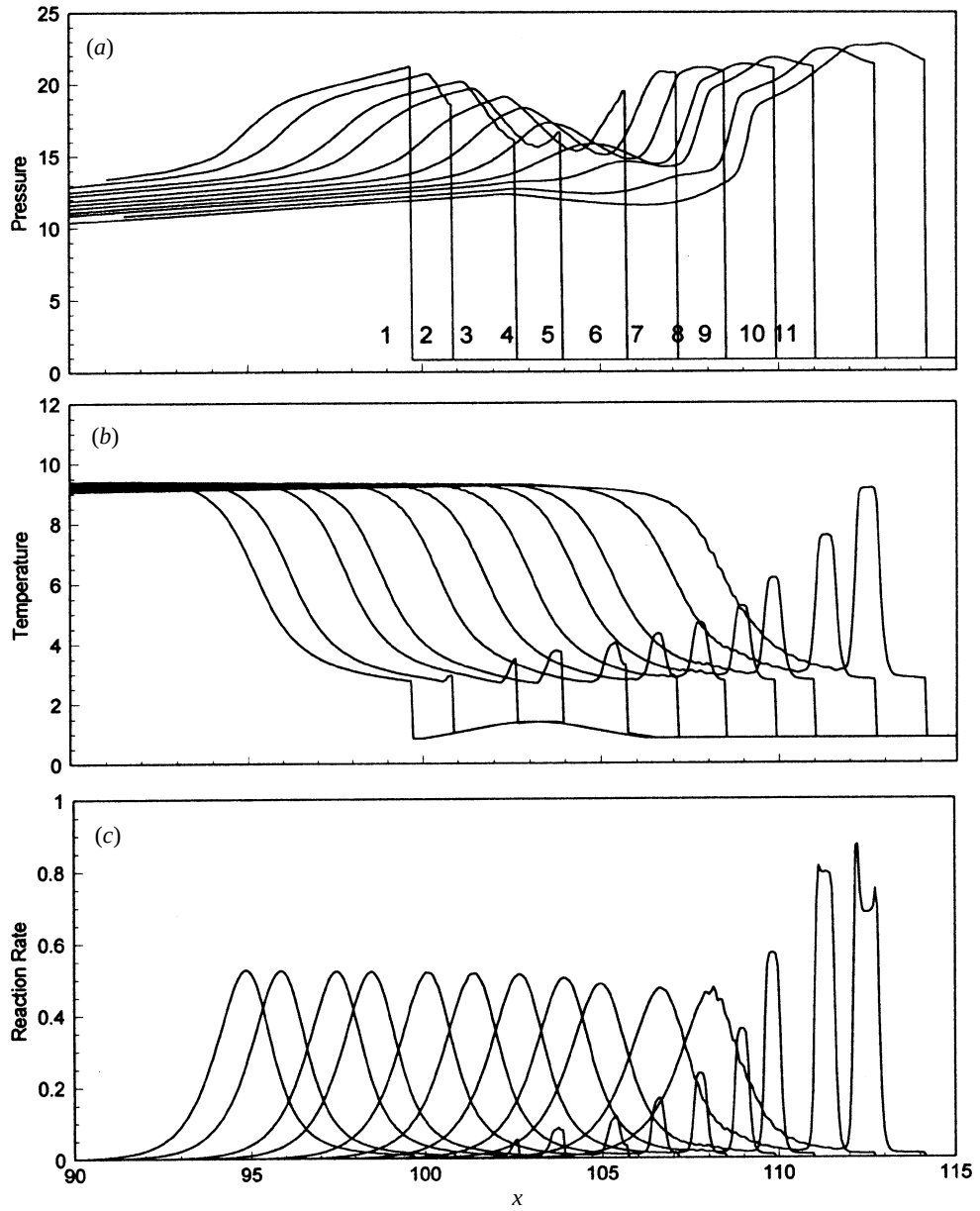

Figure 8. Profiles behind the blast wave in the presence of a perturbation showing (*a*) pressure, (*b*) temperature and (*c*) reaction rate.

turbation is manifested as a temperature perturbation. As the shock traverses the density perturbation, the temperature, and hence the reaction rate, increases rapidly resulting in the formation of a new reaction front. Thus, a 'pocket' of unreacted mixture is 'trapped' between the two reaction fronts. When this pocket eventually burns, a strong pressure pulse is generated which then propagates and catches up with the leading shock front. The merging of the two shock waves leads to an interface where

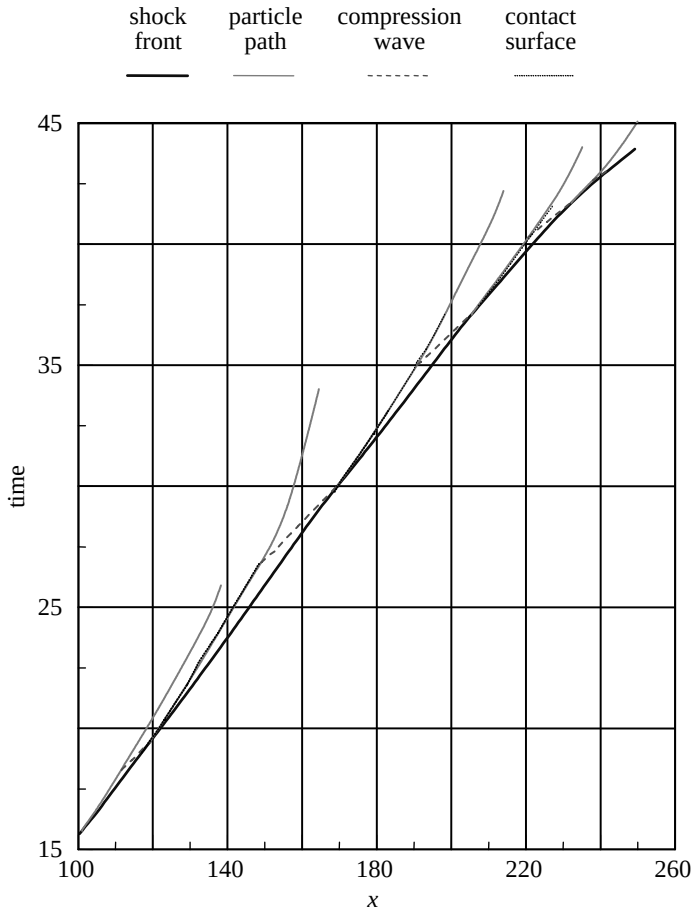

Figure 9. Wave diagram showing the mechanism for initiation with a perturbation via a series of shock mergings.

the temperature is higher than its surroundings. This leads to the formation of a new reaction front, and again a pocket of gas is trapped between the two reaction fronts. The x–t diagram shown in figure 9 illustrates the merging cycles of the shocks and formation of a new reaction front after an induction period. The leading shock is enhanced each time a shock merging occurs, and eventually the leading shock becomes sufficiently strong to result in the formation of a detonation. This mechanism of detonation initiation due to shock merging has been studied previously by Urtiew & Oppenheim (1967).

6. Directions for future investigations

Direct initiation using an ideal point, line or planar source is a well-defined problem amenable to both theoretical and numerical simulation, and can be closely approximated experimentally through the use of powerful energy sources such as condensed explosive charges or pulsed electrical and laser discharges. The direct initiation problem also contains all the essential aspects of detonation phenomena in general. Thus,

its eventual solution will elucidate the entire detonation problem. It is worthwhile to comment here on the directions that future studies could profitably take in order to reach this goal.

Experimentally, there is still a need to obtain more accurate data for the critical energy over a wide spectrum of explosive mixtures. Care must be exercised to ensure that the ignition energy sources used for initiation are of sufficiently high power, since it has been shown that critical energy can be orders of magnitude greater than the case of the ideal point source if the rate of energy deposition is below some minimum (Knystautas & Lee 1976). For this reason the spherical geometry is perhaps easiest to realize experimentally. However, the recent studies of Higgins *et al*. (1998) on quasi-cylindrical initiation using a detonating cord appear to provide a 'clean' line source of energy amenable to theoretical modelling and numerical simulation. In order to improve the current semiempirical theories, the need for more experimental data on various fuels with air and oxygen over a wide range of initial conditions cannot be overemphasized. Apart from the critical energy, the appropriate length-scales for the initiation phenomenon must also be determined. Although the cell size represents a direct characteristic length-scale for detonation structure, its measurement by the subjective soot foil technique has not been improved upon for the last four decades. Attempts to provide a more quantitative measurement of cellular structure using image-processing techniques have met with limited success. Thus, the critical tube diameter, which is a less subjective measure of detonation length-scales, could perhaps serve as the more reliable experimental parameter. With a larger database for the critical energy (for different geometries) and the critical tube diameter, better correlations could be achieved yielding more accurate semiempirical theories for the prediction of the critical energy of initiation.

Numerical simulations in the past have mostly been based on a single-step Arrhenius rate law. This often gives the non-physical result that initiation of detonation can be achieved via any arbitrary strength shock wave. Since the Arrhenius reaction rate is finite at finite temperatures, it becomes simply a question of 'waiting long enough' for sequential reactions to occur after the passage of a weak shock wave. This leads to the so-called 'fast flame' which in essence is a sequential autoignition of the explosive mixture which has been prescribed by a travelling shock. Although the subsequent amplification of pressure pulses leading to the formation of a detonation is similar to the onset of detonation as observed at the end of the quasi-steady period, the formation of the detonation from a 'fast flame' bears little resemblance to the real direct initiation problem. Similarly, in the recent numerical study by Mazaheri (1997), it was demonstrated that with a single-step rate law, a critical initiation energy no longer exists because the decaying blast wave always reaccelerates to form a detonation eventually. The single-step rate law should be abandoned in favour of more complex chemistry in further numerical or theoretical studies. While a complex set of kinetic rate equations could, in principle, be solved simultaneously with the reactive Euler equations, a two- or three-step simplified global rate law should recover the essential features of the phenomenon. Specifically, the kinetic model must be able to capture the competition between chain branching and recombination reactions. Below about 1100 K, chain-branching reactions become ineffective and hence give a sudden decrease in the global reaction rate. Thus, a simplified system of three reaction rates should be sufficient to more accurately reproduce the qualitative aspects of initiation.

Perhaps the most challenging problem is the interpretation of the large amount of detailed information that is generated by such numerical simulations. The proper reduction of all the numerically generated 'field quantities' requires the formation of analytic models. In this light, numerical simulations should be considered as experiments, where the actual analysis begins after the completion of the simulation. The use of Hugoniot representations for transient gas dynamic processes occurring in initiation, as done in the work of Clarke and co-workers (Singh & Clarke 1992), could be such an 'analytic model' wherein the numerical results can be analysed.

References

Bach, G. G. & Lee, J. H. 1970 An analytical solution for blast waves. *AIAA Jl* **8**, 271–275.

Bach, G. G., Knystautas, R. & Lee, J. H. 1969 Direct initiation of spherical detonation in gaseous explosives. In *Proc. 12th Symp. (Int.) on Combustion*, pp. 853–864. Pittsburgh, PA: The Combustion Institute.

Benedick, W. B., Guirao, C. M., Knystautas, R. & Lee, J. H. 1985 Critical charge for the direct initiation of detonation in gaseous fuel–air mixtures. *Prog. Astro. Aero.* **106**, 181–202.

Chue, R. S., Clarke, J. F. & Lee, J. H. S. 1998 Chapman–Jouguet deflagrations. *Proc. R. Soc. Lond.* A **441**, 607–623.

Clarke, J. F. & Singh, G. 1989 *A numerical simulation of shock generated ignition using the random choice method*. Springer Lecture Notes in Physics, vol. 351, pp. 22–35. Springer.

Clarke, J. F., Kassoy, D. R. & Riley, N. 1986 On the direct initiation of a plane detonation wave. *Proc. R. Soc. Lond.* A **408**, 129–148.

Clarke, J. F., Kassoy, D. R., Meharzi, N. E., Riley, N. & Vasantha, R. 1990 On the evolution of plane detonations. *Proc. R. Soc. Lond.* A **429**, 259–283.

Eckett, C. A., Quirk, J. J. & Shepherd, J. E. 1998 An analytical model for direct initiation of detonation. In *Proc. 21st Int. Symp. on Shock Waves, Great Keppel Island, Australia, 20–25 July* (ed. A. S. P. Houwing (and 10 others)), vol. 1, pp. 383–388. Springer.

Edwards, D. H., Hooper, G., Morgan, J. M. & Thomas G. O. 1978 The quasi-steady regime in critically initiated detonation waves. *J. Phys.* D **11**, 2103–2117.

Edwards, D. H., Thomas, G. O. & Nettleton, G. O. 1979 The diffraction of a planar detonation wave at an abrupt area change. *J. Fluid Mech.* **95**, 79–96.

Gilbert, R. B. & Strehlow, R. A. 1966 Theory of detonation initiation behind reflected shock waves. *AIAA Jl* **4**, 1777–1783.

He, L. 1996 Theoretical determination of the critical conditions for the direct initiation of detonations in hydrogen–oxygen mixtures. *Combust. Flame* **104**, 401–418.

He, L. & Clavin, P. 1994*a* On the direct initiation of gaseous detonation by an energy source. *J. Fluid Mech.* **277**, 227–248.

He, L. & Clavin, P. 1994*b* Theoretical and numerical analysis of the photochemical initiation of detonations in hydrogen–oxygen mixtures. In *Proc. 25th Symp. (Int.) on Combustion*, pp. 45–51. Pittsburgh, PA: The Combustion Institute.

Higgins, A. J. & Bruckner, A. P. 1996 Experimental investigation of detonation initiation by hypervelocity blunt projectiles. AIAA paper 96-0342. In *Proc. 34th AIAA Aerospace Sciences Meeting, Reno, NV*.

Higgins, A. J., Radulescu, M. I. & Lee, J. H. S. 1998 Initiation of cylindrical detonation by rapid energy deposition along a line. In *Proc. 27th Symp. (Int.) on Combustion*, pp. 2215–2223. Pittsburgh, PA: The Combustion Institute.

Knystautas, R. & Lee, J. H. S. 1976 On the effective energy for direct initiation of gaseous detonations. *Combust. Flame* **27**, 221–228.

Knystautas, R., Lee, J. H., Moen, I. & Wagner, H. G. 1978 Direct initiation of spherical detonation by a hot turbulent gas jet. In *Proc. 17th Symp. (Int.) on Combustion*, pp. 1235–1245. Pittsburgh, PA: The Combustion Institute.

Lee, J. H. S. 1984 Dynamic parameters of gaseous detonations. *A. Rev. Fluid Mech.* **16**, 311–336.

Lee, J. H. S. 1997 Initiation of detonation by a hypervelocity projectile. *Prog. Astro. Aero.* **173**, 293–310.

Lee, J. H. S. & Moen, I. O. 1980 The mechanism of transition from deflagration to detonation in vapor cloud explosions. *Prog. Energy Combust. Sci.* **6**, 359–389.

Lee, J. H. & Ramamurthi, K. 1976 On the concept of the critical size of a detonation kernel. *Combust. Flame* **27**, 331–340.

Lee, J. H., Knystautas, R. & Yoshikawa, N. 1978 Photochemical initiation of gaseous detonations. *Acta Astronaut.* **5**, 971–982.

Lundstrom, E. A. & Oppenheim, A. K. 1969 On the influence of non-steadiness on the thickness of the detonation wave. *Proc. R. Soc. Lond.* A **310**, 463–378.

Mazaheri, K. 1997 Mechanism of the onset of detonation in blast initiation. PhD thesis, McGill University.

Montgomery, C. J., Khokhlov, A. M. & Oran, E. S. 1998 The effect of mixing irregularities on mixed-region critical length for deflagration-to-detonation transition. *Combust. Flame* **115**, 38–50.

Oshima, K. 1960 Blast waves produced by exploding wire. Aeronautic Research Institute, University of Tokyo. Report 358.

Sakurai, A. 1953 On the propagation and structure of the blast wave. Part I. *J. Phys. Soc. Jap.* **8**, 662–669.

Sakurai, A. 1954 On the propagation and structure of the blast wave. Part II. *J. Phys. Soc. Jap.* **9**, 256–266.

Sedov, L. I. 1946 Propagation of strong blast waves. *Prikl. Mat. Mekh.* **10**, 241–250.

Sileem, A. A., Kassoy, D. R. & Hayashi, A. K. 1991 Thermally initiated detonation through deflagration to detonation transition. *Proc. R. Soc. Lond.* A **435**, 459–482.

Singh, G. & Clarke, J. F. 1992 Transient phenomena in the initiation of a mechanically driven plane detonation. *Proc. R. Soc. Lond.* A **438**, 23–46.

Soloukhin, R. I. 1969 Nonstationary phenomena in gaseous detonation. In *Proc. 12th Symp. (Int.) on Combustion*, pp. 799–807. Pittsburgh, PA: The Combustion Institute.

Taylor, G. I. 1950 The formation of a blast wave by a very intense explosion. *Proc. R. Soc. Lond.* A **201**, 159–174.

Urtiew, P. A. & Oppenheim, A. K. 1966 Experimental observations of the transition to detonation in an explosive gas. *Proc. R. Soc. Lond.* A **295**, 13–28.

Urtiew, P. A. & Oppenheim, A. K. 1967 Detonation ignition induced by shock merging. In *Proc. 11th Symp. (Int.) on Combustion*, pp. 665–670. Pittsburgh, PA: The Combustion Institute.

von Neumann, J. 1941 The point source solution. National Defense Research Committee, Div. B, Report AM-9.

von Neumann, J. 1962 *Collected works of J. Von Neumann*, vol. IV, pp. 219–237. New York: Pergamon.

Whitham, G. B. 1950 The propagation of spherical blast. *Proc. R. Soc. Lond.* A **203**, 571–581.

Yoshikawa, N. & Lee, J. H. 1993 Formation and propagation of photochemical detonations in hydrogen–chlorine mixtures. *Prog. Astro. Aero.* **153**, 95–104.

Zeldovich, Ya. B., Kogarko, S. M. & Simonov, N. N. 1957 An experimental investigation of spherical detonation in gases. *Sov. Phys. Tech. Phys.* **1**, 1689–1713.