

The Influence of Local Disturbances on the Direct Initiation of Detonations

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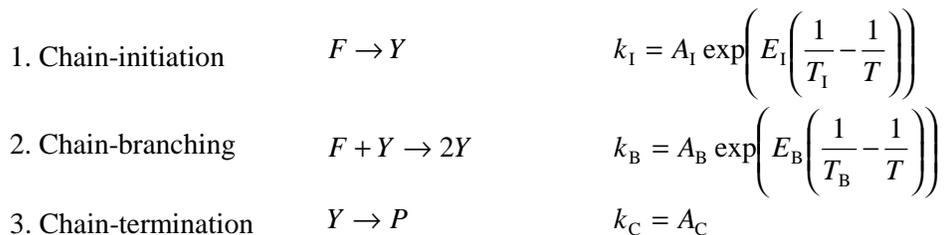
Introduction

In general, direct or blast initiation of detonations is characterized by a single parameter, i.e., the critical blast energy, which describes the global transient flow field associated with the decaying blast wave. However experimental observations [1] indicate that the onset of detonation is not a global phenomenon. Near the critical regime of direct initiation, the onset of detonation is invariably found to originate from localized hot spots in the reaction zone during the so-called “quasi-steady” period. “Detonation bubbles” are developed from these local hot spots, which eventually evolve to form a global self-sustained detonation front. Therefore, the onset of detonation appears to be a local event, yet the initiation process is characterized by a global parameter that determines the overall transient flow field. To reconcile this dilemma, it appears that the critical blast wave decay is responsible to set the appropriate flow field in order for local hydrodynamics fluctuations to be amplified and form the “detonation bubbles”. Thus the existence of a critical energy is to ensure that the blast wave generates a flow field appropriate for the rapid growth of hydrodynamic perturbations leading to the onset of detonation.

The effect of density perturbations on the initiation phenomenon has been studied previously by Chue *et al.* [2] and Mazaheri [3]. However, they used a simplistic single-step Arrhenius rate law, which cannot describe chemical quenching when the temperature drops below a certain critical value. Thus the use of a single-step rate law failed to describe the existence of a critical initiation energy. For this reason, a more realistic chemical kinetics model is used in the present study, which permits a definitive value of critical initiation energy to be defined [4]. Apart from density perturbations, perturbations due to local fluctuation in the reaction rate by free radical sensitization as well as in the magnitude of the chemical energy release itself are being investigated. The study of different types of local disturbances also permits us to determine if the onset of detonation is dependant on the nature of the perturbation itself or on the subsequent amplification of the shock wave resulting from these local perturbations (i.e., SWACER mechanism [5]).

Mathematical model

The direct initiation phenomenon is modelled by the one-dimensional reactive Euler equations (see [3] for details on the governing equations and the underlying assumptions). The initial flow field is given by the similarity solution for a non-reacting strong blast wave. The chemical kinetics scheme used for the present study is a generalized three-step chain-branching reaction model [6]. This reaction scheme involves two temperature-sensitive radical producing reactions and a temperature-independent exothermic chain-termination reaction. It can be represented by the following three main-stages:



where F , Y and P correspond to the amount of reactants, radicals and products, respectively. The chain-initiation and chain-branching rate constant k_I and k_B have an Arrhenius temperature-dependent form $A_i e^{-E_i/RT}$. The chain-termination is assumed to be first order, independent of temperature and has a fixed rate constant k_C . The pre-exponential constants A_i are used to adjust the length scale of each reaction step. The characteristic length scale is chosen as the half-reaction zone length of the steady ZND detonation. Denoting the variable f and y to be the mass fraction of the fuel F and radical Y , the consumption equations for fuel and radical can be written as:

$$\begin{aligned}\frac{\partial(\rho f)}{\partial t} + \frac{\partial(\rho u f)}{\partial x} &= -\rho f k_I - \rho^2 f y k_B \\ \frac{\partial(\rho y)}{\partial t} + \frac{\partial(\rho u y)}{\partial x} &= \rho f k_I + \rho^2 f y k_B - \rho y k_C\end{aligned}$$

and the local chemical energy release can be written as $q = Q_{\text{total}} \cdot f \cdot Q_{\text{total}} - y \cdot Q_{\text{total}}$ where Q_{total} is the total amount of chemical energy released by the fuel. Here, values of $Q_{\text{total}} = 22.5$, $E_I = 20$, $E_B = 8$, $T_I = 3T_{\text{shock}}$, $T_B = 0.70T_{\text{shock}}$ and a polytropic equation of state with $\gamma = 1.2$ are used throughout. The choice of the parameters corresponds to a stable self-sustained detonation.

To simulate the effect of local disturbances (hence hot spot formation) on the initiation process, an initial perturbation (either density, free radical concentration or chemical energy release) in the form of a half sinusoidal profile is superimposed upstream of the leading shock. The perturbation is applied when the blast wave decays to a shock temperature close to the chain-branching cross-over temperature T_B (i.e., the temperature limit below which no initiation occurs [4]). In the following discussion, the perturbation is basically characterized by its length and amplitude. The subsequent interaction of the leading shock with the perturbation is described by the numerical integration of the reactive Euler equations together with the chemical rate laws. They are numerically solved using a combination of the Piecewise Parabolic Method, the Conservative Shock Tracking and the Adaptive Mesh Refinement [3,7].

Numerical results and discussion

1. Density perturbation

Numerically, hot spots can be artificially created via small density perturbations. When the blast wave propagates through the density perturbation, a hot layer behind the shock is created causing local temperature (hence reaction rate) fluctuations. The role of an artificially induced hot spot in the ideal blast initiation has been studied by Mazaheri [3]. However, in his study he used a single-step Arrhenius rate law to model the chemical kinetics. It is known that for single-step chemistry, a system without losses will always react to completion. Therefore, initiation always occurs after a sufficiently long period. Hence, it is not clear whether the transition process is really triggered by the presence of the artificially induced hot spot. Therefore, it is worthwhile to repeat his calculation using the present three-step chemical kinetics model, which provides a switch-off mechanism to cause chemical quenching that is not present in the ideal single-step Arrhenius rate law.

Figure 1 shows the pressure of the shock front versus distance from the ignition source, showing both perturbed and unperturbed cases. The amplitude of the density perturbation is 30% decrease with respect to the unburned mixture and the length of the perturbation is about the chemical reaction zone length. For the same ignition source energy, the perturbed case leads to initiation whereas detonation initiation fails when the density perturbation (or hot spot) is not present. From this figure, it is also observed that transition to detonation is induced from a series of oscillations of the leading shock front pressure. This transition process is based on a multi-step shock merging mechanism, also observed by Mazaheri [3].

2. Non-uniformity in free radical concentration by sensitization

The origin of localized hot spots is due to a local reaction rate fluctuation inside the reaction zone. Beside a density (or temperature) perturbation, reaction rate fluctuation can also be effected via sensitization of a small region in the reactive mixture, leading to the formation of localized explosion centers. In this paper, sensitization refers to an initial decomposition of an amount of fuel into some intermediate species (free radicals) without actually release the chemical energy associated with the mixture. With the use of the present three-step chemical kinetics description, it is possible to impose a non-uniformity of free radicals into the flow field.

From the present numerical simulation, it is found that a small free radicals sensitization can also assist in triggering the onset of a self-sustained detonation with the same initiation energy as for the subcritical regime. For instance, this can be seen in figure 2, which shows the shock pressure history for a perturbed and unperturbed case. In this figure, the dashed curve corresponds to a subcritical initiation with initiation energy less than the critical value without the presence of initial free radicals non-uniformity. The blast wave thus continues to decay to a weak shock. However, when a small free radicals concentration is present ahead of the shock, detonation initiation is promoted. The solid curve corresponds to the same initiation energy but a small free radical gradient is put in front of the leading shock. The amplitude of the perturbation is only an increase of 1% in the free radicals mass fraction, resulted from the decomposition of 1% of fuel mass fraction. Similar to the density perturbation, the length of the sensitized region is about the chemical reaction zone length. It is observed that a sudden increase in free radicals concentration causes a local explosion within the reaction zone and generated a hot spot. This can be easily observed from the temperature profiles (see figure 3).

Free radicals have a direct effect on the rate of each reaction step. A sudden rise in free radicals concentration inside the reaction zone will increase the rate of chain-branching reaction resulting a reduction of the chain-branching induction zone length. More free radicals are ready to recombine, and hence cause a sudden increase in the global heat release rate. When the leading shock enters the region of free-radical non-uniformity, the sudden increase in the overall rate of chemical heat release produces a local explosion (or hot spot) behind the leading shock and a new reaction front is created. Pockets of unburned mixture and free radicals are left behind these local explosion centers. When these pockets eventually burn, strong pressure pulses are generated and the subsequent shock merging between these pressure pulses and the leading shock front triggers the onset of detonation. The interaction of these pressure pulses with the shock and the formation of temperature waves cause the proper coupling between the chemical heat release and hydrodynamic flow, leading to the formation of a self-sustained detonation. This multi-shock merging process can be observed from the pressure profiles (see figure 4).

3. Chemical energy perturbation

The last type of perturbation investigated in the present study is due to a fluctuation in chemical energy release Q_{total} . Physically, this may be due to the inhomogeneities of the reactive mixture. A small region having a higher overall chemical energy release Q_{total} is introduced upstream of the leading shock. The amplitude of the perturbation is 30% increase in the overall chemical energy release with respect to the unperturbed mixture and the length of the perturbation is also about the chemical reaction zone length. The propagation of the leading shock after hitting this perturbation and its transition to detonation is illustrated in figure 5. Similar to the other type of disturbances considered previously, a fluctuation in chemical energy release also assists in triggering the detonation. The mechanism leading to the transition of detonation is also due to a repeating process of pressure pulse amplification.

Conclusion

During the quasi-steady period of direct initiation, hot spot or localized explosion can be induced due to different disturbances or hydrodynamic fluctuation in the reactive fluid. Three types of

disturbances have been considered in this study. A hot spot was artificially created by introducing a temperature (density) perturbation in the media, which sensitizes a region of the reactive mixture to give a different reaction rate. Furthermore, using the present 3-step chemical kinetics model, it is also possible to sensitize the mixture by putting a non-uniform distribution of free radicals in the flow field. Lastly, a chemical energy release perturbation is also carried out. The present numerical results shows that all types of disturbances will lead to the formation of hot spots which can assist in triggering the transition process to detonation. The transition process for all disturbances is shown to be via a SWACER type mechanism and multi-step shock merging process as observed by Mazaheri [3]. Thus, the subsequent shock amplification appears to be the universal mechanism for hot spot initiation. The nature of the perturbation itself, that results in the hot spot formation, is not important. Therefore, successful initiation depends globally on whether the initiation energy is enough such that the blast wave can set an appropriate stage for these local disturbances to get amplified and trigger the onset of detonation.

In the first type of hot spot formation, i.e., induced by the temperature perturbation, the unburned mixture must be heated up to more than 30% increase with respect to the value of the initial temperature. While in the second type, only a very small amount of free radicals distribution (about an amount of 1%) is required. The chemical energy perturbation also required a high value of amplitude (more than 30% increase) to trigger the onset of detonation. Therefore, the present study shows that sensitization of the mixture by free radicals is a more effective way to trigger the onset of detonation than other kinds of perturbations in the media.

References

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Figures

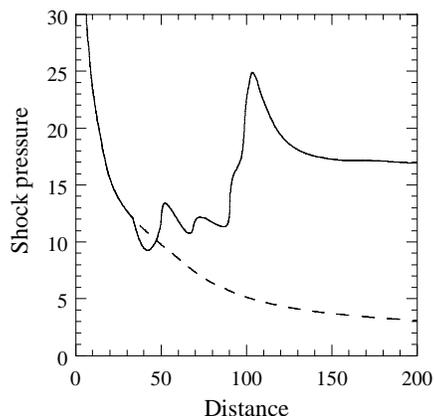


Figure 1: Effect of a density (temperature) perturbation on the initiation process. Dashed line corresponds to the subcritical regime of initiation without perturbation. Solid line represents the case with perturbation of a 30% decrease in density with respect to the unperturbed mixture.

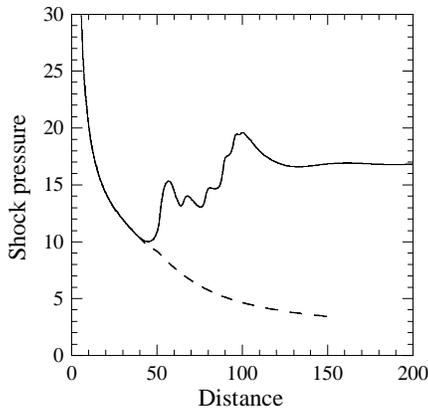


Figure 2: Effect of sensitization on the initiation process. Dashed line corresponds to the subcritical regime of initiation without perturbation. Solid line represents the case with perturbation of a 1% increase in free radical mass fraction.

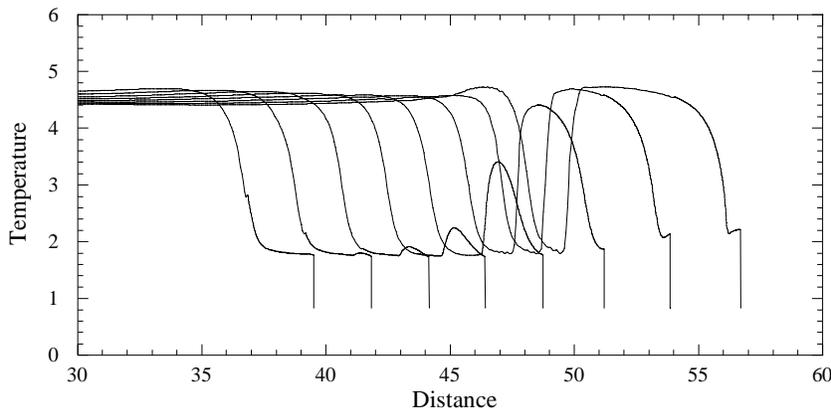


Figure 3: Temperature profiles behind the leading shock in the presence of a 1% free radical perturbation.

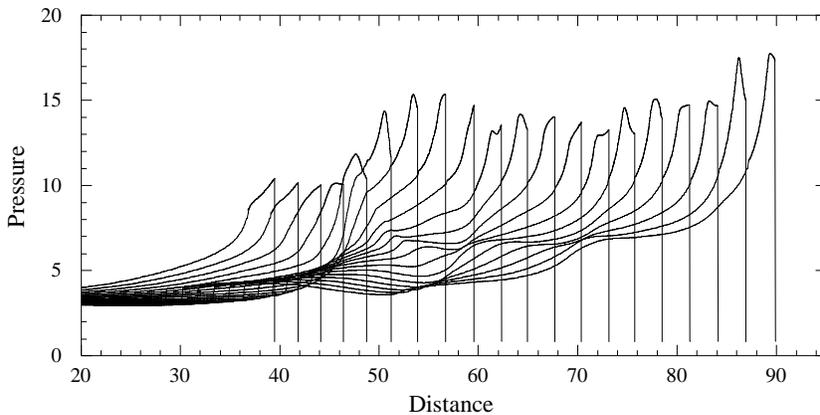


Figure 4: Pressure profiles behind the leading shock in the presence of a 1% free radical perturbation.

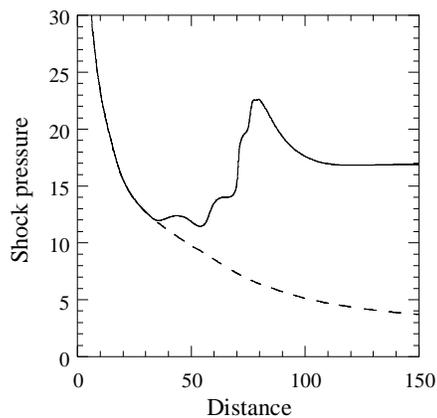


Figure 5: Effect of chemical energy release perturbation on the initiation process. Dashed line corresponds to the subcritical regime of initiation without perturbation. Solid line represents the case with perturbation of a 30% increase in the amount of chemical energy release with respect to the unperturbed mixture.