Numerical Simulation on Propagating Process of H_2/O_2 Cylindrical Detonation with Detailed Reaction Model

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1 Introduction

Detonation is a supersonic combustion wave propagating with a leading shock wave and flame front in reactive mixture. It has been studied for safety engineering such as fuel explosions or for scientific interests such as star explosions. These days, detonation is expected to provide a new aerospace propulsion system which has a high-impulse and high-efficiency characteristics. However, despite many studies on detonation, the basic physical phenomena of spherical detonation are not clear.

The spherical detonation occurs by a direct initiation which generates the detonation instantaneously. When a large amount of energy is released in a small region of the reactive mixture gas, a shock wave expanding spherically is generated while it couples with a reaction surface. The shock wave reaches an overdriven state after the initial ignition. The critical energy to initiate the detonation has been investigated by many researchers. Zel'dovich *et al.* [1] reported a theory of the critical energy based on the experimental observations which is defined by the relationship between the time in which the shock wave decays to CJ state and the characteristic time of the chemical reaction. This theory, which explained the concept of a detonation kernel was developed by Lee *et al.* [2], [3]. After these studies, many experimental studies were conducted to understand the phenomena of spherical detonation. However, there is limited information on the detailed propagation mechanism of the curved detonation by experimental studies. Therefore, numerical study is nessesary to understand such mechanism. He *et al.* [4] showed the curvature effect and the critical radius using the quasi-one-dimensional steady analysis. As the recent numerical studies, Eckett *et al.* [5] who used a one-step reaction model on the one-dimensional coordinate system demonstrated that the unsteadiness of the induction zone was dominant in the failure of spherical detonation. Watt *et al.* [6] performed one- and two-dimensional simulations of the spherical and cylindrical detonations in order to determine the cellular stability. They indicated that the cellular structure depends on the grid resolution and it becomes irregular on the higher grid resolution. Nirasawa and Matsuo [7], [8] showed that the grid resolution does not affect the critical energy and that the numerical disturbance due to orthogonal grid increases the all cellular size further in comparison with that due to the circular grid.

Our future goal is to clarify the propagation mechanism of the three-dimensional spherical detonation at the critical and supercritical conditions. However, in this paper, the propagating process of the cylindrical detonation is investigated numerically using one- and two-dimensional simulations.

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2 Numerical Method and conditions

The governing equations are the compressible Euler equations with a chemically reacting gas system in a one-dimensional cylindrical coordinate system and a two-dimensional Cartesian coordinate system. The reaction source terms are treated in a linearly point-implicit manner in order to avoid a stiff problem. A second-order Harten-Yee non-MUSCL type TVD scheme is used for the reaction source terms. The averaged state on a computational cell boundary is given by the generalized Roe's average to evaluate the numerical flux in the convective terms.

In the present simulation, a Petersen and Hanson model, containing 8 species (H_2, O_2, H, O, OH, HO_2, H_2O_2 and H_2O) and 18 elementary reactions, is used as the chemical reaction mechanism to solve a cylindrical detonation problem. This model includes the pressure dependence on a forward reaction coefficient with third body collisions of H_2O_2 decomposition and recombination reactions. The present simulation neglects viscous effects such as turbulence and boundary layer interactions. Local vortices or scales may be affected by the viscous effects, however, the largest scales generated by the shock wave should not be affected by neglecting viscosity.

The initial condition is separated into two computational regions; one near the center of the cylinder with the source energy and another with the ambient values. The pressure and temperature of source energy region are 10 MPa and 2000 K, respectively. The initial energy depends on the radius of the source energy region, which is defined by a radius of the source, r_s. The pressure and temperature of the ambient region are 0.1 MPa and 300 K, respectively. The gas in both regions consists of a stoichiometric(ϕ= 1) H_2/O_2 mixture gas.

For the one-dimensional case, the grid size, Δx, is 1.0 μm, which corresponds to the resolution of 42 grid points in the half reaction length, $L_{1/2}$. The half reaction length is defined as the distance from the shock wave to the place where the mass fraction of hydrogen is equal to the average of the free stream value and the equilibrium steady state value. In this ambient condition, $L_{1/2}$, is 41.8 μm.

For the two-dimensional case, Δx is 2.5, 5.0, or 10.0 μm to estimate the influence of the grid resolution, which corresponds to 16, 8, or 4 points/$L_{1/2}$, respectively. The present grids for Δx = 2.5 and 5.0 μm are 2401x2401 of the orthogonal system. The grids for Δx = 10.0 μm are 1201x1201 of the orthogonal systems. The boundary conditions at the x and y axes are treated as symmetry and the upper and right sides of boundaries are treated as outlet.

3 Results and Discussions

The initiation energy to start detonation has been investigated from the viewpoint of grid resolution. The initiation energy depends on r_s. Figure 1 shows the time histories of the detonation velocity and shock pressure for various r_s. r_s is 100, 300, 500, or 700 μm. The detonation velocity and shock pressure are normalized by the CJ velocity (D_{CJ} = 2841.8 m/s) and upstream pressure, respectively. The gray lines in Fig. 1 (a) and (b) denote the CJ velocity and the pressure at von Neumann spike (P_{vN} = 3.3 MPa). The one-dimensional cylindrical detonation oscillates around the CJ detonation state and does not continue to propagate at any initial condition. The maximum velocity in Fig. 1 (a) is about $1.6D_{CJ}$ and the maximum pressure in Fig. 1 (b) is about $128P_0$. The velocity for r_s = 100 μm decelerates immediately after the initial ignition. It is found that cylindrical detonation is not initiated for this condition. The velocity for $r_s \geq$ 300 μm reaches the overdriven state quickly and starts to oscillate. The velocity for r_s = 700 μm continues to oscillate around D_{CJ}. The shock pressure to oscillate around P_{vN} is also observed. It is concluded that one-dimensional cylindrical detonation can propagate if r_s is over 700 μm at this initial condition. Hence, r_s for two-dimensional simulation is adjusted to 700 μm which corresponds to $16L_{1/2}$.

The influence of the grid resolution on the detonation structure is estimated using two-dimensional simulation. Figure 2 shows the maximum pressure histories for Δx = 2.5, 5.0, and 10.0 μm. The pressure range is between 2.5 and 5.0 MPa. The white lines denote the triple point trajectories. The cell patterns are observed clearly for Δx = 2.5 and 5.0 μm. On the other hand, the cellular structure does not appear for Δx = 10.0 μm because the peak pressure decreases due to the numerical viscosity by the large grid size. Therefore the present study on the two-dimensional cylindrical detonation with the detailed cellular structure requires a grid size finer than 5.0 μm.

The influence of the initiation energy on the cylindrical detonation is investigated two-dimensionally. Figure 3 shows the maximum pressure histories for Δx = 5.0 μm and (a) r_s = 500, (b) 700 and (c) 900 μm. The small cells appear just after the initiation of detonation to increase as time passes. The grid alignment affects the cell size because the cells propagating along the diagonal direction are larger than those along the horizontal or vertical direction in Figs. 3 (a) and 4. For the relation between the initiation energies and the mean pressure, when the initiation energy becomes large, the mean pressure increases. Figure 4 shows the maximum pressure history, the shock pressures, and the shock velocity profiles for Δx = 4.2 μm and r_s = 672 μm. The red line in Fig.4 (a) denotes the pressure or velocity along the *x* or *y*-axis. The blue line in this figure denotes those along the direction of 45 degrees from the *x*-axis. The peaks of the profiles indicate the cell boundaries. The cell length along the direction of 45 degrees from the *x*-axis is longer than that along the *x* or *y*-axis. It might be affected by the difference between the grid density and the grid alignment.

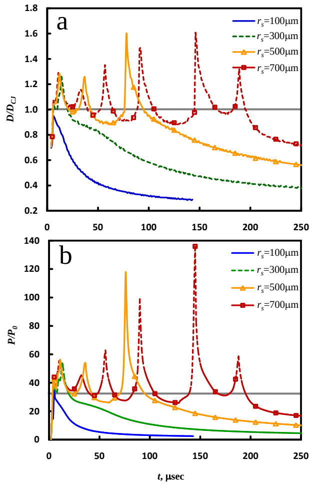

Figure 1. Time history of (a) velocity and (b) pressure.

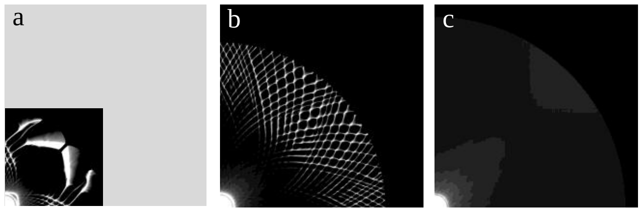

Figure 2. Maximum pressure histories in the case of r_s = 700 μm. The grid sizes are (a) 2.5μm, (b) 5.0μm, and (c) 10.0μm for each case.

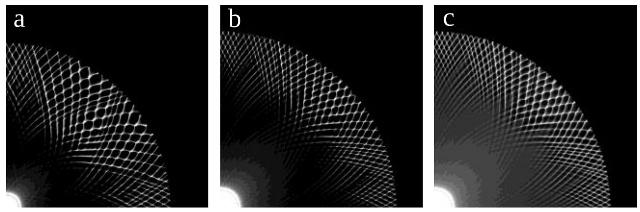

Figure 3. Maximum pressure histories for Δx = 5.0 μm in the case of (a) r_s = 500 μm, (b) r_s = 700 μm, and (c) r_s = 900 μm.

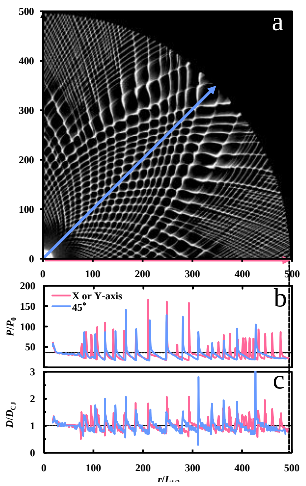

Figure 4. Maximum (a) pressure, (b) pressure and (c) velocity histories r_s = 672 μm and Δx = 4.2 μm.

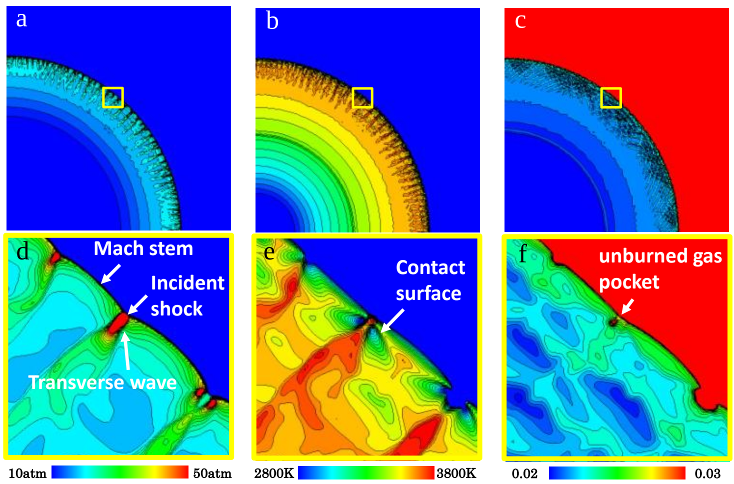

Figure 5. Contours near the detonation front for r_s = 700 μm and Δx = 5.0 μm. (a)pressure, (b)temperature and (c)H_2 mass fraction distribution.

Figures 5 show the instantaneous contours of pressure, temperature, and H_2 mass fraction for r_s = 700 μm. The present shock structure in the detonation is similar to that in a constant channel [9] . In this case, the present cylindrical detonation has the double Mach reflection where the comlex Mach reflection does not appear. An unburned gas pocket is observed near the detonation front in Fig. 5 (f). The local pressure of the cylindrical detonation wave is lower than that of the detonation propagating in a constant channel because the detonation wave expands two-dimensionally in the cylindrical detonation. The strong circulation is observed along the diagonal direction because of the grid alignment effect.

5 Conclusions

The cylindrical detonation with the cellular structure by the direct initiation was simulated one- and two-dimensionally with the detailed chemical reaction model in the stoichiometric H_2/O_2 gas mixture. As a result of the grid resolution study in the two-dimensional simulation, the grid size in the cylindrical detonation in a stoichiometric H_2/O_2 gas mixture is finer than 5.0 μm when the pressure and temperature of the ambient region are 0.1 MPa and 300 K, respectively. For the influences of the initiation energy, the higher initiation energy gives the smaller cell size. However, the cells propagating along the diagonal direction are affected by the numerical dissipation in the orthogonal grid system.

Acknowledgments

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