A Numerical Study of Hydrogen/Air Detonation Using a Pressure Dependent Stanford Model : Formation and Burning of Unreacted Gas Pocket

Nobuyuki Tsuboi*, Hiroshi Shimizu, A.Koichi Hayashi*** and Yoichiro Matsumoto†**

*Institute of Space and Astronautical Science, E-mail:tsuboi@flab.eng.isas.ac.jp

**Dept. of Mech. Eng., Aoyama Gakuin Univ., E-mail:shimizu@cow.me.aoyama.ac.jp

***Dept. of Mech. Eng., Aoyama Gakuin Univ., E-mail:hayashi@me.aoyama.ac.jp

†Dept. of Mech. Eng., The University of Tokyo, E-mail:ymats@mech.t.u-tokyo.ac.jp

1. Introduction

Detonation wave, a compound wave of shock and flame, propagating with a supersonic speed has been studied since more than a hundred and twenty years and its some detailed structure and various properties have been revealed through experiments and numerical simulations.

The reasons to study the detonation can be classified into two; fundamental and application. The former is to elucidate further detailed mechanism in fundamental characteristics of the detonation wave such as propagating mechanism of self-sustained detonation, deflagration-to-detonation transition (DDT), and the existence of irregular cell structure. The latter is to study on the source of propulsion for the supersonic aircraft such as a scramjet engine and a pulse detonation engine (PDE) as well as safety problems. Recently, the field of computational fluid dynamics (CFD) has provided remarkable advances.

One of the earliest numerical detonation studies was presented in 1978 by Taki and Fujiwara [1]. Oran, Kailiasanath, and Gamezo [2]-[6] studied for two decades about a formation of unreacted pocket behind the detonation wave, cell structure, and transverse wave as well as other detonation features. In our laboratory [7],[8], a structure of H_2/Air detonation wave has been studied by 1D and 2D numerical simulations by using some detailed chemical reaction models that have 9 species and 18 or 19 reaction steps.

In this study, numerical simulation for H_2/Air detonation was conducted by using a detailed chemical reaction model such as a pressure dependent Stanford model [9] to evaluate the detonation cell size and reveal the detonation propagation mechanism.

2. Numerical Method

In order to study the effect of the chemical reaction models on the detonation structure, the Stanford detailed chemical reaction model was investigated in the 1D and 2D simulations for H_2/Air detonation. 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) viscosity is neglected. Reactions for N_2 are not included because N_2 reaction would be slower than hydrogen/oxygen reactions.

On the basis of the assumptions, the governing equations are made from the Euler equations with the mass conservation of 9 species and with 18 elementary reactions. 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 [10] is used.

The computational grid system for 1D has 6000 points and that for 2D simulations is orthogonal grids with (x, y) = (1601, 401). The grid size for 2D case in x direction and y direction is 5.0 μm which has 32 points in half-reaction zone of H_2. Half-reaction zone of H_2 is about 1.6 $\times 10^{-4}$m for 0.1 MPa. Accordingly the computational domain is 8.0$\times$2.0 mm. The reason to use such a long computational domain is to reduce a interaction the flow behind the detonation with the downstream boundary. The wall boundary conditions are adiabatic, slip, and non-catalytic. The outflow condition is a zeroth-order extrapolation of conservative values.

For the initial conditions in the 1D simulation, physical values are given in two computational domains such as shock tube problem. One domain has 3.8 MPa and 1400 K, and another domain has 0.1 MPa and 298K. For the initial condition in the 2D simulation, 1D results are pasted in the computational domains and a rectangular pocket of unburned gas mixture is located in a symmetrical position behind the detonation front.

The Stanford model was constructed by Petersen and Hanson[9] and has 9 species and 18 elementary reactions with pressure dependence. The model includes H_2O_2 and HO_2 chemistry near the second and third explosion limit, which is necessary for ignition at ram accelerator pressures but lacking in certain finite chemistry models currently in use. The rate coefficients for H_2O_2 and HO_2 reactions has a pressure dependent rate coefficient defined by method of Troe[11].

3. Results and Discussions

Figure 1 shows formation of a new triple point and an unreacted pocket near the detonation frond. At 17.44 μs, three triple points appear near the detonation front. The detonation is the strong shock configuration as shown in Ref. [2]. In this results, it is difficult to understand the shock refraction reported by Oran et al. In the vicinity of the transverse shock, a region with slightly higher temperature behind the incident shock begins at C and continues downstream to point D. An ignition 1 due to the interaction of the transverse shock is generated behind the unreacted pocket 2 which appears vicinity of the detonation front at 17.51 μs. The unreacted pocket 4 is isolated and moves downstream, and a rapid explosion 3 behind the unreacted pocket occurs at 17.57 μs. The rapid explosion penetrates from the rear side of the unreacted pocket at 17.62 μs. Then the unreacted pocket burns from its center and the unreacted pocket burns at 17.67 and 17.72 μs. Gamezo et al. [6] revealed the formation of the unreacted pocket by using a onstep reaction, however, the detailed mechanism of the formation and the explosion of the unreacted pocket could not elucidated clearly. Present simulation can resolve it by using the detailed reaction model.

Figure 2 shows the maximum pressure history and the local specific energy release for one cellular detonation pattern. 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 all the time step in the computation as shown in Ref. [2],[12]. The maximum pressure history contours show that a weak longitudinal 1 and transverse 2,3 tracks are captured at the vicinity of the triple point collision. The weak longitudinal track 1 is generated by the intersection of the transverse shock and local ignition behind the unreacted pocket as shown in Fig. 1. The transverse tracks 2,3 are formed due to the local explosion of the unreacted pocket 5 as shown in Fig. 1. Figure 1(b) also reveals that the energy release behind the shock BC is smaller than that behind the shock AB. The results would be similar to the results reported by Oran et al. [2], but they showed that the energy release for shock AB was larger than that for shock BC. The high energy release contours are terminated at location 4 clearly due to the triple point collision and the local explosion of the unreacted pocket as shown in Fig. 1.

4. Conclusions

Numerical simulation for H_2/Air detonation was conducted by using the pressure dependent Stanford model. The results showed that the detailed mechanisms of the formation and the explosion of the unreacted pocket was revealed and that the isolated unreacted pocket were ignited from its rear side by the intersection of the transverse shock. The maximum pressure history and the local specific energy release history showed that the transverse shock intersection and the explosion of the unreacted pocket cause the weak longitudinal and transverse tracks.

References

[1] Taki,S. and Fujiwara,T., AIAA Journal 16, pp.73-77, 1978.

[2] Oran, E.S. et al., Combustion and Flame, pp147-163,1998.

[3] Oran, E.S., et al., 19th International Symposium on Combustion/The Combustion Institute, pp.573-582, 1982.

[4] Kailasanath, K., et al., Combustion and Flame 61,pp199-209, 1985.

[5] Guirguis, R., et al., 21th International Symposium on Combustion/The Combustion Institute, pp1659-1668, 1986.

[6] Gamezo, V.N., et al., Shock Waves, 9,pp.11-17, 1999.

[7] Hishida, M., Hayashi A.K., 14th ICDERS, C9.3.1-10, 1993.

[8] Shimizu, H., et al., AIAA paper 2001-0487, 2001.

[9] Petersen, E.L. and Hanson, R.K., J. Propulsion and Power Vol.15, No.4, July-August, pp.591-600, 1999.

[10] Yee, H.C., NASA Technical Memorandum 89464, 1987.

[11] Troe, J., J. Physical Chemistry, Vol.83, No.1, pp.114-126, 1979.

[12] Clifford, L.J., et al., Combustion and Flame 104, pp311-327, 1996.

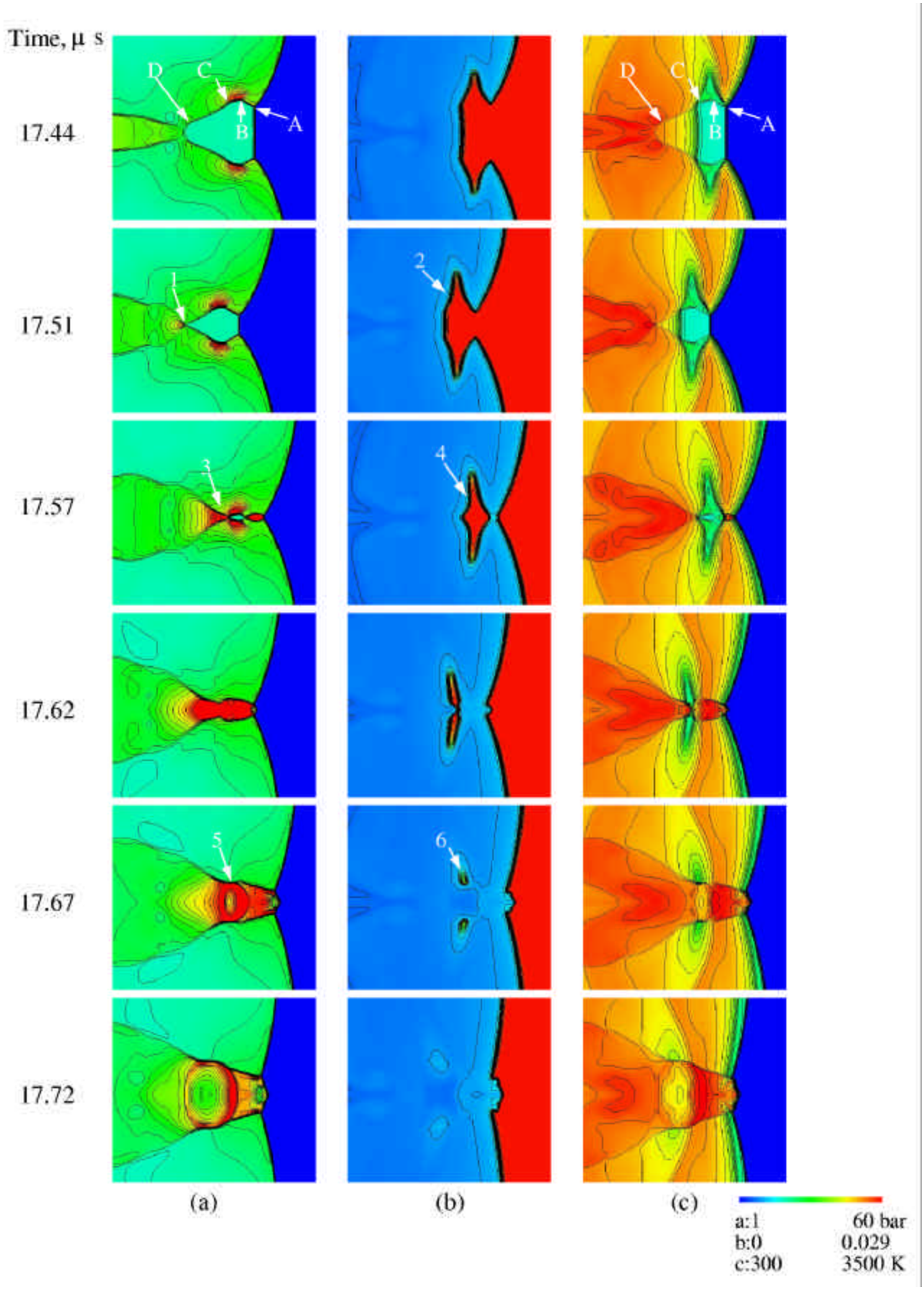

Figure 1. Contours near the formation of a new triple point and an unreacted pocket: (a) pressure; (b) H_2 mass fraction; (c) temperature. 1 - ignition behind the unreacted pocket, 2 - formation of the unreacted pocket, 3 - rapid explosion behind the unreacted pocket, 4 - unreacted pocket moving downstream, 5 - explosion of the unreacted pocket, 6 - remain of the unreacted pocket, A,B,C - triple point, D - tail of the shock wave.

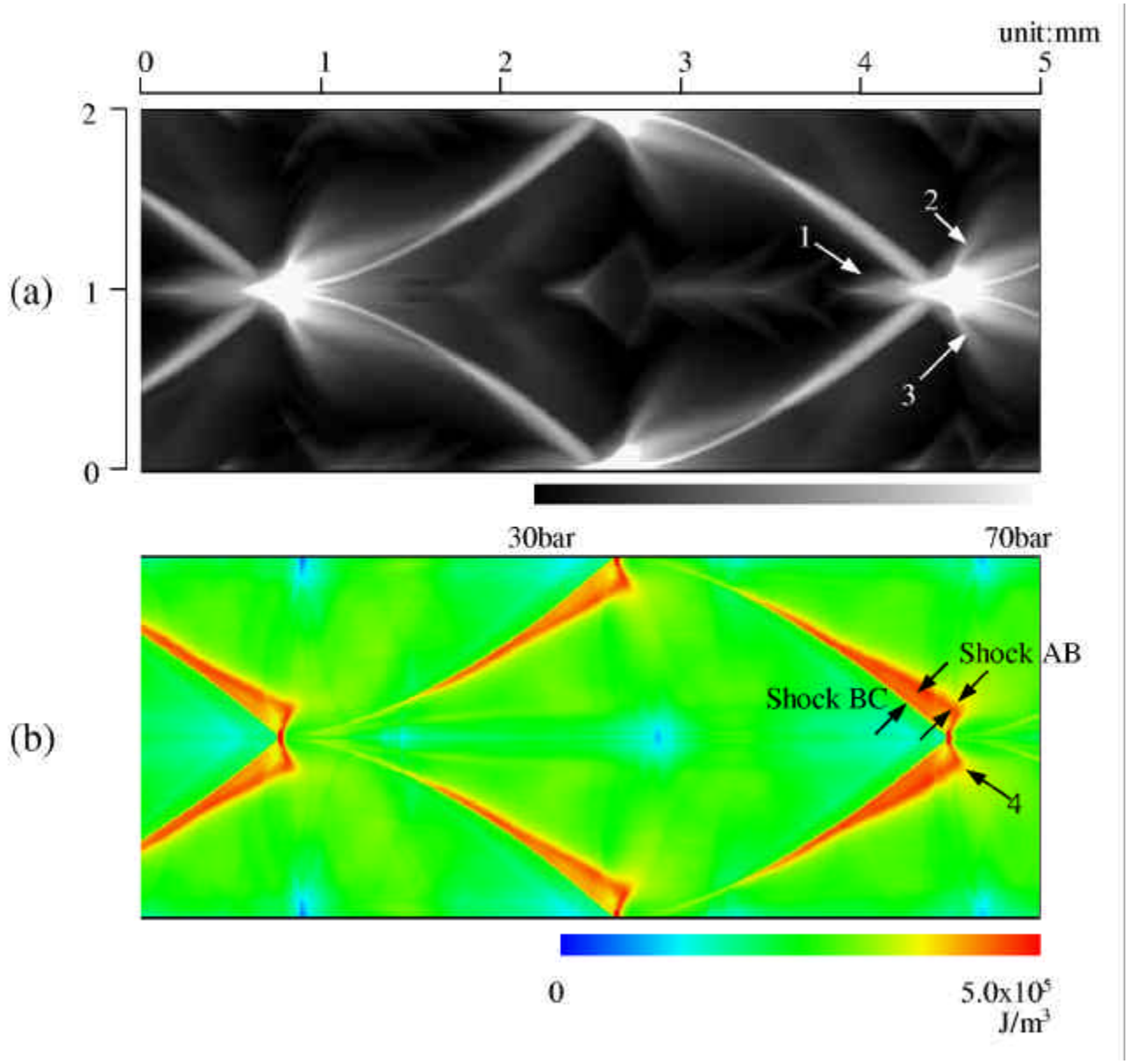

Figure 2. Time history of the detonation cellular pattern: (a) maximum pressure history; (b) local specific energy release. 1 - weak longitudinal track, 2,3 - transverse track, 4 - terminated location due to burning of the unreacted pocket.