Three-dimensional Numerical Simulation of Hydrogen/Air CJ Detonation : Diagonal Structure

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1. Introduction

Detonation waves consist of a combination of a shock wave and a flame propagating at supersonic speed; they have been studied for over a hundred and twenty years. Their detailed structure and properties have been revealed in experiments and numerical simulations as well as theoretical analysis. Motivations to study detonation are driven by both fundamental understanding and applications such as pulse detonation engine (PDE). Experimental research on the three-dimensional detonation structure in rectangular tubes has been carried out by many researchers. However, it is difficult to reveal the detailed three-dimensional structure by the experimental approaches[1]. Williams et al. studied the three-dimensional simulations and presented the rectangular mode[2, 3]. The authors had been presented the three-dimensional simulations for both rectangular and diagonal modes, however, the detonation was a overdriven case [4]. The purpose of the present study is to investigate the three-dimensional detonation cell structure for diagonal mode by using unsteady three-dimensional simulations with a detailed chemical reaction model for hydrogen/air gaseous detonation.

2. Numerical Method

The governing equations are the Euler equations with 9 species (H_2, O_2, H, O, OH, HO_2, H_2O_2, H_2O, N_2) and 19 elementary reactions. The governing equations are explicitly integrated by the Strang type fractional step method. The chemical reaction source terms are treated in a linearly point-implicit manner. A Harten-Yee non-MUSCL type TVD scheme is used for the numerical flux. In the present simulation, the Nagoya model proposed by Hishida and Hayashi [5] is used for chemical kinetics. Inflow conditions are pressure of 1.0 atm, temperature of 300K and velocity of 1980 m/s. Results of one-dimensional simulations are used as the initial conditions for the three-dimensional simulations. The mesh used in the three-dimensional simulations is orthogonal, with $401 \times 101 \times 101$ grid points and the grid size is also 5 μm. This corresponds to a resolution of 32 grid points in the theoretical half reaction length which for H_2 at atmospheric pressure equals 1.6×10^{-4}m. Accordingly, the computational domain is $2.0 \times 0.5 \times 0.5$ mm.

3. Results and Discussions

Figure 1 shows maximum pressure history for two-dimensional and three-dimensional results. The channel width is 0.5 mm, and each bottom figure is mirror image. For the two-dimensional simulations in Fig. 1(a), a slight unstable detonation is observed because of narrow channel width. Figure 1(b) shows the results for the diagonal mode (mode D). Lines of triple points propagate diagonally in this mode. The cell length for mode D is three-fourths of that for two-dimensional results. Its ratio agrees well with the experimental results [1].

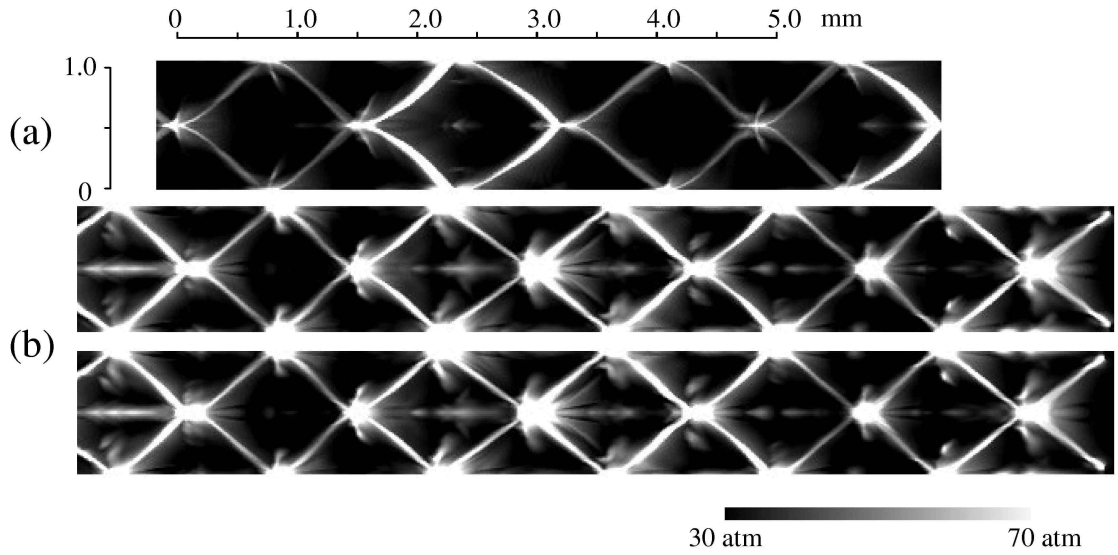

Figure 1. Comparison of maximum pressure history. (a) Two-dimensional results; (b) three-dimensional results for the diagonal mode (mode D), respectively. The top part in (b) is the lower (horizontal) wall of the tube, and the bottom part is the side (vertical) wall of the tube, respectively.

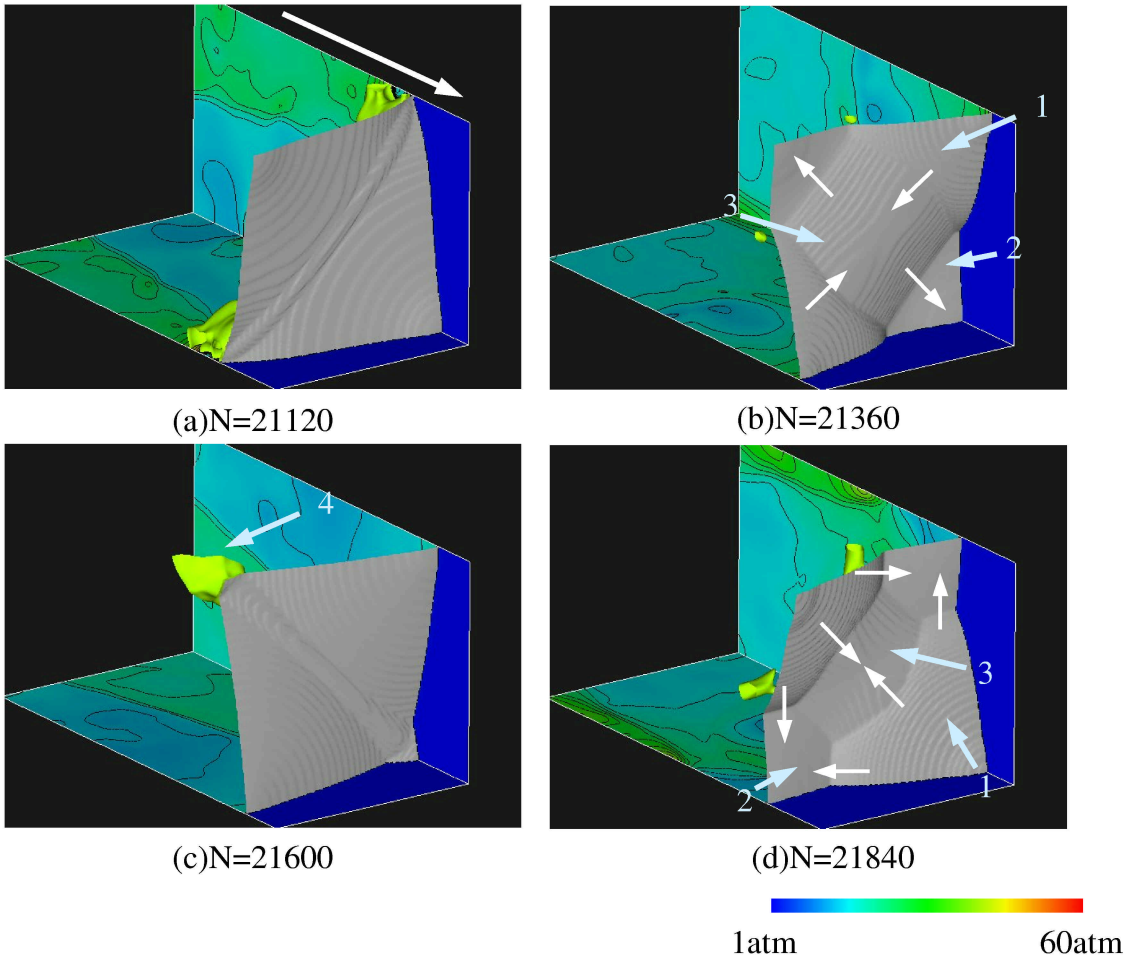

Figure 2. Instantaneous pressure space isosurface and contours in front of the detonation for the diagonal mode. The lime green space isosurface is pressure of 40 atm. The gray space isosurface denotes detonation front. The white arrows near the detonation front denote the propagation direction of line of triple points: 1,3 - Mach stem, 2 - incident shock, 4 - high pressure area behind the front.

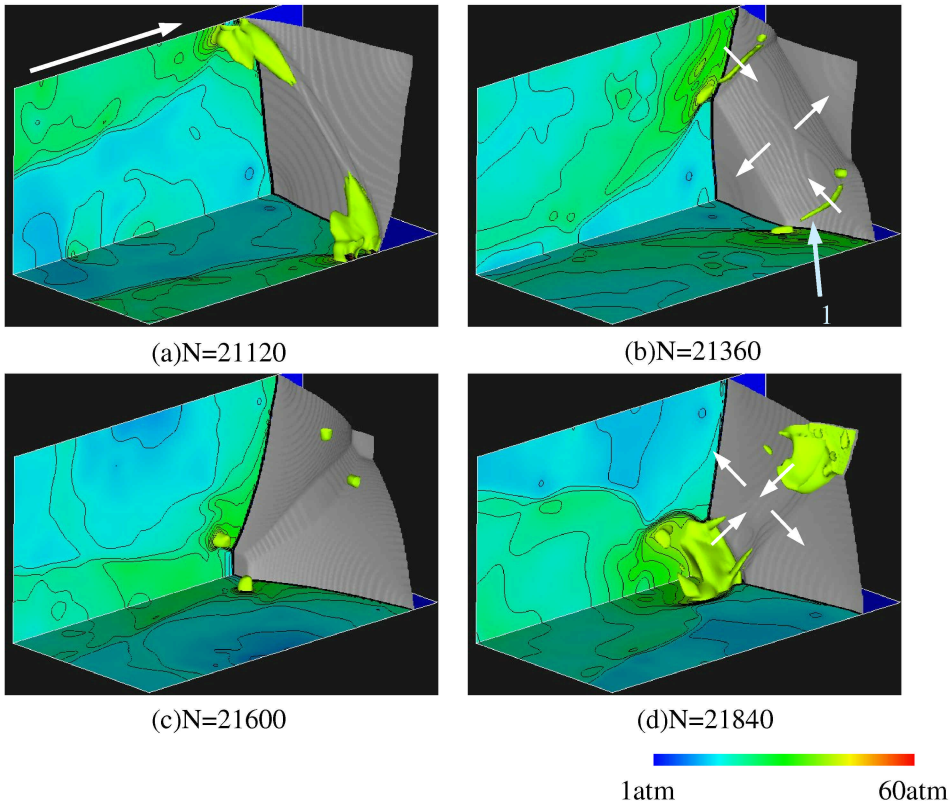

Figure 3. Instantaneous pressure space isosurface and contours behind the detonation for the diagonal mode. The lime green space isosurface is pressure of 40 atm. The gray space isosurface denotes detonation front. The white arrows near the detonation front denote the propagation direction of line of triple points: 1 - high pressure area near the transverse wave.

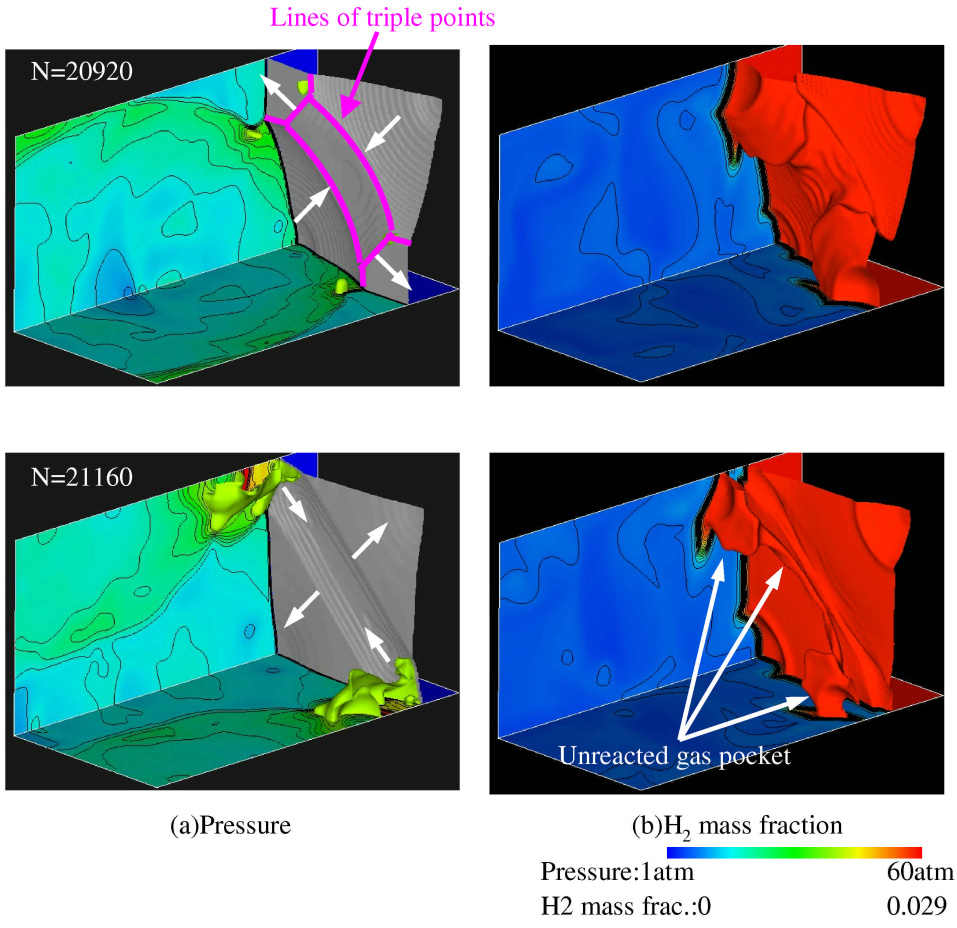

Figure 4. Instantaneous pressure and hydrogen mass fraction space isosurface contours behind the detonation front for the diagonal mode.

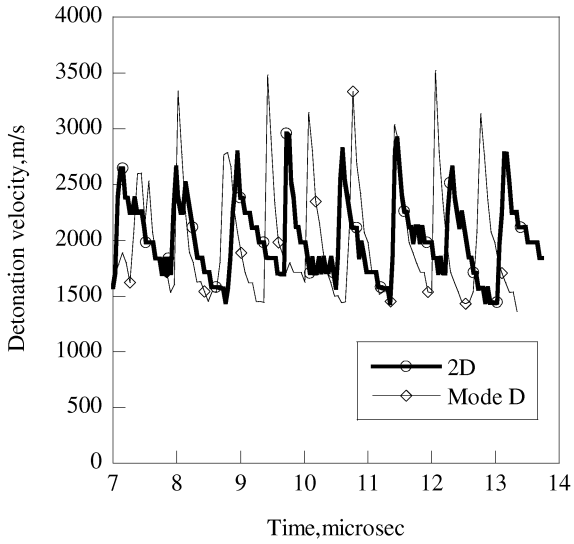

Figure 5. Instantaneous detonation velocity for both results.

Figures 2 and 3 show a periodic pattern of pressure contours for mode D. The lines of triple points appear at the boundary between Mach stem and incident shock, and they propagate toward the diagonal direction. In Figs.2(a) and 3(a), lines of triple points collide at the diagonal line in the tube. Explosions are also observed near the tube corner. Then Mach stems (labeled 1 at N=21360) are generated and spread from the tube corner, and another Mach stems (labeled 3 at N=21360) appear from the diagonal line in the tube. Symmetrical front pattern such as Figs. 2(a) and (c) are successively repeated.

In the present simulations, a detailed chemical reaction model is used to evaluate formation of unreacted pockets in detail. An example of formation of an unreacted pocket is shown in Fig. 4. This figure shows pressure and H_2 mass fraction space isosurface and contours just before and after the lines of triple points collide with the walls for mode D. When the lines of triple points focus onto the cube corner or tube center, unreacted pockets are generated in the vicinity of the detonation front. It is observed that the unreacted pocket near the corner has larger domain than that near the tube center.

Instantaneous detonation velocities for both results are plotted in Fig. 5. The detonation velocity for mode D is calculated at tube corner. Both detonation velocities decay almost exponentially in the first half of a cellular cycle and then gradually decay in the latter half of a cellular cycle. Maximum velocity for mode D is higher than that for two-dimensional results and the former cycle is shorter than the latter cycle. The average detonation velocity for mode D is approximately 1987 m/s whereas that for two-dimensional simulation becomes 2000 m/s because of slight unstable detonation.

4. Conclusions

Unsteady three-dimensional simulations were performed for hydrogen/air CJ detonations in a rectangular tube. One of three-dimensional modes, a diagonal mode, is simulated. A comparison of maximum pressure histories between two-dimensional and three-dimensional simulations shows that the cell length of the diagonal mode was only about 3/4 of that of the two-dimensional simulations.

The detonation front for the diagonal mode is characterized by complex three-dimensional time-dependent patterns. The patterns obtained in the simulations are qualitatively the same observed in experiments reported by many researchers.

References

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