Numerical Study on Direct Initiation of Cylindrical Detonation in H_2 /O_2 Mixture: Influence of Higher-order Scheme

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1 Introduction

Gaseous detonation is one type of combustion phenomena in premixed gas, and has an aspect of self-sustaining propagation with interacting between shock and combustion waves. Detonations can cause explosion accidents because of its high temperature and high pressure. A lot of studies have been carried out for the safety engineering. After detonations were founds in 1880s, many researchers have been trying to understand the phenomenon or investigate the wave structures by experimental and numerical studies [1] [2].

On March, 2011, an explosion accident occurred at the Fukushima nuclear power plant. It is thought that the detonation occurs in the nuclear power plants. The fuel-cladding Zircaloy is oxidized by high-temperature steam, then it generates hydrogen gas. Hydrogen and atmospheric oxygen react, and the DDT (deflagration-to-detonation transition) occures and the detonation are generated [3]. In order to prevent from such the accident, it is necessary to find out the cause of DDT or direct initiation of detonation in the nuclear power plants.

There has been considerable investigation on DDT and direct initiation of detonation in the nuclear power plants [4]. It is difficult, however, to understand the phenomenon in detail only in the experimental researches because the detonation propagates with supersonic speed. If one would find out the cause of DDT or direct initiation of detonation in the nuclear power plant, large-scale experimental facilities would be essential and it would requires huge cost and time.

Therefore, the numerical researches are necessary to find the feature of DDT and direct initiation of detonation in a premixed hydrogen/oxygen gas mixture. However, the numerical analysis of the detonation should be performed with finer grid and small time step in order to resolve the rapid variation of the physical values in a short time in a narrow area. The detailed chemical reaction mechanics among many chemical species requires high grid resolution and small time step. In order to reduce the computational cost, the reduction of the number of grid points by increasing the grid width is effective. Grid width is one of the important factors involved both in the calculation cost and in the

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numerical accuracy. Numerical accuracy decreases if the grid width is too large, hence it is necessary to know the adequate grid width to preserve the numerical accuracy. If one introduces a scheme with a high spatial resolution, it will be able to increase the grid width while preserving the accuracy. Tsuboi and Hayashi reported that the numerical grid cell size affects the detonation cell size, and that the finer grid produces the large detonation cells [5]. Watt and Sharpe analyzed the direct initiation of detonation with varying grid resolution in the orthoganal grid, and indicated that the regular cellular pattern appears in the case of low resolution, and the irregular cells, which are similar to cellular pattern obtained experimentarlly, are observed in the case of high resolution. If we need the detailed feature like the experimental results, we must use very small grid cells. One of the higher-order accurate schemes is WCNS (Weighted Compact Nonlinear Scheme). WCNS has the following three advantages compared with WENO:(1) various flux splitting method can be used; (2) interpolation of flow variables can be used despite the finite difference formulation; and (3) free-stream and vortex preservation properties are superior on a wavy grid [6].
This study aims to investigate the effect of the grid resolution on the two-dimensional cylindrical detonation by using the recent four higher-order accurate schemes.

2 Numerical Method and Simulation Conditions

The governing equations are the compressible Euler equations with a chemically reacting gas system in a two-dimensional orthgonal coordinate system. The equations considers compressible fluid dymamics and chemical kinetics of multi-component system, and each equations are separately solved in each time step. For the convection terms, AUSMDV scheme [7] is applied, and its spatial accuracy is increased with 2nd-order MUSCL including minmod limiter, or 3rd, 5th, and 7th-order WCNS. The time integration method is 3rd-order TVD Runge-Kutta method [8]. The source term is integrated by the point implicit method.
In the present simulation, the detailed chemical reaction model UT-JAXA [9] containing 8 species (H_2, O_2, H, O, OH, HO_2, H_2O_2 and H_2O) and 21 elementary reactions are adopted. This model considers third-body efficiencies of elementary reactions, which are very important and sensitive under high-pressure and no-diluent conditions.
The initial condition is separated into two computational regions; one is located 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 100 atm and 2000 K, respectively. Lee proposed the semi-empirical model about the critical initiation energy, which depends on the radius of the source energy region [10]. According to this model, the initiation energy is given by

$$E = \frac{\pi (r_s)^2 p_s}{\gamma - 1},$$

where p_s and r_s are the pressure and radius in the source energy region and γ is the ratio of specific heat in the source energy region, respectively. The critical initiation energy of detonation in this condition is approximately 4.3 kJ. Thus, the radius of the source energy region in this study is fixed to 0.65 mm to reproduce the critical ignition energy. Since it is assumed that the hydrogen is generated by steam, the pressure and temperature of the ambient region are 1 atm and 373.15 K, respectively. The present computational grid system uses the orthogonal grid with the constant size, Δx, of 1.25 μm, 2.5 μm, and 5.0 μm, which correspond to the resolution of 32, 16, and 8 grid points in the half reaction length in hydrogen, $L_{1/2}$, respectively. The half reaction length is defined as the distance from the shock wave front to the place where half of the reactant is consumed by combustion. In this ambient condition, $L_{1/2}$ = 40.3 μm. For each grid size, we simulated four cases by changing the numerical scheme for convection terms; 2nd-order MUSCL method, 3rd, 5th, and 7th-order WCNS methods. Table 1 indicates the present computational conditions.

Table 1 Computational conditions for varisou grid resolutions and schemes.

Case	A1	A2	A3	A4
Numerical method	2nd MUSCL	3rd WCNS	5th WCNS	7th WCNS
Grid size [μm]	1.25	1.25	1.25	1.25
Case	B1	B2	B3	B4
Numerical method	2nd MUSCL	3rd WCNS	5th WCNS	7th WCNS
Grid size[μm]	2.5	2.5	2.5	2.5
Case	C1	C2	C3	C4
Numerical method	2nd MUSCL	3rd WCNS	5th WCNS	7th WCNS
Grid size[μm]	5.0	5.0	5.0	5.0

3 Results and Discussions

Figure 1 shows the maximum pressure history obtained from the two-dimensional numerical analysis performed in the conditions of Table 1. The maximum pressure history shows the transition of the detonation front, and it corresponds to the soot foiled records in the experiments. The black line indicates the track of the triple points where the local instantaneous pressure increases. In this work, the cellular structure for the higher grid resolution becomes irregular and the cell size increases. Furthermore, in the same grid size, it is found that the higher-order schemes generates the irregular and larger cells. Black line near the irregular cell is thicker. Transverse cells appear in that line.

Figure 2 shows the instantaneous detonation front at the lower right area in the computational domain where the detonation is fully developed. Fig. 2 indicates the density gradient contours near the wave front in each resolution and scheme, which corresponds to Schlieren photographs in the experiments. The detonation front for the higher-order resolution has a complex shape. In the cases of A1-4, B3-4, C4, the circulation structures due to Kelvin-Helmholtz instability appear behind the flame front. Fig. 3 shows a schematic view of the detonation wave front. In the cases of B1 and C1-4, the Mach stem and the incident shock do not appear. Fig. 4 indicates the instantaneous temperature contours near wave front. In the cases of A1-4, B2-4, C4, the reaction induction zone is observed clearly. When the reaction zone is sufficiently wide, the transverse cells appear in the black line in Fig. 2.

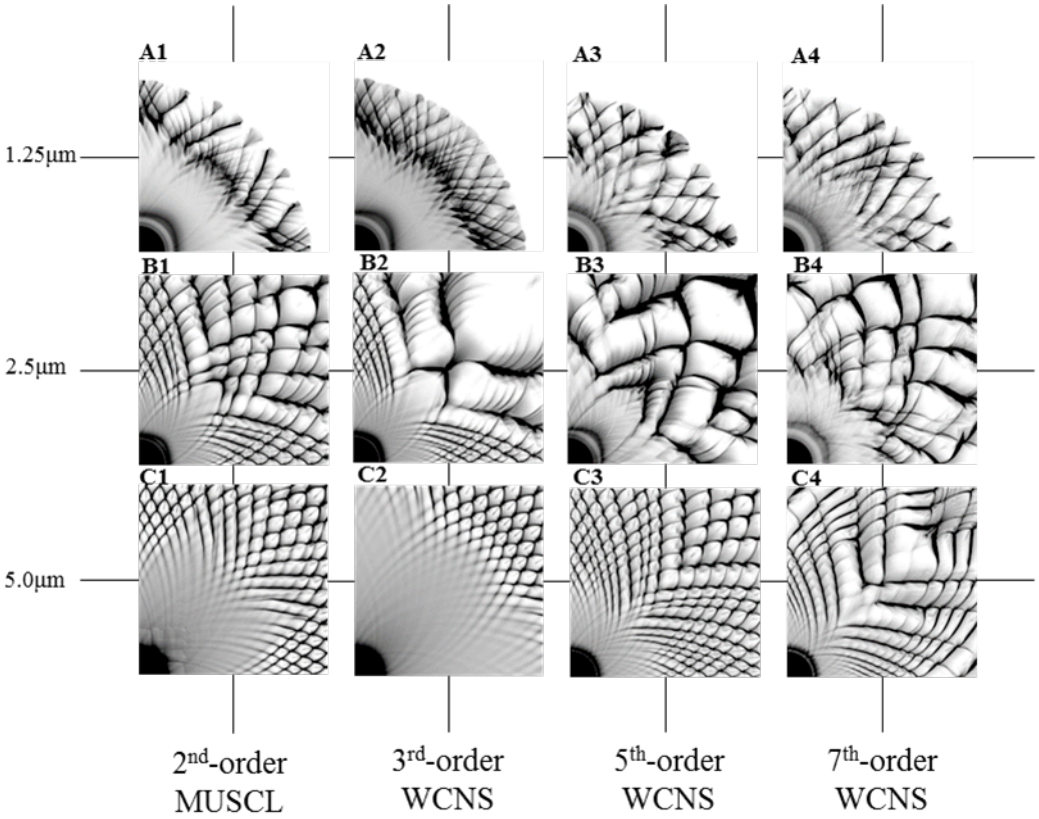

Figure 1 Maximum pressure history for various grid resolutions and schemes.

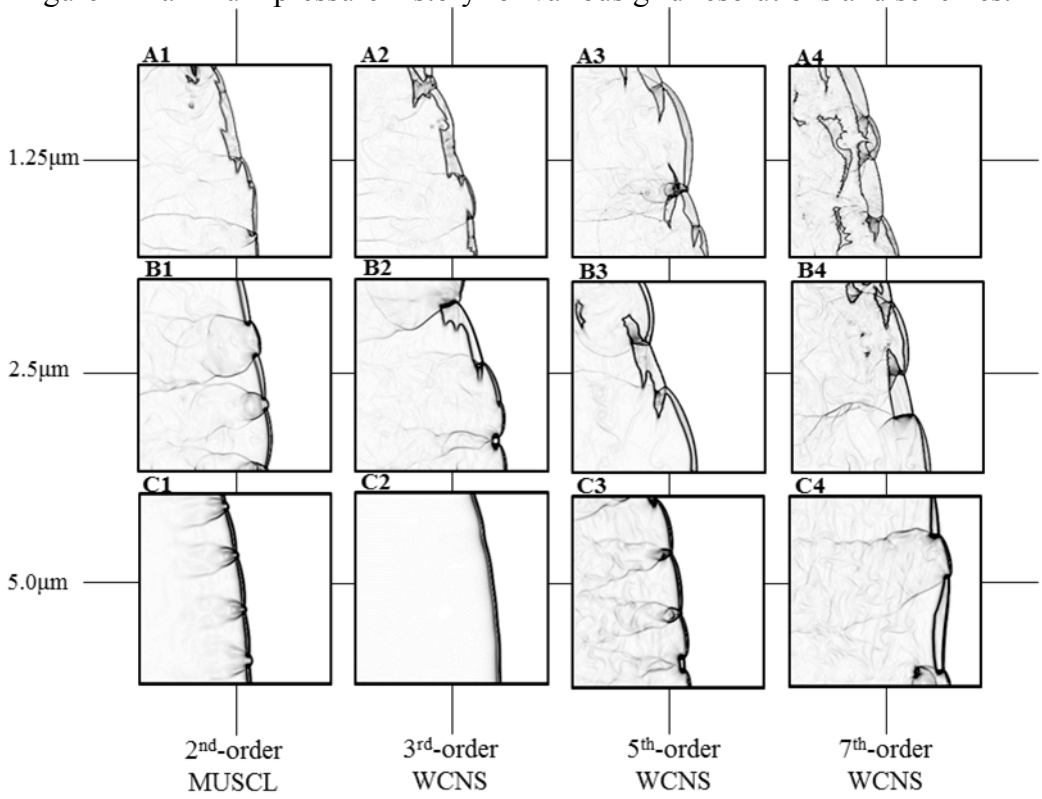

Figure 2 Density gradient contours near detonation front.

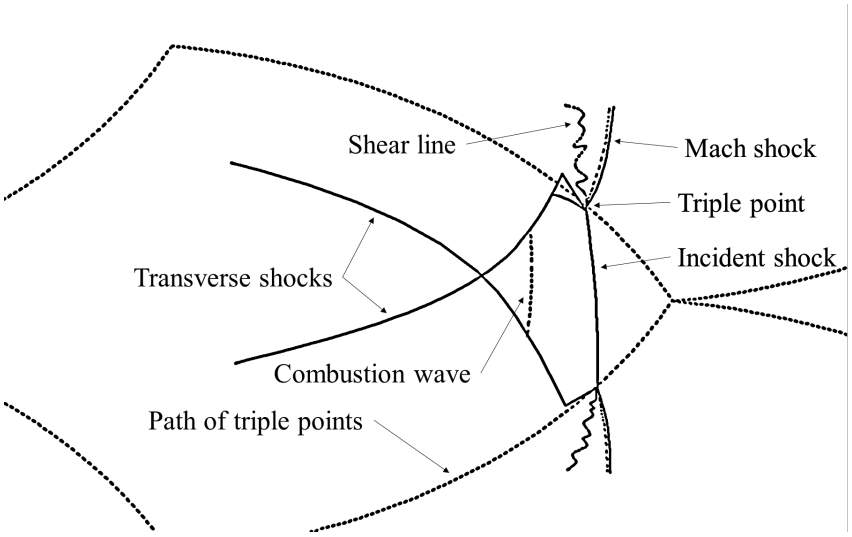

Figure 3 Schematic view of the detonation wave front.

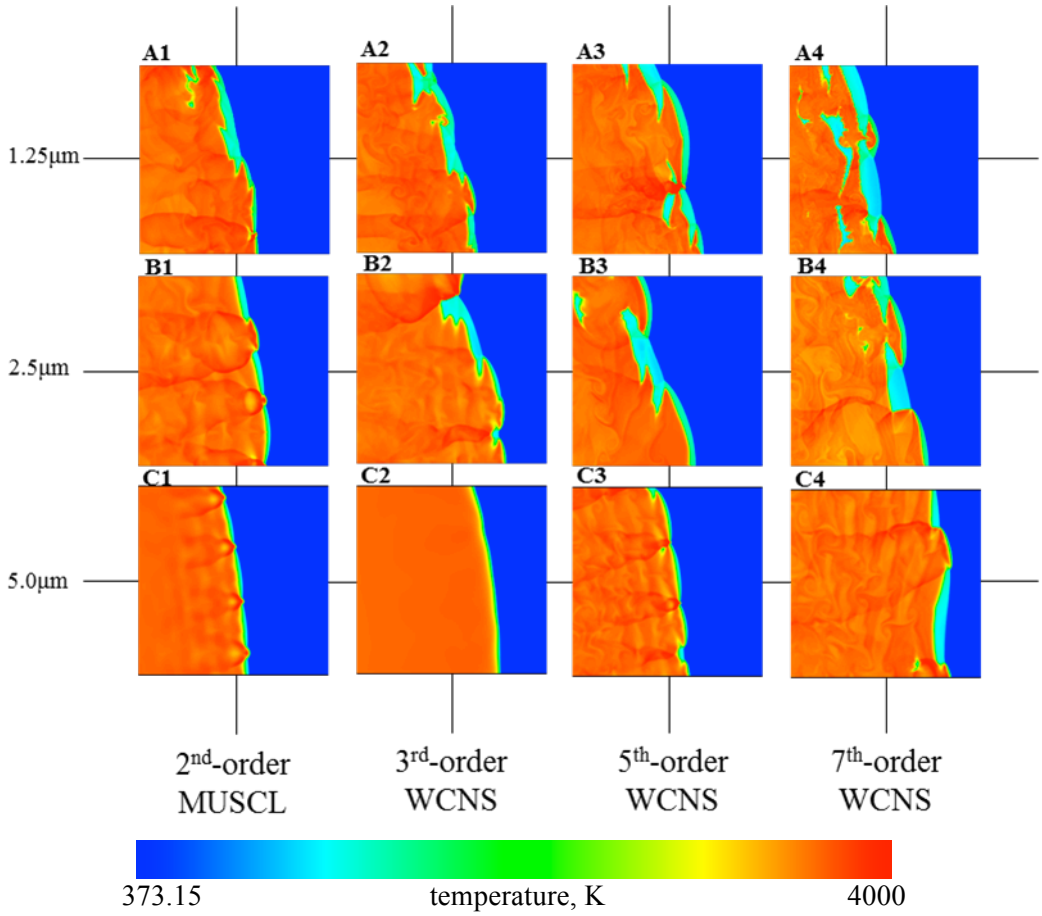

Figure 4 Instantaneous temperature contours near detonation front.

4 Conclusions

The two-dimensional cylindrical detonations by the direct initiation were simulated by a combination of three grid widths and four higher-order schemes. The higher grid resolution can be produced to be the irregurer and larger cellular structure. Further, In the same grid resolution, it is found that the higher-order scheme generates the irregurer and larger cellular structure. In the case of low resolution, Mach stem, incident shock, and unburned gas pockets cannot be observed.

Acknowledgments

This numerical analysis was carried out in the Super Computing system on the Osaka University.

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