Numerical Analysis on the Correlation between Transverse Wave Strength and Detonation Velocity

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1 Introduction

Detonation is a shock-induced combustion wave propagating in a combustible gas. Although this phenomenon has been studied for more than 120 years since its discovery in 1880's, there is still considerable room for future investigation such as Deflagration-to-Detonation Transition problem, velocity deficit, and so on. The detailed structures and properties of the detonation have been studied by the experimental and numerical methods as well as theoretical approaches.

It is known that a detonation propagation limit exists in terms of pressure, tube diameter and concentration of the mixture. Near the propagation limit, the single-headed spinning detonation occurs and a detonation velocity slower than the Chapman-Jouguet (CJ) velocity is observed in experiments. The reason of the velocity deficit has been thought to be the friction and heat losses at the tube wall; Kitano et al.[1] showed that the prediction by the modified Zel'dovich-von Neumann-Doering model, which incorporates those loss effects, matches the result obtained by their experiment. However, the numerical simulation performed by Tsuboi et al.[2] also demonstrated a velocity deficit despite the use of Euler equations, concluding that the energy release in the mixture affects the strength of the transverse detonation significantly.

It is thought that the strength of the transverse wave relates to the detonation velocity. However, there is no passed data that compared them. The objective of this study is to estimate the relationship between the strength of transverse shock and detonation velocity deficit using two-dimensional numerical simulations.

2 Numerical method

The governing equations are Euler equations with 9 species (H_2, O_2, H, O, OH, HO_2, H_2O_2, H_2O and N_2) and 18 elementary reactions, which are explicitly integrated by the Strang type fractional step method. The chemical 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 numerical flux in the convective terms [3]. The Petersen and Hanson model [4] is used for chemical kinetics to solve detonation problems. This model contains 18 reactions and 9 species, and it is based on the H_2/O_2 sub-mechanism of the RAMEC/Gas Research Institute GRI-Mech 1.2 methane-oxidation

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mechanism. The significance of this model is the pressure dependence on a forward reaction coefficient included in the collision reaction with a third body: HO_2 and H_2O_2 chemistries near the second and third explosion limits, which are necessary for ignition at extremely high pressure, are considered while lacking in certain finite rate chemical models currently in use.

Four computations are carried out by varying the initial pressure in order to observe the detonation velocity difference depending on the strength of the transverse wave. Those four cases are with initial pressures of 1.0, 0.5, 0.2 and 0.1 atm, while the temperature and the mixture are fixed as 298.15K and stoichiometric mixture of H_2/air, respectively. The computational grid is a rectangular system with 801×201 grid points. Each of the grids has a size of 5μm×5μm for an initial pressure of 1.0 atm, and scales are proportional to the inverse of the initial pressure. The boundary conditions are as follows: the upstream conditions are the initial conditions explained earlier; the side wall boundary conditions are adiabatic, slip, and non-catalytic; and the downstream boundary is a non-reflection boundary proposed by Gamezo et al.[5].

3 Results and discussions

Figure 1 is the plot of the normalized detonation velocity histories for all four initial pressures. They are averaged on the symmetry axis during a half cycle. At the initial stage of the calculations, the detonation waves are overdriven for all cases. However, their velocities later decreased as the time advances until they reach the velocities lower than the CJ detonation velocity; the detonation velocities for 1.0, 0.5, 0.2 and 0.1 atm cases reached and stabilized at approximately $0.99D_{CJ}$, $0.98D_{CJ}$, $0.97D_{CJ}$ and $0.95D_{CJ}$, respectively. This plot clearly shows that the lower the initial pressure, the slower the detonation velocity, which is the same trend with one in the three-dimensional calculation results by Tsuboi et al.[2].

The transverse wave is thought to affect the velocity of overall detonation significantly. It is because most of the chemical reactions take place behind the transverse shock producing the highest pressure as seen in Figure 2 and obviously, it is driving the transverse wave. Therefore, there is no doubt that the transverse wave plays a very important role upon detonation wave propagation.

In order to estimate the relations, detonation velocity deficit and the strength of the transverse wave are compared to each other. In the present study, the strength of a transverse wave is defined as the pressure ratio across the transverse shock (i.e. p_{max}/p_1 in Figure 2 (b)). The strengths of a transverse wave at ten time steps during a half cycle of the detonation were averaged to be compared with the velocity deficit averaged and measured during the same half cycle, which are indicated by the black data points in Figure 1. However, it must be noted that the ten points used to calculate the average shock strength are not taken from the vicinity of the side walls (within two grid points) because it is difficult to distinguish the shock on which to be focused in the explosion at the wall. As the result of the analysis, some correlation was observed between them as shown in Figure 3. It is difficult to perform a quantitative reasoning for this relation; however, it is implied that the weakening of the transverse wave is the source of detonation velocity deficit in this simulation because generally, larger detonation velocity deficits occur with weaker transverse wave.

4 Conclusions

Two-dimensional numerical simulations on detonation are performed in order to predict the relation of transverse wave with detonation propagation. As the result of the analysis, strong relations between the strength of a transverse wave and detonation velocity deficit are implied.

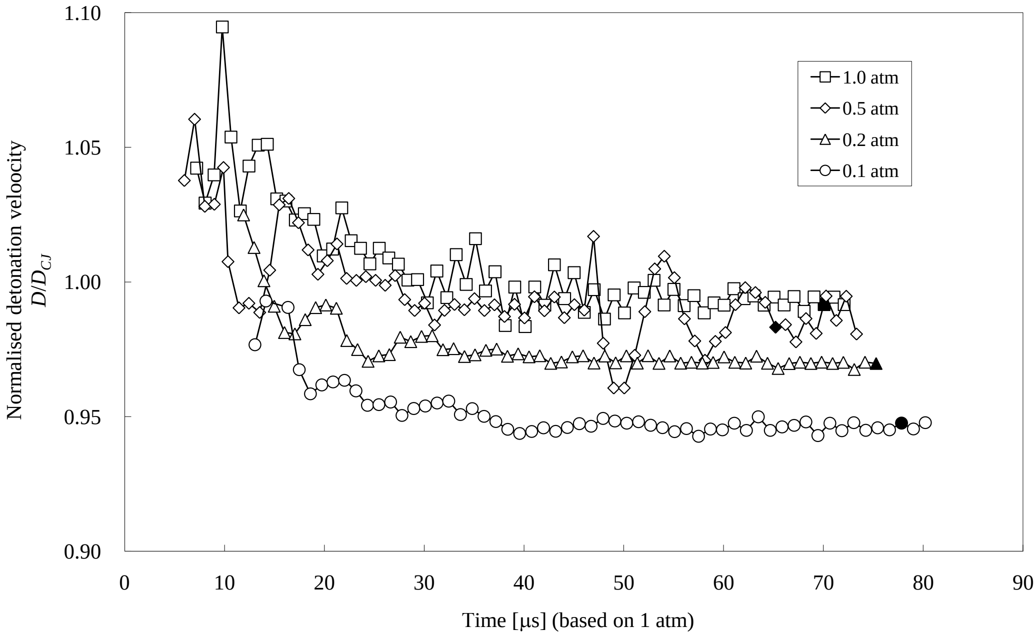

Figure 1 Calculated average detonation velocity on symmetry axis during half cylce. Data of the half cycle used to calculate black points are used to plot Figure 3.

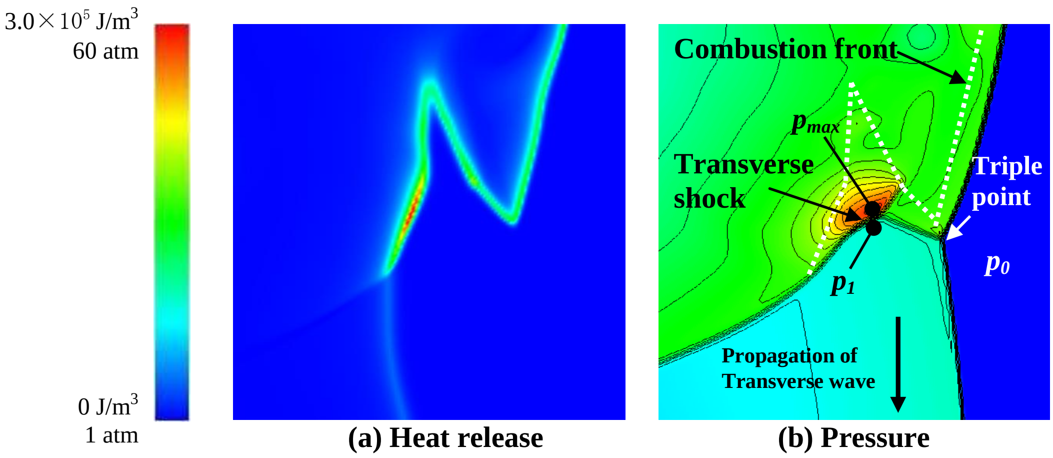

Figure 2 Istantaneous simulation results around the triple point.

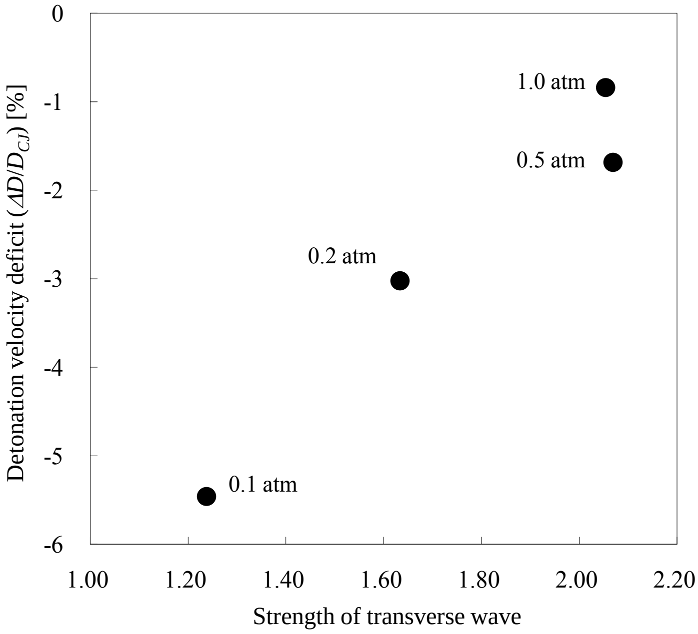

Figure 3 Relation between detonation velocity deficit and strength of transverse wave.

Acknowledgements

This research was performed in collaboration with the Center of Planning and Information Systems at ISAS/JAXA.

References

[1] Kitano, S. et al. (2009). Spinning detonation and velocity deficit in small diameter tubes. Proc. Comb. Inst. 32: 2355.

[2] Tsuboi, N., Hayashi, A.K., Koshi, M. (2009). Energy release effect of mixture on single spinning detonation structure. Proc. Comb. Inst. 32: 2405.

[3] Yee, H.C. (1987). Upwind and symmetric shock-capturing schemes. NASA TM-89464.

[4] Petersen, E.L., Hanson, R.K. (1999). Reduced Kinetics Mechanisms for Ram Accelerator. Combustion. J. Propul. Power 15: 591.

[5] Gamezo, V.N., Desbordes, D., and Oran, E.S. (1999). Two-dimensional reactive flow dynamics in cellular detonation waves. Shock Waves 9: 11.