Three-dimensional Numerical Simulation of H_2/Air Detonation in a Circular Tube : Structure of Spinning Mode

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1. Introduction

Detonation waves consist of shock waves with reaction zones propagating at supersonic speed, and they have been studied from safety engineering point of view for over a hundred years. The detailed structures and properties of the detonation have been studied experimental and numerical ways as well as theoretical approach. In a circular tube, spinning mode and multi-headed mode have been observed in the past experiments. The spinning mode is the lowest one propagating in a circular tube and it propagates with a helical track on the wall and rotates around the tube axis. Campbell and Woodhead first observed as the reproducible striations produced on high-speed photographic records of detonations in stoichiometric mixture of carbon monoxide and oxygen in 1926 [1, 2, 3]. Bone and co-workers systematically investigated the phenomenon and they concluded that spin was connected with the mode of coupling of the leading shock front and reaction zone[4, 5, 6].

Recent computational fluid dynamics (CFD) has yielded remarkable insight in these problems. Our group have simulated three-dimensional hydrogen/air detonation with a detailed chemical reaction model in a rectangular tube for about four years, and have revealed two modes, namely a rectangular mode in phase and a diagonal mode[7, 8]. On the other hand, numerical simulation in a circular tube has not been simulated well because of an existence of singular point in a tube center. Washizu et al. [9] simulated a spinning detonation in a co-axial tube by using a two-step chemical reaction model, however, their results do not mean a pure spinning detonation in a circular tube. We computed a cornstarch/oxygen two-phase detonation in a cylindrical tube and revealed a structure made up of a periodic two-headed detonation [7]. However, a spinning detonation could not be observed.

In this paper, we presented simulation of a spinning detonation in a circular tube after the spinning mode was discovered in 1928, and we revealed a three-dimensional shock structure.

2. Numerical Method

The governing equations are the Euler equations with 9 species ($H_2, O_2, H, O, OH, HO_2, H_2O_2, H_2O$, and N_2) and 18 elementary reactions and are explicitly integrated by the Strang type fractional step method. The chemical reaction source term is treated in a linearly point-implicit manner. A Harten-Yee non-MUSCL type TVD scheme is used for the numerical flux [10]. In the present simulation, the Petersen & Hanson model is used for chemical kinetics to solve detonation problems, which was proposed by Petersen and Hanson [11] as a new detailed chemical reaction model.

The computational mesh is a cylindrical system with 601x41x213 grid points. The grid sizes are 5μm in the propagating direction, 10μm near the wall and 20 μm close to the center in the radial direction, and 15μm in the circular direction along the tube wall. Therefore, computational domains are 3mm in length and 1mm in diameter. The present computed domain is small in order to maintain high resolution, however, the three-dimensional propagating structure can be revealed in the present simulation.

The boundary conditions are as follows: the upstream conditions are at pressure of 0.1 MPa and temperature of 300K, and the inflow gas is stoichiometric with H_2/air gas mixture; the wall boundary conditions are adiabatic, slip, and non-catalytic; and the downstream condition is that pressure is fixed at the boundary and other variables are extrapolated. The value of the pressure at the downstream boundary is 1.78 MPa (C-J theoretical value).

The initial conditions for the one-dimensional simulations are given in two computational domains with high pressure in the vicinity of a closed end wall and low pressure. In the three-dimensional calculation the results from the one-dimensional simulations are used as an initial condition, and sheets of unburned gas mixture behind the detonation front are artificially created. These sheets are asymmetrically formed on the circular direction. Present simulations requires about 150 hours on 8 processors of a NEC SX-6 to obtain a steady detonation.

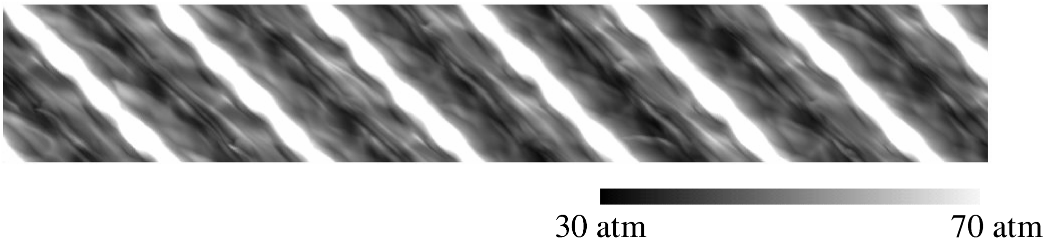


Figure 1. Maximum pressure history on the tube wall. Detonation propagates from left to right.

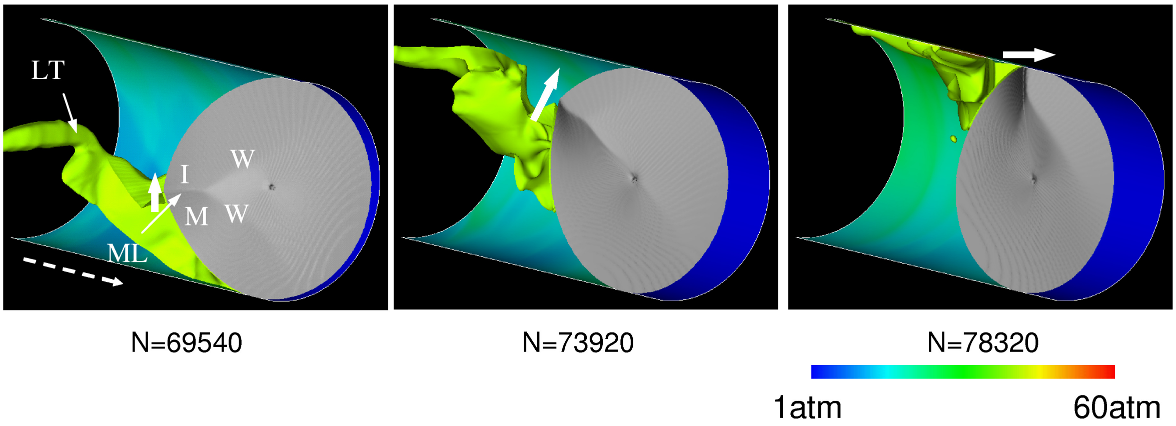


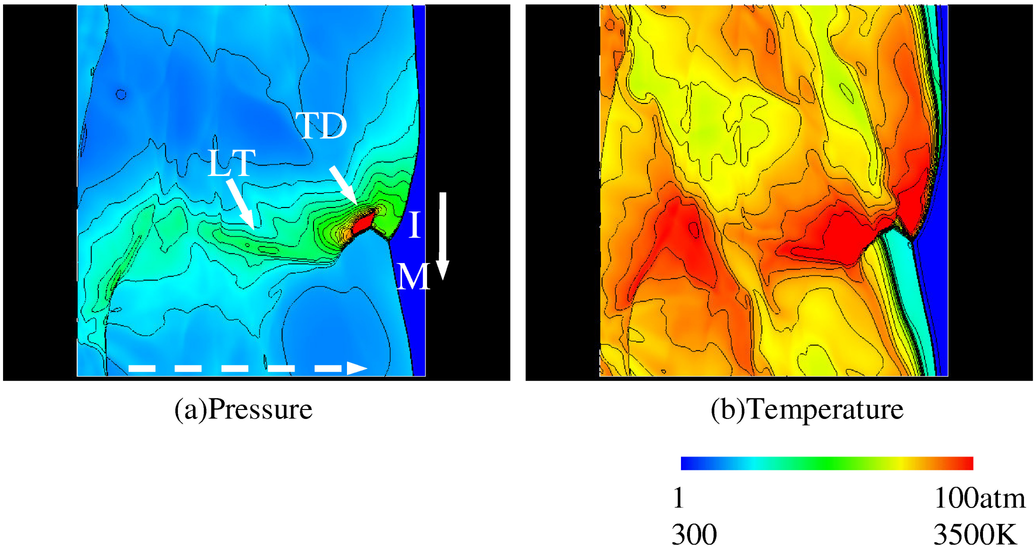
Figure 2. Instantaneous pressure space isosurfaces and contours in the tube at various times. The lime green space isosurface is pressure of 40atm. The gray space isosurface denotes the detonation front. The white broken arrow denotes the propagating direction of the detonation front, and the white arrow near the detonation front denotes rotating direction. I - incident shock side, M - Mach stem side, ML - Mach leg, W - "whisker", and LT - long trail, respectively.

3. Results and Discussions

Figure 1 shows the maximum pressure history on the tube wall. A spinning detonation pattern, which is observed experimentally, is represented, and it resembles a "ribbon" wrapped in a loose spiral. Present result is not a uniform spin, but periodically irregular spinning detonation. Schott [12] measured both uniform spin and irregular spin. He mentioned the periodically irregular spin commonly observed under his experimental conditions.

The ratio of the pitch to the tube diameter in the experiments were approximately 3 and its theoretical value is 3.13[13]. The ratio in the present simulations equals 3.0 and the results would be reliable.

The periodical motion of the spinning detonation is shown in Fig. 2. The detonation velocity is approximately 2020 m/s, and its value is 2% larger than 1980 m/s which is Chapman-Jouguet value because the present downstream boundary affects. At N=69450, a triple line shaped a stationary Mach configuration with a strongly developed "leg" is observed near the wall. The Mach configuration consists of "leg" and one or two "Whiskers"[14]. "Leg" is called as Mach leg[14]. Incident and reflected waves similar to "Whiskers" adjoining the leg at the triple point are obviously shock waves and their intensity drops rapidly with increase of distance from wall of tube. The Mach leg is orthogonal to the tube wall. At N=73920, one whisker disappears, and the other and the Mach leg are joined. The inboard part of the Mach leg travels faster than the outerboard part of the Mach leg. The former overtakes the latter at N=73920. Then the Mach leg also separates into a Mach leg and two whiskers such as at N=78320 again. The Mach leg rotates at the counterclockwise direction in the present results.



(a)Pressure

(b)Temperature

Figure 3. Instantaneous pressure and temperature contours. The white broken arrow denotes the propagating direction of the detonation front, and the white arrow near the detonation front denotes rotating direction. I - incident shock side, M - Mach stem side, TD - transverse detonation, and LT - long trail, respectively.

Figure 3 shows pressure and temperature contours on the tube wall. The transverse detonation rotates from top to bottom in this figure. While the transverse detonation oscillates slightly, the overall shock structure maintains same structure. The incident shock wave is strongly curved, and it keeps overdriven detonation. The long pressure trail is observed downstream of the transverse detonation. The long trail is diffused and it become a weak pressure wave far from the detonation front.

Thus far, we have simulated a spinning detonation in a circular tube and reveal its structure after a single spinning detonation was experimentally discovered in 1926 by Campbell and his colleagues.

4. Conclusions

Unsteady three-dimensional simulations were performed for hydrogen/air detonations in a circular tube. The lowest mode, namely, a single spinning detonation, was simulated. The maximum pressure history shows the ratio of the pitch to the tube diameter equals 3, and it agrees well with the experimental results and theoretical prediction. The transverse detonation and the long pressure trail appeared in the present simulation. They are experimentally observed, however, their three-dimensional structure and unsteady motion were unclear. Present simulation would discover new physics about the spinning detonation after the single spinning detonation was discovered in 1926.

Acknowledgements

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