Numerical Simulation of Two-Dimensional Hydrogen/Air C-J Detonation Waves: Dependence of Detailed Chemical Reaction Models on Detonation Cell Size

Keitaro ETO*, Nobuyuki TSUBOI, A. Koichi HAYASHI*****
*Dept. of Mech. Eng., Aoyama Gakuin Univ., E-mail: eto@cow.me.aoyama.ac.jp
**The Institute of Space and Astronautical Science, E-mail: tsuboi@flab.eng.isas.ac.jp
***Dept. of Mech. Eng., Aoyama Gakuin Univ., E-mail: hayashi@me.aoyama.ac.jp

Keyword: Detonation, CFD, Detailed chemical reaction model, C-J detonation

1. Introduction

The detonation studies have been done from safety engineering point of view for over a hundred and twenty years. Detonation wave has particularly supersonic and high pressure compared with deflagration wave, and has profitable factors in respect of combustion time and combustion pressure that decides thermal efficiency of thermal engines. Therefore the next generation propulsion devices such as pulse detonation engine (PDE) and oblique detonation wave engine (ODWE) etc. [1] [2] have been studied actively in recent years. It's very important that characteristics of a detailed chemical reaction model should be estimated for detonation problems because pre-mixture gas has various equivalence ratios. For example, mixture gas changes equivalence ratio in multi-cycle PDE. Though there exits PDE with H_2-O_2 pre-detonator and H_2/Air combustion chamber, conventional one- or two-step reaction model cannot simulate such a case.

Nagoya model [3] has been used to simulate detonation by our group, however, ignition delay would be smaller than the other model, therefore detonation cell become too small. Recently, Petersen & Hanson model (PH model) [4] was proposed as new detailed chemical reaction model. But there are few researchers [5] to apply for detonation problems. In this study, two-dimensional hydrogen/air C-J detonation waves are conducted by using both reaction models in order to estimate characteristics of PH model.

2. Numerical Method

The governing equations are made from the Euler equations with the mass conservation of each chemical species. The following assumptions were made to simplify the problem: 1) the species of gas are H_2, O_2, H, O, OH, HO_2, H_2O_2, H_2O, N_2; 2) specific heats at constant pressure of chemical species are functions of temperature and each gases follow a state equation of perfect gas; 3) viscosity of each chemical species is neglected. The equations are explicitly integrated by second-order Strang type fractional step method. The source terms with chemical reaction are treated in a linearly point-implicit manner. As for a numerical flux scheme, Harten-Yee non-MUSCL type TVD scheme [6] is used. In this simulation, two detailed chemical reaction models are used. One is Nagoya model with 9 species and 19 elementary reactions. The other is Petersen and Hanson model with 9 species and 18 elementary reactions with pressure dependence.

The computational grid system for 1D-simulation has 60000 points and that for 2D-simulation is orthogonal grid as shown in table 1. Accordingly the computational domain is 8.0x2.0 mm. The reason to use such a long computational domain is to reduce an interaction of the flow behind the detonation

with the downstream boundary. The wall boundary conditions are adiabatic, slip, and non-catalytic. The outflow condition is a zero-order extrapolation of conservative value without pressure and temperature. Pressure is fixed at the boundary and temperature is calculated from pressure and density.

For the initial condition in the 1D-simulation, physical values are given in two computational domains such as shock tube problem. One domain has 38bar and 1400K, and the other domain has 1.0132bar and 298.15K. For the initial condition in the 2D-simulation, 1D-results are posted in the computational domains and a rectangular pocket of unburned gas mixture is located in a symmetrical position behind the detonation front.

Table 1: 2D-simulatin cases for computational grid system.

No.	reaction model	grid space μm	channel width mm	the number of grids	
				x	y
(1)	Nagoya	10	2	801	201
(2)	Nagoya	7.5	2	1067	267
(3)	Nagoya	5	2	1601	401
(4)	Nagoya	4	2	2001	501

No.	reaction model	grid space μm	channel width mm	the number of grids	
				x	y
(5)	Petersen and Hanson	10	2	801	201
(6)	Petersen and Hanson	5	2	1601	401

3. Results and Discussions

It's confirmed that average detonation velocity is equal to C-J theoretical value (about 1980m/sec). It shows the validity of these simulation results.

With respect to the dependency of reaction model, the detonation cell size for PH model becomes twice of that for Nagoya Model as shown in Figs. 1 and 2. Irregular detonation cells are observed for Nagoya model. Detonation cell size would be dependent on ignition delay, and ignition delay for PH model is larger than that for Nagoya model. Cell size width for experiments in the present conditions is approximately 10mm, and these calculated cell sizes are smaller than the experimental value.

Then grid size dependency or the detonation cell sizes estimated for Nagoya model as shown in Figs. 2 and 3. Many researchers have been reported that detonation cell significantly dependent on grid spacing, and poor resolution cause small cell size. The present results also show that the detonation cell size increase with smaller grid spacing.

Figure 4 shows the comparison of local specific energy release between PH model and Nagoya model. The energy release is given by the difference in enthalpies due to the chemical kinetics during a time step at constant pressure, and the summation is over the entire time step in the computation. The energy release increase in the vicinity of triple point and transverse wave, and it is depend on the grid resolution and the reaction model. The comparison of PH model and Nagoya model with grid spacing of 5μm in Fig. 5 (a) and (b) show that there are no differences between them is shown. However, the grid dependency for Nagoya model is significantly large as shown in Fig. 4 (b) and (c).

Measured detonation cell width is plotted in Fig. 5. The dependency of grid spacing is clearly observed for both models. For the Nagoya model, maximum width is approximately 2mm with grid

spacing of 4μm though the channel width is 4mm.

Figure 6 shows maximum energy release for both models. There also exists the grid spacing dependency on maximum energy release for both models. It's shown that the gradient for Nagoya model is larger than that for PH model. However, a convergent tendency at grid spacing of 4-5μm can be observed for Nagoya model. Therefore optimum grid spacing for Nagoya model is approximately 5μm. For PH model, a convergent tendency didn't appear in the present simulations. Further study is required to estimate the dependency of grid spacing for PH model.

4. Conclusions

Two-dimensional Hydrogen/Air C-J detonation waves with two detailed chemical reaction models were simulated to estimate the dependency of the reaction models. And the validity of PH model was evaluated by comparing to Nagoya model and experimental results. As a result, the cell size for PH model becomes larger than that for Nagoya model. Furthermore cell size tended to become larger by using smaller grid spacing.

The maximum energy release and its history are also shown to depend on the grid resolution and the reaction model.

It's thought that PH model has the validity enough for the simulation of detonation waves from the present results, however, more resolution studies would be required for PH model.

Reference

[1] A.K. Oppenheim, N. Manson, and H.Gg. Wagner, “Recent Progress in Detonation Research”, AIAA Journal Vol.1, pp.2243-2251, 1963.

[2] R. A. Strehlow, “Gas Phase Detonations: Recent Developments”, Combustion and Flame Vol.12 No.2, pp.81-101, 1968.

[3] M. Hishida and A.K. Hayashi, “Numerical Simulation of Pulsed Jet Plume Combustion”, AIAA Vol.152, pp.343-361, 1993.

[4] L. Petersen and K. Hanson, “Reduced Kinetics Mechanisms for Ram Accelerator Combustion”, Journal of Propulsion and Power Vol. 15, No. 4, July-August, 1999.

[5] H. Shimizu, N. Tsuboi, A. K. Hayashi, “Study of Detailed Chemical Reaction Model on Hydrogen-Air Detonation”, AIAA paper, 2001-0478, 2001.

[6] H. C. Yee, "Upwind and Symmetric Shock-Capturing Schemes”, NASA Technical Memorandum 89464, 1987.

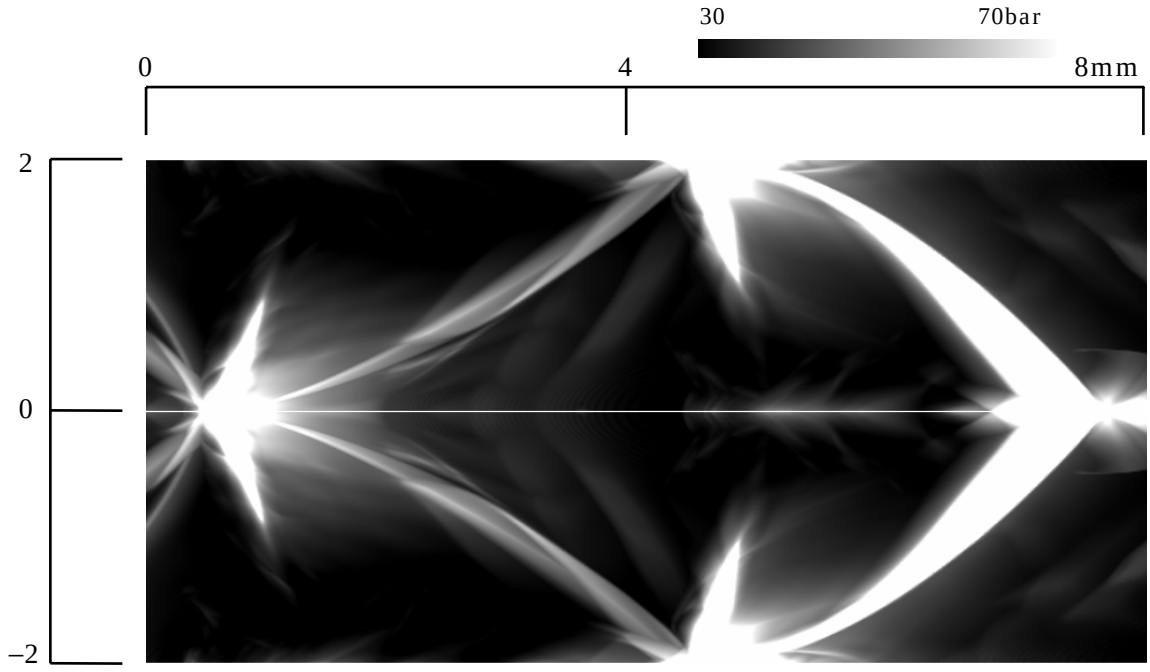

Fig. 1: Maximum pressure history by using Petersen & Hanson model, grid spacing of 5μm.

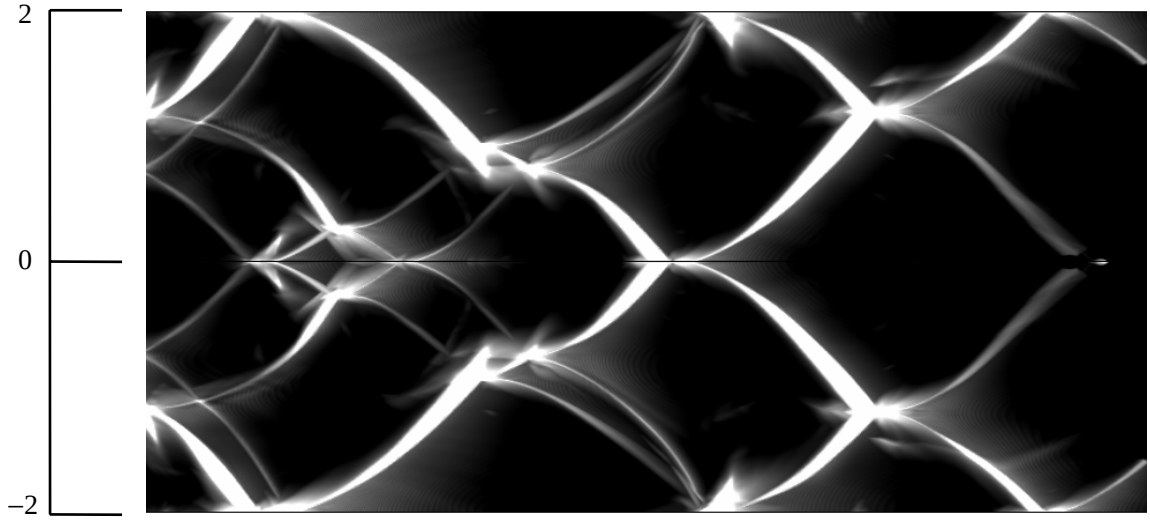

Fig. 2: Maximum pressure history by using Nagoya model, grid spacing of 5μm.

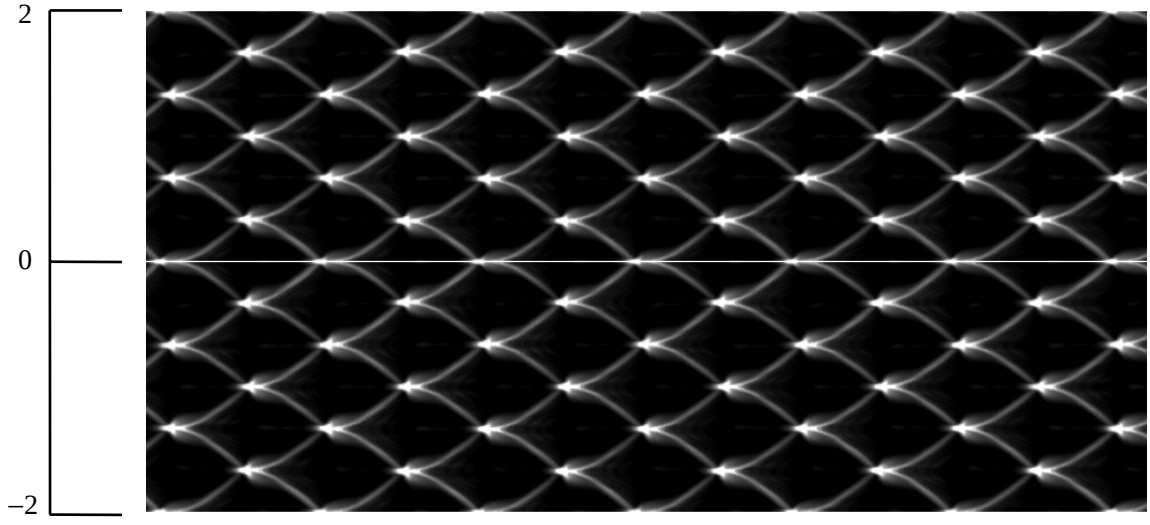

Fig. 3: Maximum pressure history by using Nagoya model, grid spacing of 10μm.

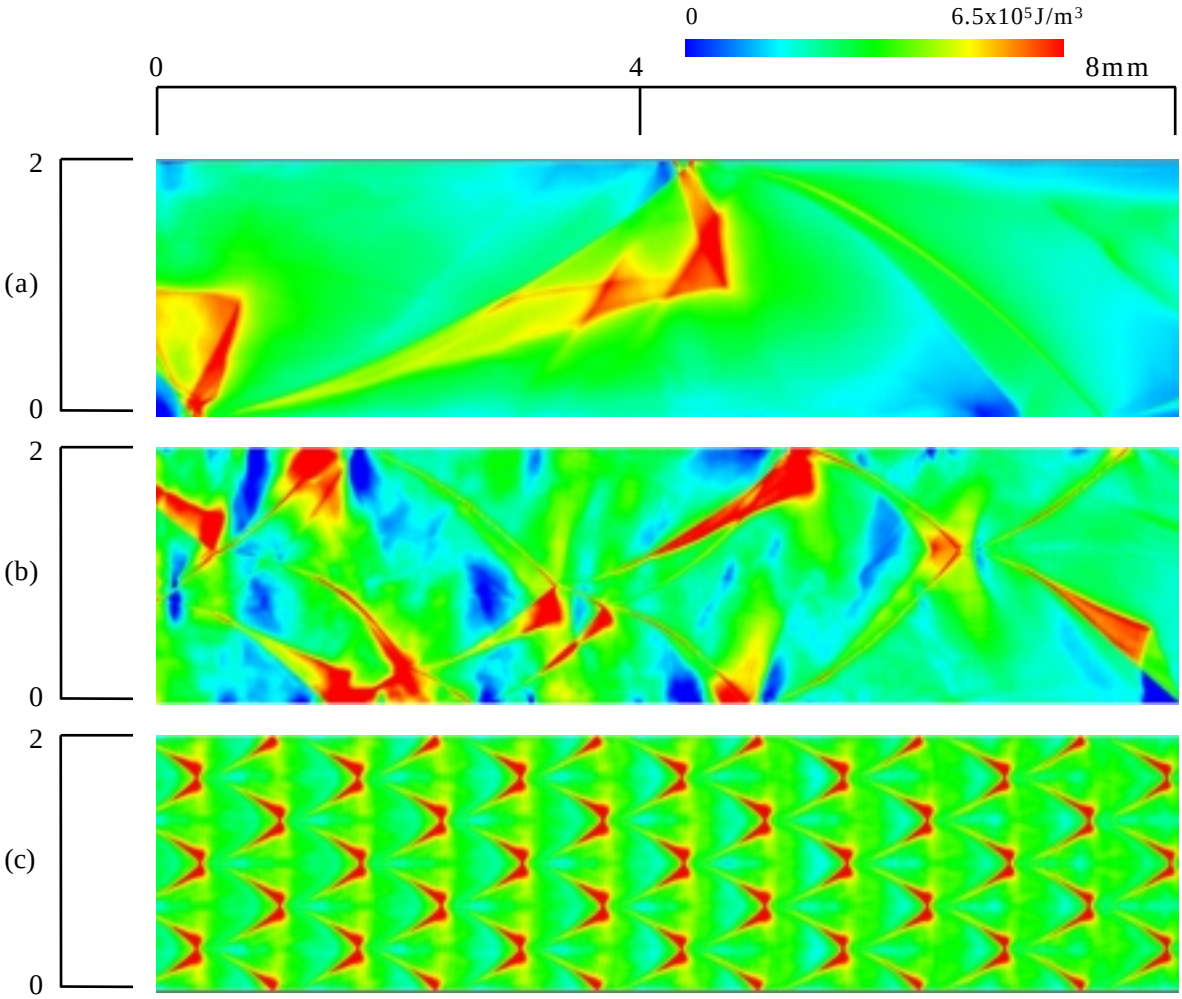

Fig. 4: Energy release histories: (a) Petersen & Hanson model, grid spacing 5μm, (b) Nagoya model, 5μm, (c) Nagoya model, grid spacing 10μm.

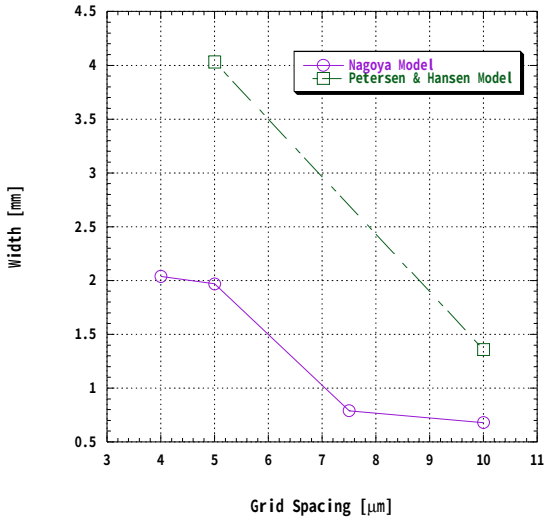

Fig. 5: Detonation cell size plot.

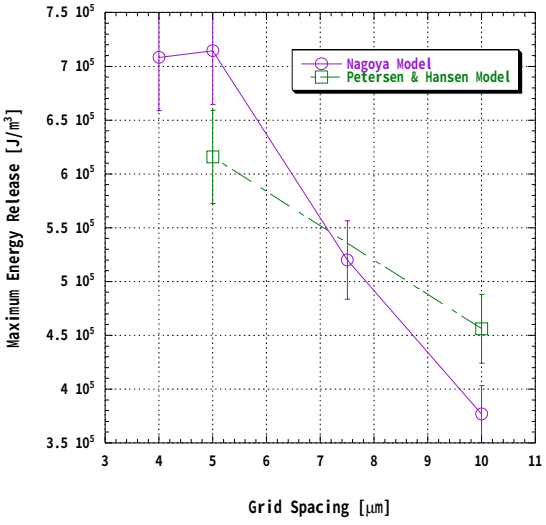

Fig. 6: Maximum energy release plot.