Numerical Study on Detonation Initiation through a Uniform Energy Source

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1 Introduction

Hydrogen as a clean energy carrier, is already used extensively in many industrial applications. However, wide spread use of hydrogen energy requires significant efforts to resolve safety issues. For the purpose of addressing hazard assessment of Hydrogen detonation, thorough understanding of the mechanism of detonation initiation through different means is required. Detonation initiations, in general, can be categorized into two fundamental modes, i.e. indirect or direct initiation. The indirect initiation refers to a category that the reactive mixture can be ignited by a weak energy source, which is followed by a deflagration to detonation transition process (DDT). Comprehensive reviews on DDT can be found in many literatures [1-4]. The direct initiation is that the detonation is formed instantaneously via rapidly depositing a large amount of energy in unconfined combustible mixture of a small volume [5,6].

Since the pioneering work of Zeldovich et al. [7]who proposed a qualitative relationship between the critical energy and the induction zone length first, the problem of direct initiation has been studied extensively for the past five decades [8]. Note that only numerical studies concerning detonation initiation is reviewed in the present section. The experimental studies on blast initiation can be found in [9]. Numerical simulations of detonation initiation can be carried out readily, and much more detailed information on the transient process can be obtained than from experiments. In the numerical simulations, chemical reaction models from single-step Arrhenius rate law to full detailed chemistry of the reactions are implemented.

The present study focuses on the shock/reaction interaction process associated with the detonation ignition process by using a uniform source energy (a uniformly distributed section with high initial pressure and temperature). Therefore, the main objective of this paper is to elucidate more physics and extend the research scope of ununiform detonation ignition.

2 Numerical methodology

The governing equations employed to describe the detonation dynamics are one-dimensional reactive Euler equations, which have the following form:

$$\frac{\partial \mathrm{U}}{\partial t} + \frac{\partial \mathrm{F(U)}}{\partial x} = \mathrm{S(U)} \tag{1}$$

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where the vector U, the flux F, and source the term S are defined as:

$$\mathrm{U} = \{\rho, \rho u, E, \rho_1, \rho_2, \dots, \rho_{N-1}\}^T, \quad (2)$$

$$F(U) = \{\rho u, \rho u^2 + p, (E + p)u, \rho_1 u, \rho_2 u, \dots, \rho_{N-1} u\}^T, \quad (3)$$

$$S(U) = \{0,0,0, \omega_1, \omega_2, \dots, \omega_{N-1}\}^T \quad (4)$$

where ρ, u, p and E denote the density, velocity, pressure and the total energy, respectively. N is the number of species, and $\rho_i = \rho Y_i$ in which Y_i is the mass fraction of the i-th species (Note that $Y_N = 1 - \sum_{i=1}^{N-1} Y_i$). ω_i is the mass production rate of the i-th species. The total energy and the equation of state are given by,

$$E = \rho h - \mathrm{p} + \frac{\rho u^2}{2}, \; h = e + \frac{\mathrm{p}}{\rho} \quad (5)$$

where h, p and e represent the enthalpy per unit mass, pressure and specific total energy, respectively. A detailed chemical reaction model comprised of 9 species and 48 elementary reactions [10] is employed to describe a hydrogen-oxygen-argon detonation.

To resolve the detailed structures during the detonation initiation process, it is necessary to use a very fine resolution in the numerical simulation. To fulfill this requirement, a parallel AMROC code [11] with a block-structured adaptive mesh refinement (AMR) method after Berger and Colella [12] was used in the present work to dramatically reduce the computation time and memory requirement. A resolution test was conducted to validate the convergence of the numerical methods associated with the detailed chemical reaction mechanism in the present study using AMR. Five different resolutions, $33\,\mathrm{pts}/\Delta_\mathrm{I}$, $66\,\mathrm{pts}/\Delta_\mathrm{I}$, $264\mathrm{pts}/\Delta_\mathrm{I}$, $528\mathrm{pts}/\Delta_\mathrm{I}$, $1056\mathrm{pts}/\Delta_\mathrm{I}$, were tested for a benchmark case with T_s=1800 K and p_s=300 kPa. It is clearly observed in Figure 2, in order to resolve the unsteady process during the detonation initiation in the near field, a grid resolution as high as 528 $\mathrm{pts}/\Delta_\mathrm{I}$ is required to ensure convergence.

As shown in Figure 1, a uniform energy source with high temperature T_s and high pressure p_s is set to describe a uniform energy source to the left of the interface. The initial temperature and pressure in the driven section to the right of the interface for all cases are set as $T_0 = 298$ K and $P_0 = 6670$ Pa, respectively. The pre-mixed combustible mixture used in the present study is $\mathrm{H_2}$: $\mathrm{O_2}$: Ar=2:1:7. The left boundary is set as a solid wall in the present study unless specified. The right boundary is set as an outflow condition.

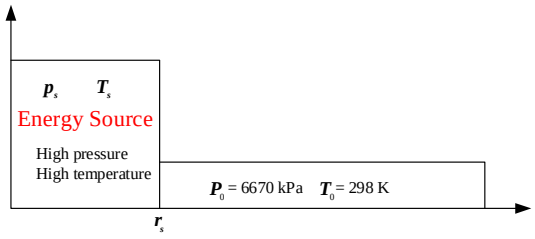


Figure 1. A schematic of simulation setup

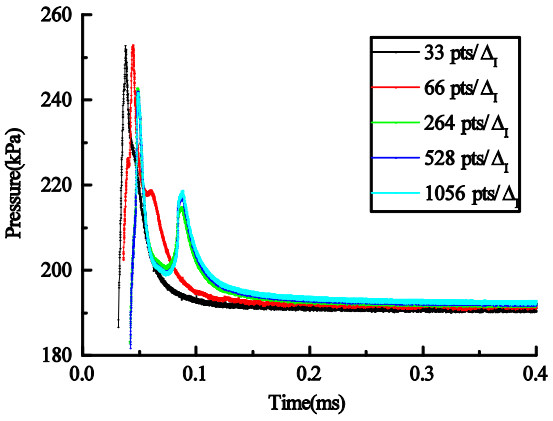


Figure 2. Pressure of the shock front in different resolutions

3 Results and discussions

A series of cases with constant driver length (r_s=10 cm) is studied here first. The initial temperature of reactants in the energy source is set as 1800 K. The initial pressure of reactants in the energy source is varied

in order to generate thermal explosions of different intensity. Three different regimes, corresponding to so-called subcritical (Figure 3(a)), critical (Figure 3(b)) and supercritical (Figure 3(c)) regimes, are observed in the present numerical study as shown in Fig.2, where a sequence of pressure profiles is plotted as a function of distance.

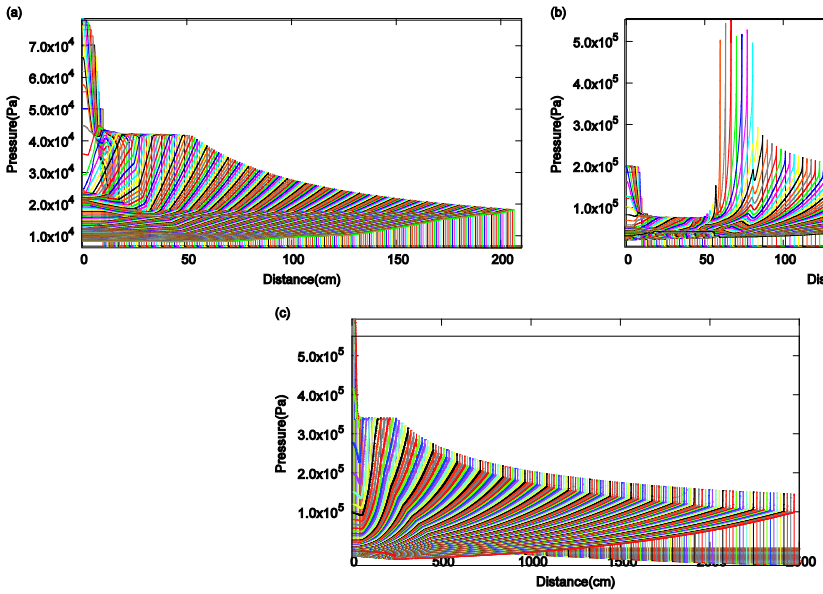


Figure 3. Different regimes of detonation initiation with r_s=10 cm and T_s=1800 K, (a) subcritical case (p_s=50 kPa), (b) critical case (p_s=122 kPa), (c) supercritical case (p_s=2000 kPa)

The corresponding initial pressures in the energy source for the above three cases in Figure 3 are 50 kPa, 122 kPa, and 2000 kPa, respectively. The critical pressure is found to be 122 kPa in the present cases with r_s=10 cm and T_s=1800 K. For a subcritical regime as plotted in Figure 3(a), the pressure in the energy source increases to about 76 kPa from 50 kPa abruptly as a result of a thermal explosion. However, the thermal explosion of energy source is not sufficiently strong to form a CJ detonation subsequently. Finally, the leading shock wave relaxes to an acoustic wave due to the influence of rarefaction wave. If the initial pressure in the energy source is increased to 2000 kPa which is greatly beyond the critical pressure (122 kPa), an overdriven detonation is immediately formed by the strong thermal explosion, and then asymptotically decays to a self-sustained CJ detonation subject to rarefaction wave, as shown in Figure 3(c). This is referred to the supercritical regime. For the critical regime, after the thermal explosion, the reactive shock wave undergoes a state with constant velocity ($\approx 0.68 V_{CJ}$) and pressure ($\approx 0.5 p_{VN}$) prior to re-accelerating to an overdriven reaction front. Eventually, the overdriven reaction front catches up with the leading shock front to form an overdriven detonation which asymptotically decays to a self-sustained CJ detonation, as shown in Figure 3(b).

As shown in Figure 4, the initial process in the vicinity of the interface consists of two mutual interaction processes, i.e. a Riemann problem and a chemical reaction. The former influences the spatial distribution of the auto-ignition delay time and the subsequent reaction progress. The latter affects the flow state through temperature increase by heat releasing. At the interface, a shock wave is immediately generated and propagates towards right; a rarefaction wave is also generated in an opposite direction to attenuate the pressure and the temperature. Between the rarefaction wave and the rear wall, a CV explosion process occurs. The thermal explosion in the energy source is completed before the rarefaction wave arrives at the rear boundary, as shown in Figure 4(a). After the initial thermal explosion, as shown in Figure 4(b), there exists a period of state where the pressure and the temperature of the shock front almost remains unchanged, but

the distance between reaction front and shock front increases, referring to the quasi-steady period. This quasi-steady period terminates when a rapid pressure pulse appears due to localized explosion behind the

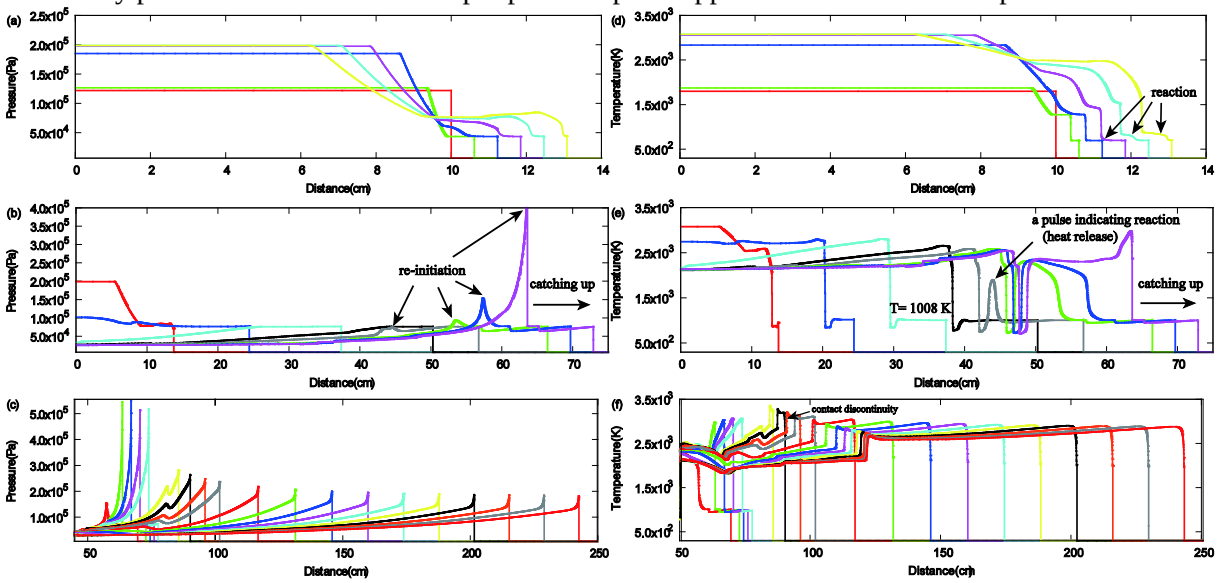
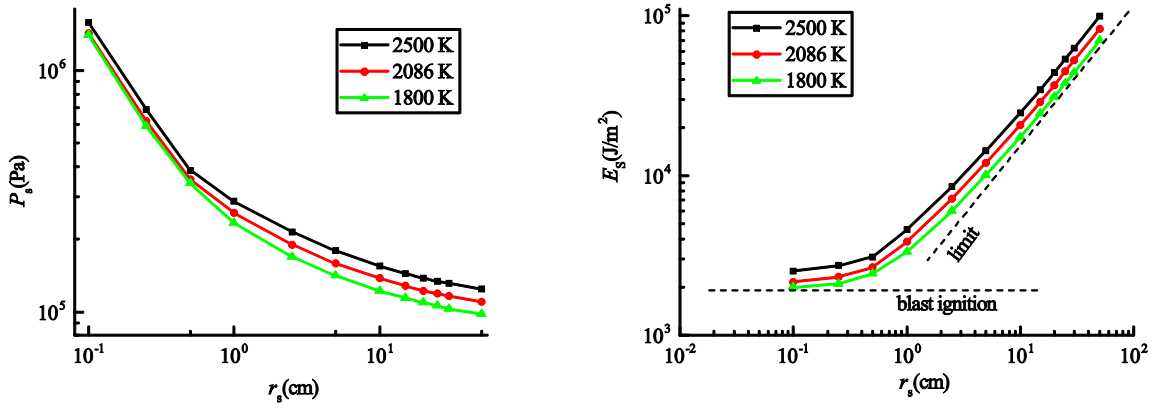


Figure 4. Pressure and temperature profiles for a critical case with r_s=10 cm, p_s=122 kPa and T_s=1800 K.

shock front. After the rarefaction wave reaching the pre-shocked gas, the localized explosion is formed when a hot spot resulting from hydrodynamic instabilities is induced in pre-shocked reactants near its auto-ignition temperature. Then the reaction front (or pressure pulse) abruptly re-accelerates to a high speed and eventually merges with the leading front to form an overdriven detonation which asymptotically decays to a self-sustained CJ detonation wave after a large distance.

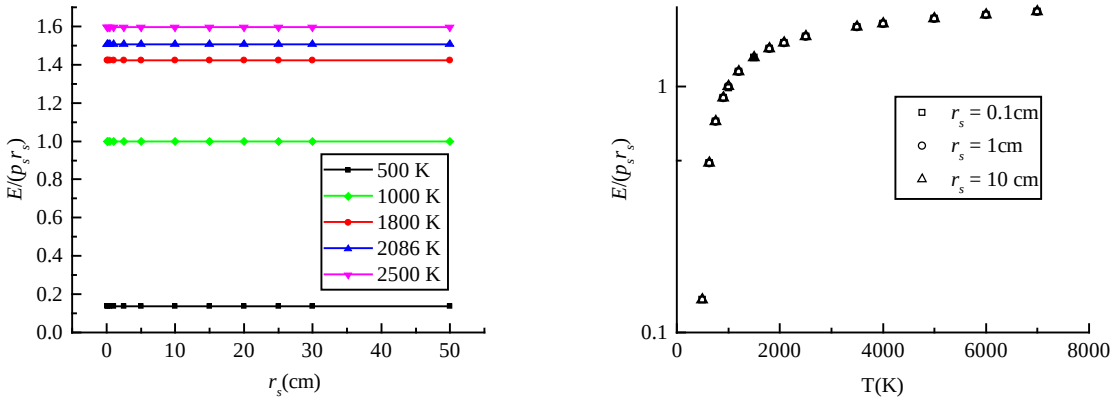


(a) (b)

Figure 5. Critical pressure and critical internal energy for the detonation ignition, (a) critical pressure, (b) critical internal energy

Figure 5 shows the critical pressure and critical internal energy as a function of distance for the detonation ignition in the present study. For cases with a constant given temperature, the shorter the driver length is, the larger the initial pressure (or equivalently the energy density) is required. This is due to the fact that the rarefaction wave originating from the interface plays a key factor to the subsequent initiation. By decreasing the driver length, the time of the rarefaction wave reflecting from the rear boundary and

pursing after the front is decreased accordingly. However, less internal energy in the energy source is needed to initiate a detonation, which can be observed in Figure 4(b). When r_s is larger than 10 cm, the critical internal energy used is proportional with the length of the energy source, which suggests that the portion of internal energy used to initiate a detonation remain the same for cases where the energy source length is large. As the driver length decreasc to zero, the critical internal energy needed asymptotically approach a constant value, indicating a blast initiation. It can also be concluded that the energy used to directly initiate a detonation in the case of blast initiation is dramatically less than that in the case of homogenous thermal explosion with large driver length.



(a) (b)

Figure 6. Non-dimensional critical internal energy in the energy source, (a) as a fuction of r_s , (b) as a fuction of T

In order to find a universal parameter to describe the initiation of detonation, a scaled critical energy $E/p_s r_s$ is used as shown in Figure 6, it is found in Figure 6(a) that the scaled critical energy keeps constant despite the change in the length of the energy source r_s. It suggests that the length scale effect of r_s can be ignored in the detonation initiation process using the homogenous explosion model in the present study. However, the initial temperature of the energy source, does have a significant effect on the scaled critical energy. As shown in Figure 6(b), the scaled critical energy increases as the initial temperature increases. However, when the initial temperature increases above about 3000 K, the increase rate of critical energy is dramatically reduced. It appears that the scaled critical energy asymptotically approaches a constant value with the increase of the initial temperature.

4 Conclusions

The detonation ignition process through a uniform energy source with stoichiometric hydrogen/oxygen diluted by 70% Argon has been systematically studied in the present study. According to the driver length and initial thermodynamic parameters, three different regimes of detonation initiation were found in the present study, namely supercritical, critical, and subcritical regimes. The initiation process is essentially a Riemann problem (shock tube problem) nonlinearly coupled with a constant-volume explosion. Depending on the auto-ignition delay time, the above two processes can be decoupled roughly. The critical internal energy in the energy source used to initiate a detonation is also analyzed. It was found that, with a short driver length, the detonation initiation process corresponds to a blast ignition process, and the critical internal energy keeps constant as the driver length decreases below a critical value. In contrast, for cases with a large driver length, the critical internal energy is proportional to the driver length. In addition, the

energy of different initial temperature at same energy source was studied. It is found that the scaled critical energy is independent of the energy source length, indicating no length scale effect is involved in the detonation initiation process with the present model. However, the scaled critical energy heavily affected by the initial temperature. The scaled critical energy $E/p_s r_s$ is found to be approximately around 1 within a wide range where the initial temperature is above the auto ignition temperature (about 1000 K). In this study we do not consider the multidemional affect for the initiation of detonation, so it is different from actual behavior in the critical condition, we will consider this factor in the future.

Acknowledgments

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