PDE 응용을 위한 H₂-O₂-Ar 혼합물에서의 직접 기폭 과정에 대한 수치 해석

임경수*, 김창기**, 황준식**

Numerical Analysis of Direct Detonation Initiation Processes in a H2-O2-Ar Mixture for Pulse Detonation Engine Applications

Kyoung Su Im*, Chang Kee Kim**, Jun Sik Hwang**

ABSTRACT

The present paper reports high-fidelity simulation of direct initiation processes of cylindrical detonation waves by concentrated energy deposition. 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, including realistic finite-rate chemistry model of the nine species and twenty-four reactions for H₂-O₂-Ar mixtures. Detailed results of sub-critical, critical, and supercritical initiation process are reported.

Key Words : Pulse Detonation Engine, Direct Detonation Initiation, CESE Method

1. INTRODUCTION

In general, there are three experimental methods to initiate detonation: (i) flame initiation, (ii) shock wave initiation, and (iii) direct initiation. In all three cases, shock waves occur prior to detonation initiation. The present paper focuses on the third initiation mode, which is relevant to the detonation initiation process in a PDE.

In the direct initiation mode, 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 (or cylindrical) 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 by sparks. They pointed out that the amount of the deposited energy, or the critical energy, is the key parameter controlling the initiation process. Later on, Bach et al. [2] summarized theoretical and experimental studies of

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* Wayne State University, Detroit, MI, USA
** 국방과학연구소(Agency for Defence Development)

spherical detonation waves initiated by a laser-induced spark. They classified the three different regimes of the initiation processes according to the magnitude of the initiation energy:(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.

Due to simplicity and computational efficiency, numerical analyses for the detonation initiation have been based on the use of (i) single-step irreversible reaction models, and (ii) the assumption of a polytropic gas mixture. However, in order to catch the essential features of real detonation initiation phenomena, Lee and Higgins [3] strongly suggested that one should abandon the single-step chemistry model and adopt real finite rate chemistry models and thermodynamics calculations.

In this paper, we focus on direct initiation of cylindrical detonation in an $H_2/O_2/Ar$ mixture. A finite-rate model of twenty-four reaction steps and nine species is adopted. Various values of initiation energy are used to simulate the supercritical, the sub-critical, and the critical processes. We analyzed the numerical solutions in the reaction zone to study the underpinning physics in the direct initiation processes.

2. MODEL EQUATION

2.1 Reacting Flow Equation

The governing equations for the numerical simulation are the one-dimensional multi-species reactive Euler equations of N_s species:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial r} = G(U) + S(U) \qquad (2.1)$$

where

$$U = (\rho, \rho u, \rho E, \rho_1, \rho_2, ..., \rho_{N_s-1})^T$$

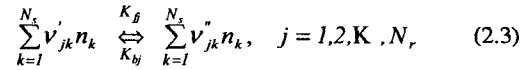$$F = (\rho u, \rho u^2 + p, (\rho E + p)u, \rho_1 u, \rho_2 u, ..., \rho_{N_s-1} u)^T$$

$$G = -\frac{j}{r}(\rho u, \rho u^2.(\rho E + p)u, \rho_1 u, \rho_2, ..., \rho_{N_s-1} u)^T$$

$$S = (0,0,0, \dot{\omega}_1, \dot{\omega}_2, ..., \dot{\omega}_{N_s-1})^T \qquad (2.2)$$

ρ, u, p, E, and ρ_k are density, velocity, specific total energy, and mass concentration of species k, respectively. $j = 0, 1, 2$ for planar, cylindrical, and spherical flows, respectively.

$\dot{\omega}_k$ is the net molar production rate of species k and can also be expressed as $\dot{\omega}_k = \rho \Omega_k / W_k$

According to the law of mass action, the stoichiometric equation of a set of N_r elementary reactions involving N_s species can be written in the following form

$$\sum_{k=1}^{N_s} v'_{jk} n_k \underset{K_{bj}}{\overset{K_{fj}}{\Longleftrightarrow}} \sum_{k=1}^{N_s} v''_{jk} n_k, \quad j = 1,2,K,N_r \qquad (2.3)$$

where $n_k = \rho_k / W_k$ is the mole concentration of species k in the gas mixture. v'_{jk} and v''_{jk} are respectively the stoichiometric coefficients of the reactants and products of species k in the jth reaction. The source terms, $\dot{\omega}_k$ for k=1,2,3,..,Ns-1, in the species equations, Eq. (2.2), are formulated in mass concentration, and they are the summation of the net rate of change of species k from all chemical reactions involved, i.e.,

$$\dot{\omega}_k = W_k \sum_{j=1}^{N_r} (\dot{\omega}_k)_j \qquad (2.4)$$

where W_k is the molecular weight of species and $(\dot{\omega}_k)_j$ is the rate change of concentration of species k by the reaction j, given by

$$(\dot{\omega}_k)_j = (v''_{jk} - v'_{jk})\left(K_{f_j} \prod_{l=1}^{N_s} n_l^{v'_{jl}} - K_{b_j} \prod_{l=1}^{N_s} n_l^{v''_{jl}}\right) \qquad (2.5)$$

2.2 Initial and Boundary Condition

The initial conditions are taken from reference [4]. A specific amount of energy, E_s, in the form of high

temperature and high pressure (with a subscript s) is deposited instantaneously into the driver section of a reactive gas mixture. On the other hand, low temperature and pressure are set for the driven section.

If $0 \le r < r_s$, $p = p_s, T = T_s, y_i = y_s, u = u_s$,

$$r \ge r_s, \quad p = p_0, T = T_0, y_i = y_i, u = u_0 \qquad (2.6)$$

Refer to Fig. 1. The radius of the driver section r_s is about 15 times smaller than the critical radius R_c [4]. Inside the driver section, pressure is set about 15-20 times higher than the peak values of the corresponding C-J detonation. Essentially, the initial condition provides a strong cylindrical expanding blast wave to be expanded in the radial direction. The species compositions at both sides are H_2+O_2+7Ar. The pressure and temperature of the driven section are 0.2 atm and 298K, respectively. Several values of E_s are selected in the present calculations: E_s = 33.0, 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 set 200 atm for all calculations.

Two boundary conditions are used in the calculation. At r=0, the boundary conditions are derived based on a limiting form of Eqn. (2.2) when r approaching null. At r=∞, the standard non-reflecting boundary conditions are employed.

3. NUMERICAL METHOD

The space-time Conservation Element Solution Element (CESE) method, originally proposed by Chang [5] has been extended for chemical reacting flows with realistic finite-rate chemistry models. The CESE method is distinguished by the simplicity of its design principle, i.e., treating space and time as one entity in calculating flux conservation.
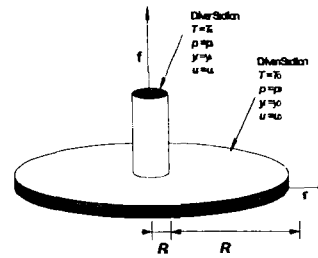

Fig. 1 A schematic of the initial condition of the direct detonation initiation process

4. RESULTS AND DISCUSSION

Fig. 2 shows the numerical simulation of three regimes of direct initiation according to different initiation energy. In a series of calculations by incrementally increasing the values of the deposited initiation energy, we can clearly observe the three regimes.

When the initial energy 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 process. Two initial energies of E_s = 43.0 J/cm and E_s = 53.0 J/cm are in the critical regime. Distinct pressure peaks are observed. The deposited initiation energies are not high enough to sustain stable detonation waves. This unstable period ends at R = 30cm, and the waves become the self-sustained CJ detonation waves. With higher initiation energy for E_s = 76.3 J/cm, the initial blast wave directly initiate the detonation wave, which expands and decays to the CJ value with mild instabilities.

Fig. 3 shows the spatial pressure profiles for E_s = 33.0 J/cm and E_s = 43.0 J/cm. In Fig. 3(a), initially, strong pressure continuously decays to be below the von Neumann pressure. At R = 13 cm, the shock wave is decoupled from the reaction front. After this separation, chemical reaction

disappears and the detonation initiation fails.

In Fig. 3(b), the initial development of the reactive wave is similar to that of Fig. 3(a). However, at R= 16 cm, pressure pulse occurs in the reaction zone, and the reactive wave becomes unstable overdriven detonation. Intermittently, the pressure peaks of this overdriven detonation wave decay to sub CJ values. As time evolves, it gradually converges to the CJ detonation, indicating a successful initiation process.

6. CONCLUSION

The numerical simulations of the direct initiation process of cylindrical detonation for a H_2-O_2-Ar mixture have been conducted using the space-time CESE method. Calculation has been done based on the use of realistic finite-rate chemistry models and comprehensive thermodynamics models. The three detonation initiation regimes were calculated according to the values of the deposited energy in the initial conditions, including sub-critical, critical, and supercritical. In the critical regime, the present result showed flow instabilities with strong pressure peaks.

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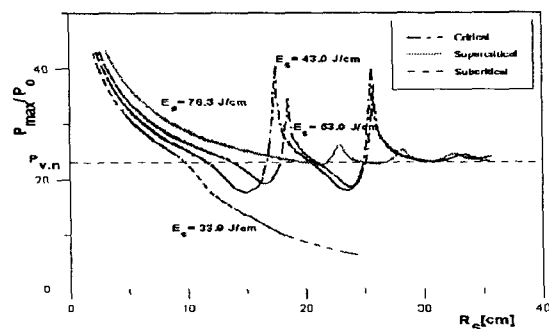
Fig. 2 The spatial histories of local maximum pressures in the three regimes of direct initiation processes of a cylindrical detonation in a H_2 + O_2 + 7Ar mixture.
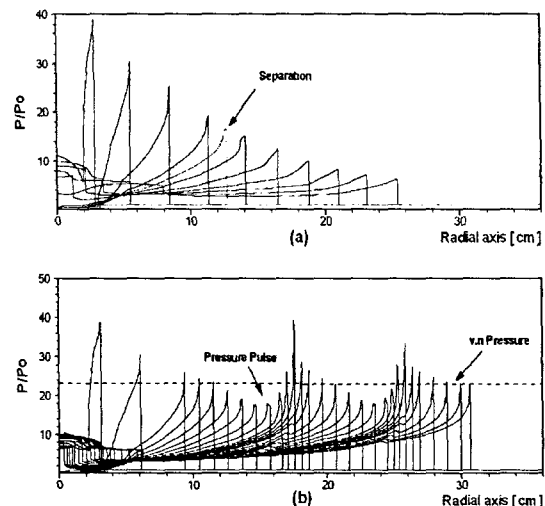

Fig. 3 Spatial pressure profiles for the failed and successful initiation processes. (a) E_s = 33.9 J/cm, and (b) E_s = 43.0 J/cm.