Analyses of Direct Detonation Initiation with Multi-Step Finite-Rate Chemistry

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Abstract

The present paper reports high-fidelity simulation of direct detonation initiation processes by depositing concentrated energy into an unconfined H_2-O_2-Ar mixture. The goal is to understand the underpinning mechanisms in failed or successful detonation initiation processes. We employed the Space-Time CESE method to solve the reacting flow equations. The chemistry model is composed of nine species and twenty-four reaction steps. Results of simulated sub-critical, critical, and supercritical detonation initiation process are reported. Competing terms in the temperature-reaction-zone equation are analyzed. We found that the unsteadiness play a critical role in the direct detonation initiation process.

1. Introduction

In the direct initiation of a detonation, a large amount of energy is instantaneously deposited to a small region of unconfined combustible mixture. Immediately, a strong blast wave is generated. This spherical shock wave expands and decays while it continues heating the gas mixture. Due to shock heating, chemical reactions occur and chemical energy is released. Under suitable conditions, detonation is initiated. The blast wave generated by igniter plays an important role because it produces the critical states for the onset of the detonation. Therefore, it is often referred to as the blast initiation.

Zeldovich et al. [1] studied the direct detonation initiation process, and they pointed out that the amount of the deposited energy is the key parameter controlling the initiation process. Bach et al. [2] reported theoretical and experimental results of spherical detonation waves, initiated by a laser-induced spark. Depending on the magnitude of the deposited energy, they classified three different regimes of the initiation processes: (i) the supercritical regime for successful detonation initiation, (ii) the sub-critical regime for failed initiation, and (iii) the critical regime for marginally sustainable detonation initiation.

Many attempts have been made to predict the critical energy for initiating detonation under various circumstances. He and Clavin [3] performed quasi-steady analysis of the direct initiation process. They developed the critical curvature model, which states that the failure mechanism of the detonation is mainly caused by the nonlinear curvature effect of the wave front. Shepherd and coworkers [4] proposed the critical decay rate model, in which they suggested that the critical mechanism of a failed detonation is due to the unsteadiness of the reacting flow. Due to simplicity and

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computational efficiency, numerical analyses for the direct detonation initiation have been based on the use of single-step global reaction models, and the assumption of polytropic gas mixtures. However, in a recent numerical study, Mazaheri [5] showed that the solution of using a single-step model could be misleading. In his calculations, the critical initiation energy does not exist because the decaying blast wave always becomes a detonation. Subsequently, Lee and Higgins [6] suggested that one should abandon the single-step chemistry model and adopt realistic finite-rate chemistry models composed of multiple species and multiple reaction steps to capture the essential features of the direct detonation initiation processes.

In this paper, we focus on direct initiation of cylindrical detonation in an $2H_2+O_2+7Ar$ mixture. A finite-rate model of twenty-four reaction steps and nine species is adopted. Three values of initiation energy are used to simulate the supercritical, the sub-critical, and the critical processes.

2. Detonation Initiation

The initial conditions are taken from reference [3]. A specific amount of energy in the form of high temperature and high pressure is deposited instantaneously to the driver section (denoted by a subscript *s*) of a reactive gas mixture. On the other hand, low temperature and pressure are set for the driven section, denoted by a subscript 0:

$$\begin{aligned} \text{If } 0 \le r < r_s, \quad & p = p_s, T = T_s, y_i = y_s, u = u_s, \\ r \ge r_s, \quad & p = p_0, T = T_0, y_i = y_i, u = u_0 \end{aligned} \tag{1}$$

Refer to Fig. 1. The radius of the driver section r_s is about 15 times smaller than the critical radius R_c. Inside the driver section, pressure is set about 15-20 times higher than the peak values of the corresponding C-J detonation. The initial condition provides a strong cylindrical blast wave, expanding into the driven section. The pressure and temperature of the driven section are 0.2 atm and 298K, respectively. The deposited energy E_s is calculated based on the internal energy equation for a perfect gas:

$$\begin{aligned} E_s &= \sigma_j r_s^{j+1} p_s / (\gamma - 1) \\ \sigma_j &= [2j\pi + (j-1)(j-2)]/(j+1) \end{aligned} \tag{2}$$

Several values of E_s are selected in the present calculations: E_s = 33.9, 43.0, 53.0, and 76.3 J/cm, corresponding to the initiation radius r_s= 0.4, 0.45, 0.5, and 0.6 cm, respectively. Pressure at the driver section, p_s, is *200* atm for all calculations.

3. Results and Discussions

In the sub-critical regime, the deposited energy is below the critical value, and the reaction front is always decoupled from the leading shock wave. In the critical regime, the deposited energy is very close to the critical value. Initially, the blast wave continuously decays such that the maximum pressure would become lower than the CJ values, and the detonation is seemingly fizzling out. Suddenly, local explosions occur in the reaction zone, and a strongly overdriven detonation wave is suddenly developed. After violent instabilities, the detonation asymptotically approaches the CJ condition. In the supercritical regime, the initiation energy exceeds the critical value. The shock

wave is always attached to the reaction front. The overdriven detonation decays continuously to become a self–sustained CJ detonation with minor instabilities.

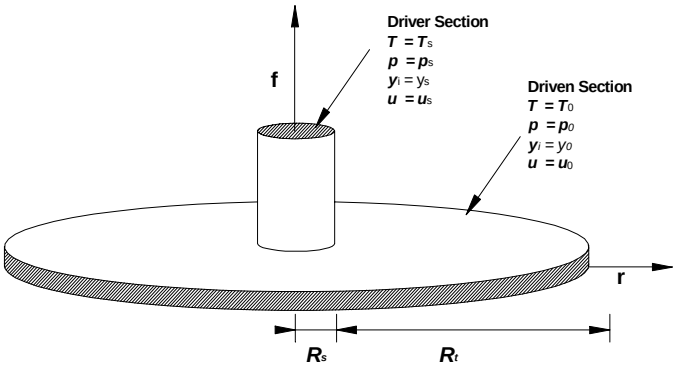

Fig. 1: A schematic of the initial condition of the direct detonation initiation process.

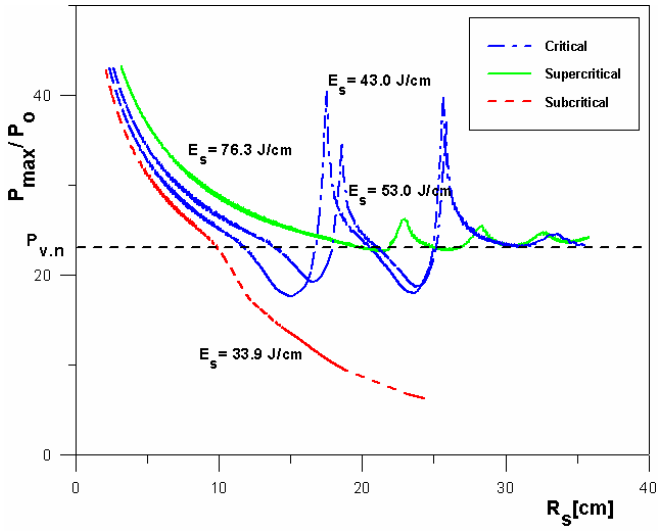

Fig. 2: Maximum pressures as a function of radius in three direct detonation initiation regimes in a $H_2 + O_2 + 7Ar$ mixture.

Figure 2 shows the numerical simulation of three regimes of direct initiation according to different initiation energy. The ratio of local maximum pressure to initial reactant pressure is plotted as a function of the radial locations of the leading shock wave. For reference, the pressure of the von Neuman spike of the corresponding self sustained CJ detonation is also plotted by dot line. For E_s = 33.0 *J/cm*, the strong blast wave decays to a wave with peak pressures much lower than the CJ value, indicating a failed detonation initiation. E_s = *43.0* and 53.0 *J/cm* are in the critical regime and distinct pressure peaks can be observed. The instability ends around R = 30 *cm*, and the waves become the CJ waves. With higher initiation energy, E_s = 76.3 *J/cm*, the initial blast wave directly initiate the detonation wave, which expands and decays to the CJ detonation. For E_s = 33.0 *J/cm*, Fig. 3 shows the temperature as a function of time of ten fluid particles initially located at different radii. As the flow develops, the leading shock wave comes across the fluid particles one by one. Due to shock heating, particles 1 to 4 rapidly heat up, and the chemical reactions occur. For the fifth to eighth particles, the ignition delay has significantly increased. The last two particles never heat up because the

blast wave becomes too weak. Although not shown, after about 100 μs, particles 1 to 4 decelerate and move backwards. The flow reversing is due to the low-pressure region at the center of the evolving detonation.

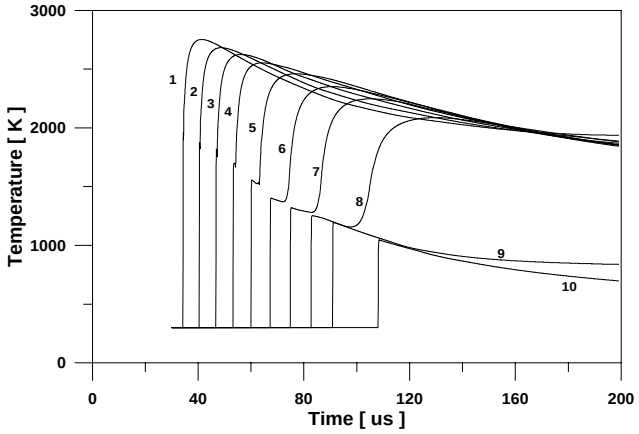

Fig. 3: Temperature histories of fluid particle paths for $E_s = 33.9$ *J/cm*.

4. Concluding Remarks

In the presentation, we will report details of the CESE method, which was employed to calculate the reacting flow equations. In particular, the analyses were based on realistic finite-rate chemistry model in conjunction with comprehensive thermodynamics models for a real detonating mixture. Three detonation initiation regimes were calculated according to the values of the deposited energies, including sub-critical, critical, and supercritical. In the critical regime, numerical results showed instabilities with strong pressure peaks. In the presentation, we will also compare the magnitude of each term in the temperature-reaction-zone equation for the evolving initiation processes. We will show that the unsteadiness plays a critical role in influencing the Lagrangian temperature profiles of fluid particles, and thus the success or failure of the detonation initiation processes.

Reference

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