

Direct Initiation of Detonation in small initiation reaction rate

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1 Introduction

In direct initiation, detonation is formed instantaneously via the rapid deposition of a large amount of energy in a small volume of the combustible mixture. If a sufficient amount of energy is released by the igniter, rapid auto ignition takes place behind the generated blast wave and the reaction-coupled shock quickly becomes a CJ detonation. For direct or blast initiation, the energy of the source is the sole parameter that governs success or failure of detonation initiation.

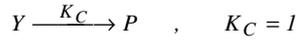
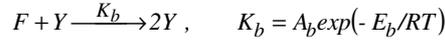
To survey the detonation phenomenon, a lot of numerical studies have used the simple one-step model with Arrhenius reaction rate to model the combustion process (Mazaheri, Eckett) [1, 2]. Because of its application simplicity the one-step model is very suitable, but it has some inconveniences. For example this model is not capable to model induction length independently and detonation decay could not be also modeled.

Stability of steady planar detonation waves has been studied by Short and Quirk [3] for the three-step reaction mechanism. This model included initiation, branching and termination steps. Since in a reaction mechanism chain branching is the most important one, Short and Quirk have studied the effect of chain branching on the stability of detonation. Ng and Lee [4] studied the role of chain branching on direct initiation of detonation for the three-step model. They have observed the different regimes of critical, sub-critical and super-critical initiation by the change in chain branching rate. They concluded that the three-step mechanism presents a more precious result in comparison with one-step mechanism.

The role of chain initiation on the stability of detonation has investigated by Mazaheri and Hashemi [5]. They compared characteristic times of some elementary reactions of H₂-O₂ reaction mechanism for different cases (i.e. stable, unstable and failure of detonation). They showed that while the characteristic times of the branching and termination reactions do not show considerable difference in these cases, the initiation characteristic times differ significantly. This suggests a crucial role for the chain initiation on the dynamic of detonation. In this study direct initiation of detonation is investigated in small reaction rate of the chain initiation.

2 Governing Equations

The chemical kinetic model used for present study is a generalized three-step chain-branching reaction model and its detailed description can be found in [3,5]. This model contains chain initiation, chain branching, and chain termination steps, as follows:



F , Y , and P represent the reactant, radical, and product of reaction. K_I is the rate constant of each reaction, and, A and E are the Arrhenius constants.

The rates of the above reactions are $r_I = k_I f$, $r_b = k_b f y$, $r_C = k_C y$, where f and y are the mass fraction of fuel and radical, respectively. In order to study the effect of the initiation step, an individual time scale is defined for each reaction step. These characteristic times are defined as:

$$\tilde{\tau}_I \propto \frac{1}{r_I} \approx \frac{1}{A_I \exp(-E_I/RT_s)}, \quad \tilde{\tau}_b \propto \frac{1}{r_b} \approx \frac{1}{\rho_s A_b \exp(-E_b/RT_s)}, \quad \tilde{\tau}_C \propto \frac{1}{r_C} \approx \frac{1}{A_C}$$

Subscript ‘‘s’’ in the above relations denotes the post shock condition. These characteristic times are used as the main kinetic parameters in this study.

Ignoring viscosity, conductive heat transfer, diffusion, and body forces, the governing equations for compressible reactive flow are reactive Euler equations. If the multidimensional character of a detonation can be also ignored, then a one-dimensional description is valid. In a fixed reference frame, the one-dimensional reactive Euler equations for a planar geometry are given by:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0, \quad \frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} = 0, \quad \frac{\partial(\rho e)}{\partial t} + \frac{\partial[\rho u(e + p)]}{\partial x} = 0$$

$$\frac{\partial(\rho f)}{\partial t} + \frac{\partial(\rho u f)}{\partial x} = \rho w_F, \quad \frac{\partial(\rho z)}{\partial t} + \frac{\partial(\rho u z)}{\partial x} = \rho w_P$$

where variables ρ , u , p , and e are the density, particle velocity, pressure, and total energy, respectively. w_F is the consumption rate of the reactant, and w_P is the production rate of the product. The mass fraction of the radicals is obtained from $y = 1 - f - z$. A calorically perfect gas equation of state is used throughout the study. Therefore:

$$e = \frac{p}{\rho(\gamma - 1)} + \frac{u^2}{2} - Q(1 - z), \quad P = \rho RT$$

where Q is the heat release per unit mass of the reactant and γ is the ratio of the specific heats. The dependent variables are non-dimensionalized with respect to the unburnt mixture properties. Thus, the density, pressure and velocity are non-dimensionalized with ρ_0 , γP_0 and the sound speed of unburnt mixture (C_0), respectively. The termination step characteristic time ($\tilde{\tau}_C$) is chosen as the time scale for non-dimensionalization. To non-dimensionalize distances, the reference length (L_C) is set to $\tilde{\tau}_C$ times the sound speed of the unburnt mixture (C_0). Q and Ea are non-dimensionalized with RT_0 .

4 Numerical Method

In the present work, PPM is chosen as the main gasdynamics solver. PPM is a third order method near the discontinuities and forth orders in smooth regions [6]. For shock front tracking, the simplest one is the conservative front tracking of Chern and Colella [7], which is utilized in the present study.

Since all reactions are completed in a narrow region close to the shock, it is more economical to use a fine grid only in this region, and a coarse grid elsewhere. To fulfill this requirement, a simple version of the ‘‘Adaptive Mesh Refinement, AMR’’ of Berger and Colella [8] is employed in the present work. In the AMR method, a coarse grid covers the entire domain. Then, fine meshes are superimposed over the coarse grid near the front. The number of meshes that are necessary depends on the behavior of the shock front [3].

In the present work, for each case, the mesh was repeatedly refined until the qualitative nature of the front and the structure behind the front were not changed. A CFL number equal to 0.5 is used in all calculations reported in this paper. The developed code for one-step chemistry is validated via several test problems [1]. This code is developed for three-step chemistry and validated by Mazaheri and Hashemi [5].

4 Results

The ideal strong blast wave is adapted as initial conditions, the same approach as in most of the previous studies [1,2,4]. Depending on initiation energy, three regimes of initiation could be observed; subcritical, critical and supercritical. These three regimes are compared here for high and low reaction rate of the chain initiation. Figure 1 shows these three regimes of initiation for a relatively high initiation reaction rate ($\tau_i=10^8$). In the subcritical regime¹ (dashed line, $E_0=780.35$), the shock pressure decreases rapidly as for a strong non-reactive blast wave. As the blast decays to larger distances, the chemical heat release starts to influence the blast wave propagation. But the chemical reaction zone fails to couple to the shock front and the blast continues to decay. If the initiation energy increase to $E_0=780.36$, the critical regime is observed. In this case, the shock front and the reaction front first decouple as the blast expands. However, unlike the subcritical case, the decoupling in the critical case stops after the blast wave has decayed to a certain shock pressure ($P_{sh}\approx 4$). During decaying period an explosion occurred in the unreacted mixture which preheated by the shock front. This explosion reaches to the shock front and amplifies it to the pressure about $P_{sh}=15$ to form an overdriven detonation wave. The overdriven wave eventually decays to a self-sustained CJ detonation wave. If the initiation energy is smaller than this critical value (e.g. $E_0=780.35$), the decoupling will continue and the shock will eventually decay and no detonation is initiated.

The regimes of direct initiation are also obtained for a relatively small reaction rate of the chain initiation. Figure 2 shows three regimes of initiation for $\tau_i=8.6\times 10^{11}$. By comparing with the previous case, some differences are observed in the critical initiation. When $\tau_i=10^8$, the shock pressure in critical initiation has decayed to $P_{sh}\approx 4$, while by $\tau_i=8.6\times 10^{11}$, the shock pressure has decayed only to $P_{sh}\approx 8$. This shows that for a successful initiation, the shock pressure during initiation is not allowed to decrease below a critical value. This critical value increases when τ_i increases. So when τ_i increases enough, critical initiation takes place without decreasing the shock pressure below the corresponding CJ detonation shock pressure. In such cases, critical initiation becomes similar to the supercritical initiation.

Another difference between these two cases (Figure 1 & 2), is that decaying period of the initial blast, is shorter for the larger τ_i . This results from the first difference, which the shock front could not decrease below a certain value and therefore the decaying period becomes short. In the decaying period the reaction zone decouples from the shock front. The longer decaying period yields more distance between the shock front and the reaction zone. So a large portion of combustible mixture which preheated by the decaying shock, is between the shock front and the reaction zone. When τ_i is small, the reaction could initiate and propagate through this medium and form a strong pressure pulse or a new detonation wave (figure 1) behind the leading shock front². The new detonation wave reaches the leading shock front and thereafter moves together as a stronger detonation wave. This phenomena is observed experimentally and numerically by many researchers e.g. [1,3,9]. When the decaying period becomes short, as a result the preheated combustible mixture behind the shock front becomes small and could not create a strong wave to amplify the leading shock. So with increasing τ_i , the amplification process during decaying period becomes weak.

¹ The failure of detonation (near the critical initiation of detonation) is considered here as subcritical regime of initiation.

² A complete description of the formation mechanisms of pressure pulse or detonation behind the leading shock could be find in [3, 5]

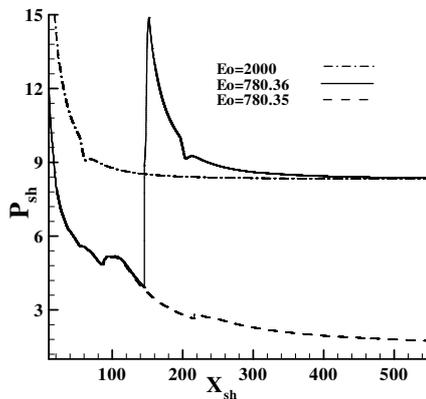


Figure 1. subcritical(dashed), critical(solid) and supercritical (dash-dotted) initiation of detonation with relatively high reaction rate of chain initiation ($\tau_i=10^8$)

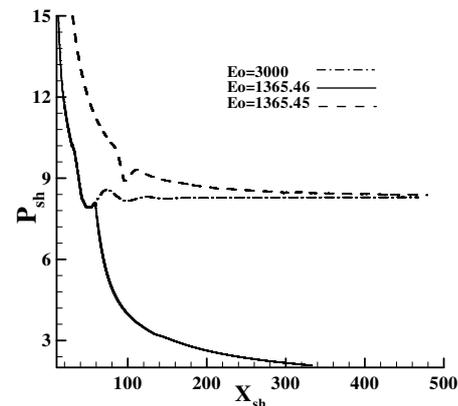


Figure 2. subcritical(dashed), critical(solid) and supercritical (dash-dotted) initiation of detonation with relatively low reaction rate of chain initiation ($\tau_i=8.6 \times 10^{11}$)

By comparing these two cases, we can determine the role of chain initiation on the direct initiation of detonation. When τ_i increases, the minimum allowable shock pressure during propagation of detonation is increased. If the shock pressure falls below this value, detonation will be quenched.

So in low reaction rate of chain initiation (large τ_i), detonation becomes more sensible to oscillation and decreasing the shock pressure (and so temperature). This also shows a detonability limit, where the minimum allowable shock pressure (in the decay period) corresponding to τ_i , becomes nearly the CJ detonation shock pressure.

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