Research paper

# Numerical study on propagation of cylindrical detonation

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## Abstract

Cylindrical detonation has been investigated numerically with a one-step reaction model to understand its propagation mechanism and the critical energy. This reaction model describes a change in physical values on reaction process to be simple. On the other hand, a detailed chemical reaction model consists of a lot of elementary reactions to deal with the detailed dynamics of heat release. In this paper, the propagating process of the cylindrical detonation with the detailed chemical reaction model is discussed. According to the grid resolution study in two-dimensional simulation, the required grid size to resolve of the cellular structure in a stoichiometric $H_2/O_2$ gas mixture is finer than 5.0 mm when the pressure and temperature of the ambient region are1atm and 300K. Furthermore, as for the relation between their cell sizes and the initiation energies, the cell size becomes smaller as the initiation energy increases. However, the cells propagating along the diagonal direction are affected by the numerical dissipation on the orthogonal grid system.

***Keywords*** : Cylindrical detonation, Spherical detonation,Stoichiometric $H_2/O_2$ gas mixture, Ignition energy, Detailed chemical reaction model

## 1. Introduction

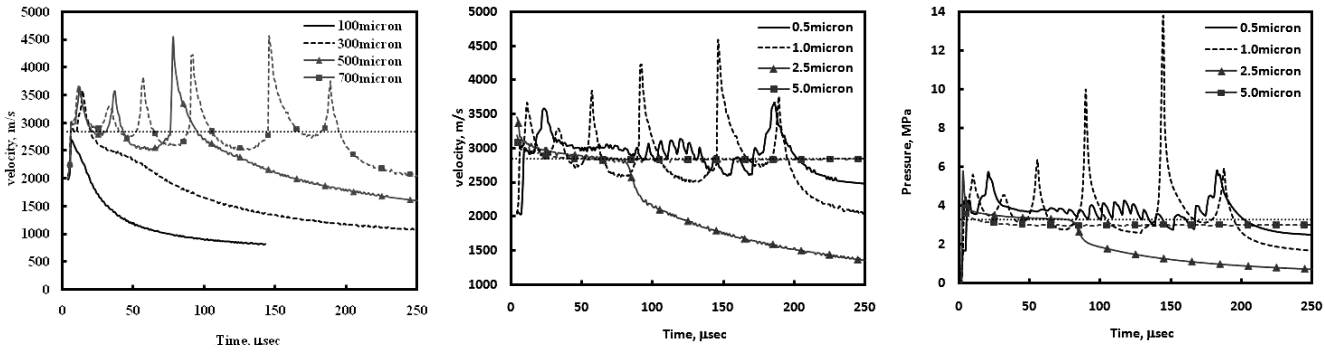
Detonation has been studied from the safety engineering points of view such as fuel explosions or from the scientific interests such as star explosions. These days, detonation is expected to provide a new aerospace propulsion system which has a high-impulse and high-efficiency characteristics. However, despite of many studies on detonation, cylindrical and spherical detonation has not been made clear much in their structure using experimental and numerical studies.

The cylindrical detonation is occurred by a direct initiation which gives a detonation instantly. The direct initiation provides a high-energy source and generates a strong shock wave. The previous experimental studies[1)2)] revealed that there is a critical energy to initiate detonation. While the recent numerical studies[3)-5)] have been performed on critical energy using one- and two-dimensional simulations with a one-step reaction model. Recently Nirasawa and Matsuo[6)7)] showed that the grid resolution does not affect the critical energy and the numerical disturbance in an orthogonal grid increases the cell size of detonation further in the comparison with that in a circular grid.

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

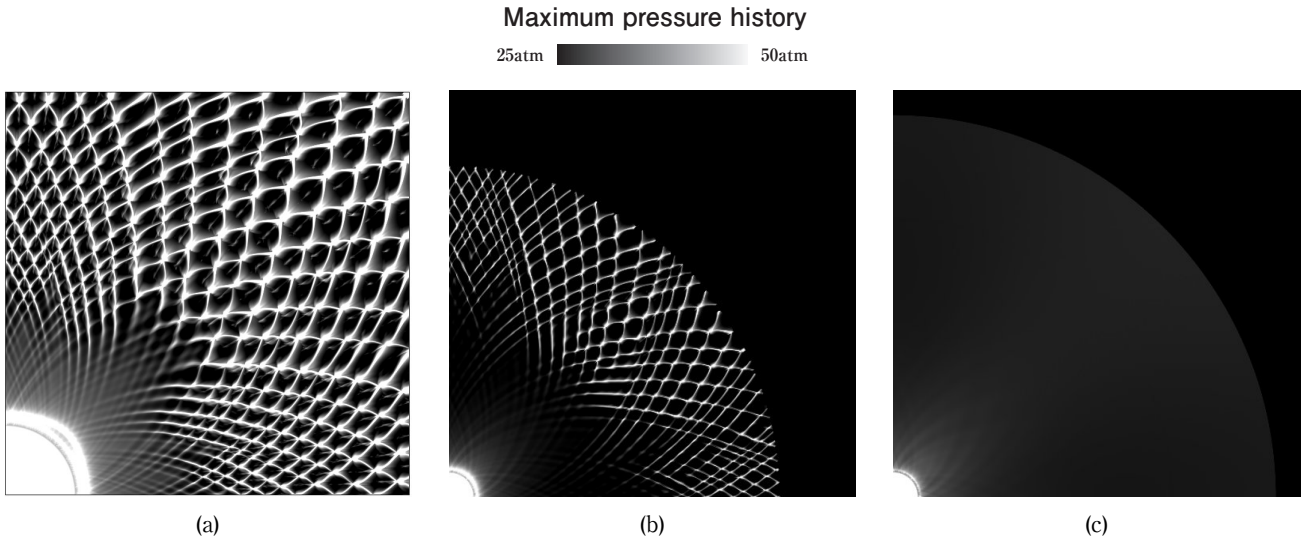
## 2. Numerical Method and Conditions

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. For the convective term, the numerical scheme is a second-order Harten-Yee non-MUSCL type TVD scheme. For the chemical reaction, a Petersen and Hanson model containing8species




(a) Detonation velocity for various $r_s$ (b) Detonation velocity for various $\Delta x$ (c) Shock pressure for various $\Delta x$

**Fig. 1** Time history of detonation velocity and shock pressure. $\Delta x$=1.0μm in Fig.1(a) and $r_s$=700μm in Fig.1(b) and (c).




(a) (b) (c)

**Fig. 2** Maximum pressure histories in the case of $r_s$=700μm. The grid sizes are (a) 2.5μm, (b) 5.0μm, and (c) 10.0μm for each case. The range of pressure is between 25 and 50atm.

($H_2$, $O_2$, H, O, OH, $HO_2$, $H_2O_2$ and $H_2O$) and 18 elementary reactions is used 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 initial conditions are separated into two computational regions ; one near the center of the cylinder with a high−energy and another with the ambient values. The pressure and temperature of high−energy region are 100 atm and 2000K, respectively. The initial energy depends on the radius of the high−energy region, which is defined by radius, $r_s$. The pressure and temperature of the ambient region are1atm and 300K, respectively. The gas in both regions consists of a stoichiometric $H_2/O_2$ gas mixture.

For the one−dimensional case, the grid size, $\Delta x$ is 1.0μm, which corresponds to the resolution of 41 grid points in the half reaction length, $L_{1/2}$. The half reaction length is defined as the distance from the shock wave to where the hydrogen mass fraction is equal to the average of the free stream value and the equilibrium steady state value.

For the two−dimensional case, $\Delta x$ is 2.5, 5.0, and 10.0μm to estimate the influence of the grid resolution. The present grid for $\Delta x$=2.5 and 5.0μm are 2401 x 2401 and that for $\Delta x$=10.0μm are 1201 x 1201.

## 3. Results and Discussions

### 3.1 One−dimensional simulations

The initiation energy to lead detonation has been investigated from the viewpoint of grid resolution, which depends on $r_s$. Figure1(a) shows the time histories of the detonation velocity for various $r_s$ which are 100, 300, 500, and 700μm. The dotted−line A−A' in Fig.1(a) denotes the CJ velocity ($D_{CJ}$=2841.8m/s). The velocity for $r_s$ =100μm decelerates immediately after the initial ignition. The velocity for $r_s \geq$300μm becomes quickly the overdriven state and observed the oscillation which implies the characteristics of a one−dimensional cylindrical detonation. The velocity for $r_s$ =700μm continues to oscillate around $D_{CJ}$ for sufficient time. This is a characteristic of the one−dimensional detonation in Cartesian coordinate. It is found that the one−dimensional detonation in Cylindrical coordinate for $r_s$ = 700μm can propagate. Therefore $r_s$ for two−dimensional simulation is adjusted to 700μm which corresponds to 16.7 $L_{1/2}$.

Figure1(b) shows the time histories of the detonation velocity. Figure1(c) shows the time histories of shock pressure for $\Delta x$=0.5, 1.0, 2.5, and 5.0μm. The dotted−line B−B' in Fig.1(c) denotes the pressure at the von Neumann spike at CJ state ($P_{vN}$=3.3MPa). Regardless of the grid size, the one−dimensional cylindrical detonation initiates immedi-

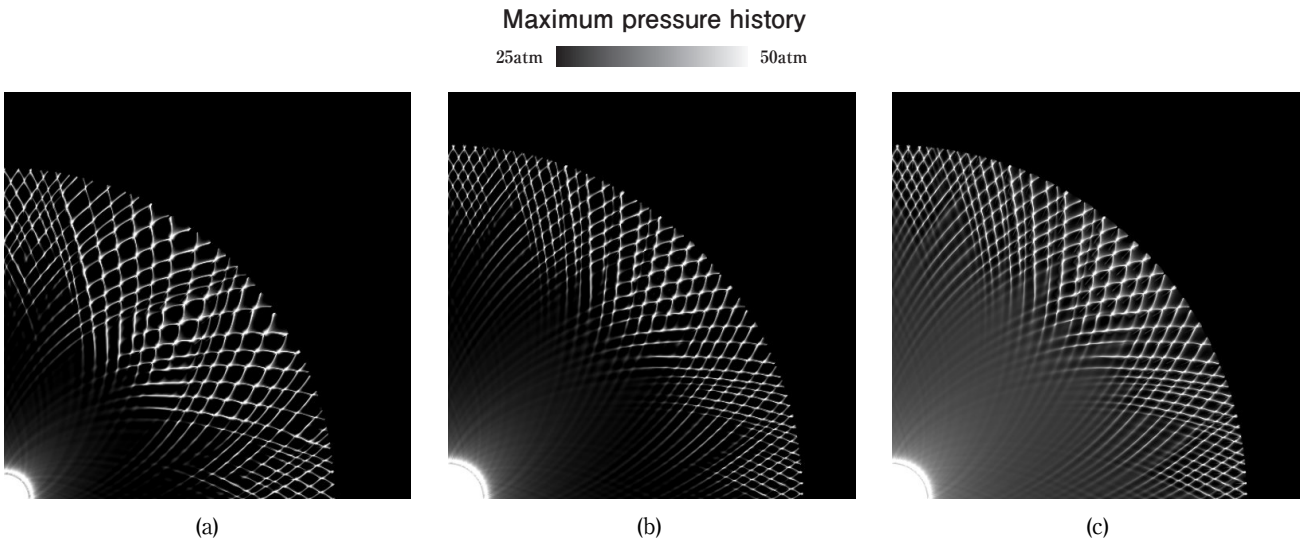



**Fig. 3** Maximum pressure histories for $\Delta x$=5.0μm in the case of (a) $r_s$=500μm, (b) $r_s$=700μm, and (c) $r_s$=900μm. The range of pressure is between 25 and 50atm. The white lines denote the tracks of triple points.

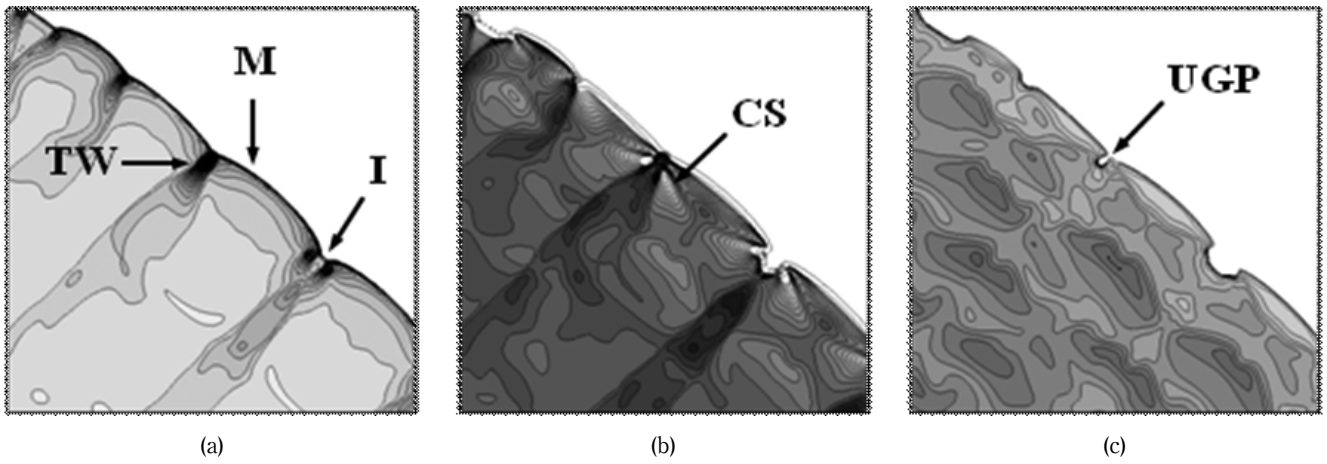



**Fig. 4** Contours near the detonation front for $r_s$=700μm and $\Delta x$=5.0μm. (a)pressure, (b)temperature and (c)$H_2$ mass fraction distribution. The gray regions in Fig.4(a) and (b) and the white regions in Fig.4(c) denote high values. I : incident shock, M : Mach stem, TW : transverse wave, CS : contact surface, and UGP : unburned gas pocket.

ately after the ignition. However, the velocity and pressure profiles do not oscillate for $\Delta x$=5.0μm due to a numerical viscosity. It is found that the grid size needs to be the finer than 1.0μm case to resolve the cyclic oscillation of the velocity in one−dimensional cylindrical detonation.

## 3.2 Two−dimensional simulations

### 3.2.1 Influence of grid size

The grid size is preferred to be coarse to reduce the computational cost. Therefore, the influence of the grid resolution on the detonation structure is estimated. Figure 2shows the maximum pressure histories for the grid size of $\Delta x$=2.5, 5.0, and 10.0μm. The pressure range of this figure is between 25 and 50atm. The white lines denote the triple point trace. The cell patterns are observed clearly for the case of $\Delta x$=2.5 and 5.0μm. On the other hand, cellular structure does not appear for 10.0μm due to the numerical viscosity. Therefore the present study on the two −dimensional cylindrical detonation with detailed cellular structure requires a grid size finer than 5.0μm.

### 3.2.2 Influence of initiation energy

The influence of the initiation energy on the cylindrical detonation is investigated two−dimensionally. Figure3 shows the maximum pressure histories for $\Delta x$=5.0μm and $r_s$ varies as 100, 300, 500, and 700μm. The small cells appear just after the initiation of detonation which cell sizes increase. The grid alignment affects the cell size because the cells propagating along the diagonal direction are larger than those along the horizontal or the vertical direction. This feature is also reported by Nirasawa and Matsuo[7]. As for the relation between their cell sizes and the initiation energies, the cell size becomes smaller as the initiation energy increases.

### 3.2.3 Detailed structure of detonation wave

Figure4shows the instantaneous pressure, temperature, and $H_2$ mass fraction contours for $r_s$ =700μm. The present shock structure of the detonation is similar to that in a constant channel[8)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.4(c). 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.

## 4. 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 two−dimensional simulation, the simulation of 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 are1atm and 300K. As 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.

## Acknowledment

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