Detailed Shock Configuration of Cylindrical Cellular Detonation

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1 Introduction

Detonation front forms a complex structure by interactions among various shock waves. Transverse wave, which propagates perpendicular to a traveling direction of detonation, is an important phenomenon to understand the mechanism of detonation. The interaction between transverse waves propagating to opposite directions each other induces a local explosion. The local explosion provides the shock wave with driving energy and new transverse waves. The shock configuration in detonation is classified into three: the single Mach interaction, double Mach interaction, and complex Mach interaction [1]. A multi-headed detonation in a tube generally forms the single and the double Mach interaction. On the other hand, the complex Mach interaction is observed particularly in a spinning detonation and an expanding detonation.

Many numerical studies about expanding detonation have performed two-dimensionally [2-3]. We calculated cylindrical detonations which deal with an expanding detonation using the Harten-Yee upwind type TVD scheme in the convective term of governing equations [4]. As the results, the cell bifurcation is observed when the sell size becomes large enough due to detonation front expansion. The shock waves form the complex Mach interaction just before the cell bifurcation. It probably implies that there is a correlation between the cell bifurcation and the complex Mach interaction. However, the correlation was not explained in our previous and many others studies because a configuration of complex Mach interaction is not clear due to lack of resolution. Furthermore, the complex Mach interaction such as the multi-headed ribbon could not be observed in the previous simulation. This result indicates that it is necessary to obtain the detailed structure to use a higher resolution performance than the past scheme. Togashi et al. [6] showed the shock configuration of detonation wave using an AUSMDV scheme which is good at shock and discontinuity capturing.

The present study is to investigate a detailed shock configuration of detonation wave, especially a complex Mach interaction. A hydrogen-oxygen cylindrical detonation is simulated to obtain a correlation between the cell bifurcation and shock configuration.

2 Numerical Method and Conditions

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The governing equations are the compressible Euler equations in two-dimensional Cartesian coordinate system with a chemical reaction. The second-order MUSCL type AUSMDV scheme is used in inviscid terms. The Shuen's limiter is used as a numerical flux limitation. The reaction source terms are treated in a linear point-implicit manner in order to avoid a stiff problem. The Petersen and Hanson model, which contains eight species (H_2 , O_2 , H, O, OH, HO_2 , H_2O_2 and H_2O) and eighteen elementary reactions, is used as a detailed chemical reaction mechanism. This model has a pressure dependence on the forward reaction coefficient related with the third body reactions of H_2O_2 . The viscous effects in the present simulation such as turbulence and boundary layer interactions are neglected.

The computational mesh is orthogonal with 8001×4001 grid points. The initial condition is set in two computational regions: the cylindrical region within r_s (=16 $L_{1/2}$ [2]) is source region and another region is ambient region. $L_{1/2}$ is the half reaction length which defined as the distance from the shock wave to the place where the mass fraction of hydrogen is equal to the average value between free stream and equilibrium steady state. A hydrogen-oxygen stoichiometric mixture is set on these regions. The pressure and temperature in the source region are 10 MPa and 2000 K, respectively, then, the pressure and temperature in the ambient region are 0.1 MPa and 300 K, respectively. The grid size in both *x* and *y* direction is $0.05L_{1/2}$ (=2.34µm). The boundary conditions on the *x* and *y* axes are treated as symmetry and the upper and right sides of the boundaries are treated as the outflow boundary.

3 Results and Discussions

As the result of simulation on cylindrical detonation, the maximum pressure history is shown in Fig.1a. The pressure range is from 0.1 to 18.0 MPa. The transverse wave which is higher pressure than the surrounding one leaves the trajectory similar to a cell pattern obtained by the experimental soot film. Although the detonation cell near the ignition source is small, the detonation cell gradually becomes larger as the detonation expands. Since the detonation front expands toward outside, the transverse wave spacing becomes larger with detonation propagating, then, the cell size becomes larger. When the detonation wave propagates at the certain distance from ignition source, the fine cells suddenly come out as shown in the right region of Fig. 1a. Gamezo et al. [7] numerically obtained the fine cells in two-dimensional detonation in a tube. They reported that the unsteadiness of marginal detonation produces the transverse cell. Figure 1b is a closeup of detailed cellular structures described by the dashed square region in Fig. 1a. The transverse wave propagates from the top left region to the bottom right one in Fig. 1b. The finer cell called as the transverse detonation cell is seen in the wide trajectory of the transverse wave (transverse detonation). The transverse detonation cell is similar to the multiheaded ribbon like trajectory of the transverse waves in the spinning detonation [8]. The transverse detonation cell becomes clearer at the right bottom of Fig. 1b. The pressure of the detonation front denoted by A is higher than that by B.



Fig. 1. The left figure (1a) is the maximum pressure history. The right figure (1b) is closeup of the region denoted with the dashed square region in Fig. 1a. The range of pressure is between 0.1 and 18.0 MPa. The hatched area from top left region to bottom right one in Fig. 1b is the trajectory of transverse wave (transverse detonation), where the transverse detonation cells are observed in. The fine cells are observed in top right region in Fig. 1b.



Fig. 2. The time sequence distributions of pressure in the dashed square region of 2 in Fig. 1b. The pressure range is between 0.1 and 12.0 MPa. The white lines in Figs. 2(i)-2(vii) are heat release contours which indicate a reaction front. The top left figure is the superimposed contours with black line of heat release in Figs. 2(i)-2(vii) on the dashed square region of 2 in Fig. 1b.

Figures 2(i)-2(vii) show the time sequence distributions of pressure in the dashed square region of 2 in Fig. 1b. The pressure range is between 0.1 and 12.0 MPa. The white line in Figs. 2(i)-2(vii) is heat release contour which indicates a reaction front. The top left figure is the superimposed contours with black line of heat release in Figs. 2(i)-2(vii) on the dashed square region of 2 in Fig. 1b. A transverse wave and a transverse detonation associated with transverse wave are observed in Fig. 2(i). The reaction front shows a wedge shape behind the transverse wave and follows the transverse detonation behind it as shown by heat release contour in Fig. 2(i). The unburned gas surrounded reacting or reacted one called as an unburned gas pocket appears due to the configuration of reaction front when a local explosion occurs by interference of the transverse waves (the transverse wave and the transverse detonation) as shown in Fig. 2(iii). Then the transverse detonation eats up the unburned gas as it propagates further. In the case of Fig. 2, the transverse wave reformed by the local explosion divides by two; one is A-B in Fig. 2(iv) to propagate along the primary detonation front, and another is C-D propagates through the unburned gas pocket.



Fig. 3. The detailed structure of detonation front in Fig.2(vii). (a) Pressure and (b) heat release contours in the dashed square region of 2 in Fig. 1b at time after local explosion.

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The detailed structure in Fig. 2(vii) is described in Fig. 3. The detonation front is composed of the incident shock, reflected shock, Mach stem, and two transverse detonation fronts in this region. The shock configuration propagating down in Fig. 4 is the double Mach interaction. The primary triple point has an incident shock, reflected shock and Mach stem, The secondary triple point exists backward soon from the primary triple point. The darker region of Fig. 3b shows a high heat release which indicates reaction front. The region between the shock and the reaction front is an induction zone. The gas behind the Mach stem reacts actively with the higher pressure by the strong shock. On the other hand, the gas behind the incident shock reacts passively with the lower pressure by the weak shock. Looking at near the reflected shock, the reaction zone in the Mach stem side involves unburned gas in induction zone in the incident shock side. As the result, the reflected shock is strengthened by the reaction. This reaction drives the transverse wave.



Fig. 4. The pressure range is between 0.1 and 12.0 MPa. The white line in Figs. 4(i)-4(vii) is heat release contour which indicates a reaction front. The top left figure is the superimposed contours with black line of heat release in Figs. 4(i)-4(vii) on the dashed square region of 4 in Fig. 1b.

Figures 4(i)-4(vii) show the time sequence distributions of pressure in the dashed square region of 4 in Fig. 1b. The pressure range is between 0.1 and 12.0 MPa. The white line in Figs. 4(i)-4(vii) is heat release contour which indicates a reaction front. The top left figure is the superimposed contours with black line of heat release in Figs. 4(i)-4(vii) on the dashed square region of 4 in Fig. 1b. The transverse detonation is observed. The transverse detonation stretches with propagating into downward region. The detailed configuration of the detonation structure is shown in Fig. 5, where the complex Mach interaction is formed. Many secondary triple points appear at the transverse detonation front and draws transverse detonation cell in Fig. 1b. The secondary triple points propagate to the Mach stem and disturb. This disturbance may develop new transverse wave. The trajectory of the new transverse wave bifurcates and show fine cells in main cellular structure.

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Fig. 5. The detailed structure of detonation front in Fig.4iii. (a) Pressure and (b) heat release contours in the dashed square region of 2 in Fig. 1b at time after local explosion.

4 Conclusions

The hydrogen-oxygen cylindrical detonation is calculated using by two-dimensional simulation. We obtain the transverse detonation cell and understand the followings.

• The transverse detonation cell appears in the area where the cell size is large due to expand of detonation front.

•The fine cell appear in the region near the transverse detonation cell.

•The secondary triple points disturb the Mach stem and develop new transvers wave.

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