Research paper

Effects of initial pressure on single spinning detonation in a square tube

Nobuyuki Tsuboi*†, Makoto Asahara**, and A. Koichi Hayashi**

*Institute of Space and Astronautical Science / Japan Aerospace Exploration Agency, 3-1-1 Yoshinodai, Sagamihara, Kanagawa 229-8510, JAPAN
† Corresponding address: tsuboi@flab.eng.isas.jaxa.jp

**Aoyama Gakuin University, 5-10-1 Fuchinobe, Sagamihara, Kanagawa 229-8558, JAPAN

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Abstract

Numerical researches for unsteady three-dimensional detonations in a square tube are presented in order to understand characteristics of single spin mode in a hydrogen / air gas mixture. The results show that the strength of the transverse detonation and the existence of the spin detonation depend on the initial pressure because the release energy in CJ state decreases as the initial pressure decreases.

Keywords: Detailed chemical reaction model, Detonation, Numerical simulation.

1. Introduction

Spinning detonations in a square tube have been observed in a few past experiments and have been studied in order to reveal its shock structure for over eighty years. The spinning detonation in a square tube, which propagates with a helical track on the wall and rotates around the tube axis, has a similar shock structure with that in a circular tube. 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)~3)]. They obtained spinning detonation in not only a circular tube but also non-circular tube such as a square tube. Oppenheim presented a smoke-film record of the spinning detonation in a square cross section tube [4)].

Recent computational fluid dynamics (CFD) has yielded remarkable insight in these problems. Three-dimensional simulations have been performed by Williams et al., who studied the rectangular mode in a square tube [5), 6)], and by the present authors [7)~9)].

There exists two modes for the three-dimensional detonation in a square tube; namely a rectangular mode and a diagonal mode. Furthermore, there are two types in the rectangular mode; in phase and partially out of phase. These rectangular modes consist of two two-dimensional waves. The three-dimensional cell length for these rectangular modes is approximately the same as the two-dimensional cell length. The diagonal mode shows a three-dimensional diagonal motion of the triple point lines and cannot be simulated by two-dimensional calculations. The single spinning detonation in a square tube, which also has a three-dimensional shock structure, has not been simulated, successfully simulated by some of the authors to find the unstable three-dimensional shock structure [10), 11)]. Some researchers experimentally tried to find the dependence of the initial pressure and composition of gas mixture on the detonation structure; however, it is not enough to understand the dependence of them on its structure.

In this paper, we presented simulations of single spinning detonations in a square tube in order to understand the effect of the initial pressure.

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 they 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 [12)]. The Petersen and Hanson model is used for chemical kinetics to solve detonation problems [13)].

The computational mesh for all cases is a rectangular system with 601x101x101 grid points. The grid sizes for initial pressure p_0 of 0.1 MPa are 5 μm in the propagating direction 10 μm in the other directions for atmospheric

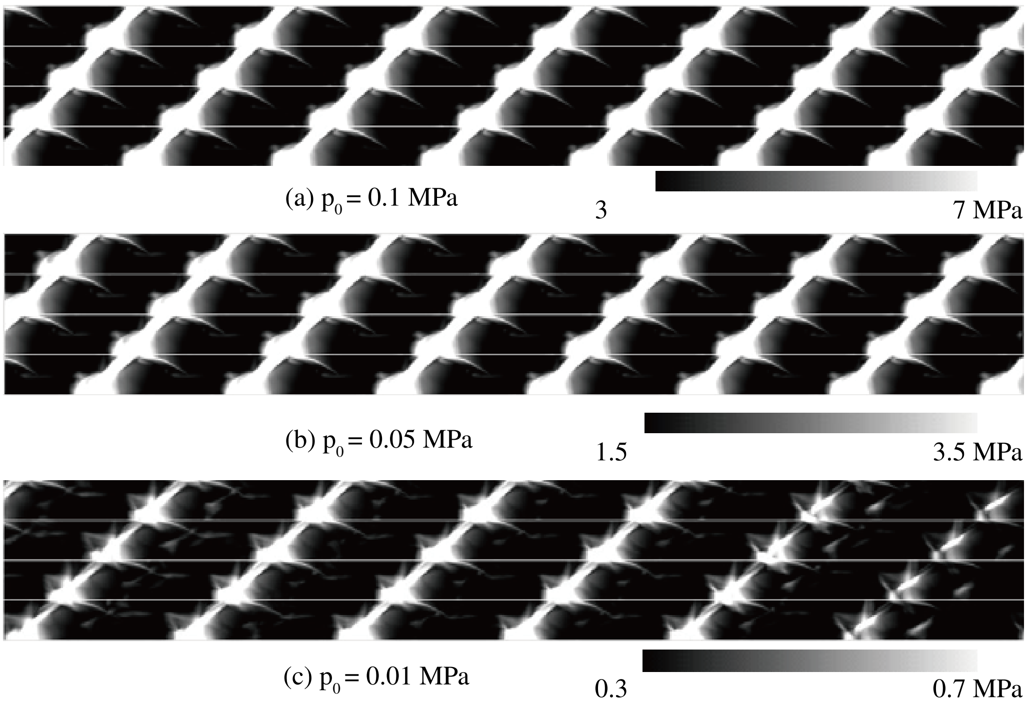

Fig. 1 Maximum pressure history on the tube wall. Detonation propagates from left to right.

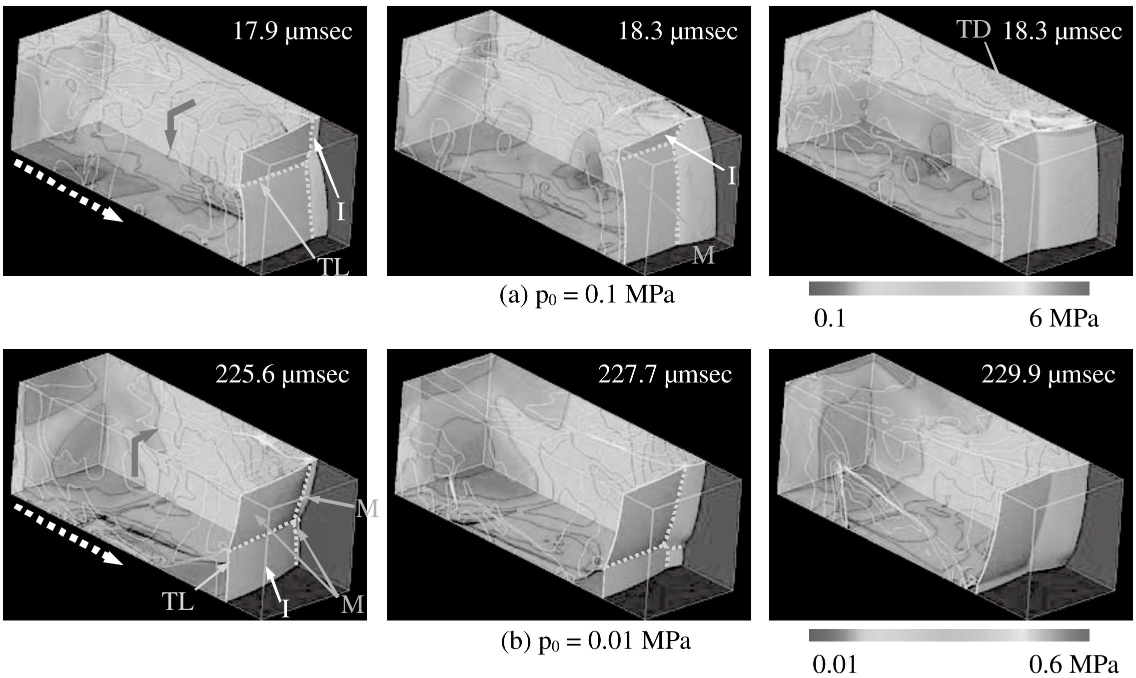

Fig. 2 Comparison of instantaneous pressure space isosurfaces and contours in the tube at various times.
The lime green space isosurface is pressure of 4 Mpa (p_0 = 0.1 MPa) or 0.4 Mpa (p_0 = 0.01 MPa). The gray space isosurface denotes the detonation front. The white broken arrow denotes the propagating direction of the detonation front, and the red arrow near the detonation front denotes the rotating direction. I-incident shock side, M-Mach stem side, TD-transverse detonation, and TL-triple line, respectively.

pressure, respectively. Five micrometers correspond to a resolution of 32 grid points in the theoretical half reaction length which equals 1.6×10^{-4} m for H_2. Therefore, computational domains are 3 mm in length and 1mm in width. For initial pressure of 0.05 or 0.01 MPa, all scales are multiplied by five or ten. The present computed domain is small in order to maintain high resolution, however, the three-dimensional propagating structure can be revealed in such a small scale.

The boundary conditions are as follows: the upstream conditions are at pressure of 0.1, 0.05 or 0.01 MPa and temperature of 300 K, 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 the non-reflected boundary proposed by Gamezo et al. [14].

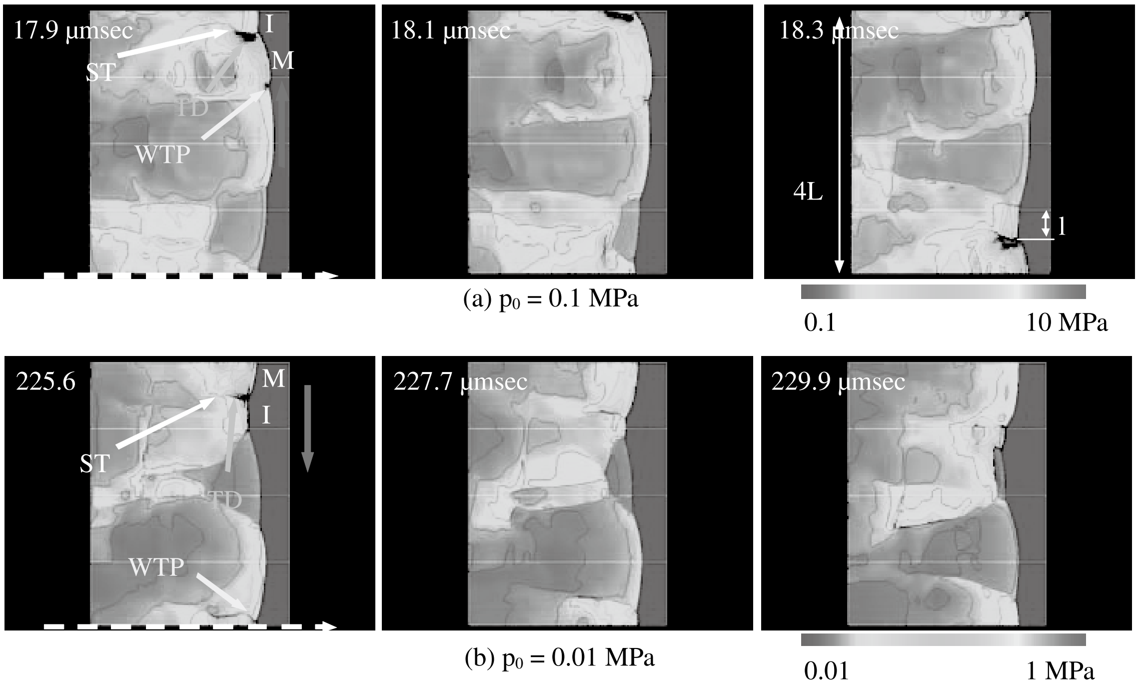

Fig. 3 Comparison of instantaneous pressure contours on the wall. The white broken arrow denotes the propagating direction of the detonation front, and the red arrow near the detonation front denotes the rotating direction. I-incident shock side, M-Mach stem side, TD-transverse detonation, ST-short pressure trail, and WTP-weak triple point, respectively.

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. Present simulations requires about 150 hours for all cases on 8 processors of a NEC SX-6 to obtain a steady spinning detonation.

3. Results and discussion

Figure 1 shows a comparison of maximum pressure histories on the wall. A spinning detonation pattern which is observed experimentally resembles a "ribbon" wrapped in a loose spiral for both cases. The calculated track angle is 47 deg. for p_0 = 0.1 and 0.05 MPa, and 44 deg. for p_0 = 0.01 MPa, respectively. The track angle for p_0 = 0.01 MPa is smaller than the experimental data which are appriximately 49 deg and the spinning detonation for p_0 = 0.01 MPa disappers because the release energy in CJ state (175.48 kJ · mol^{-1}) for p_0 = 0.01 MPa is lower than the other cases (192.36 kJ · mol^{-1} for p_0 = 0.1 MPa and 187.46 kJ · mol^{-1} for p_0 = 0.05 MPa). The effects of the initial pressure are also observed in the band width. The detailed comparison between the experimental results and numerical simulation for p_0 = 0.1 MPa is presented in Ref. 11. Cellular structures in the transverse detonation rotating along the wall do not appear in the present results because grid resolution may require higher than the present simulations.

Figure 2 presents instantaneous detonation front shapes viewed from the front side at various times. The orthogonal triple lines are always observed on the detonation front. Three Mach stems and one incident shock are separated by the triple lines. The vertical and the horizontal triple lines move partially out of phase, therefore the present spinning mode is the rectangular mode partially out of phase. These triple lines in the diagonal mode and the rectangular mode in phase move in phase in our past simulations [7], which differ from the present results. The overall shock structures do not dependent on the initial pressure.

Figure 3 shows instantaneous pressure contours on the wall. A transverse detonation is observed for both cases. Furthermore, a weak triple point which is reflected from the orthogonal wall also propagates along the wall for both cases. The transverse detonation for p_0 = 0.01 MPa is weaker than that for p_0 = 0.1 MPa because the release energy decreases as the initial pressure decreases.

The calculated averaged detonation velocities on the corner in the tube during one cycle for various initial pressures are plotted in Fig. 4. At the initial stage of starting the spinning detonation, the velocities are overdriven for all cases; however, their velocities decrease linearly to become the value lowers than the CJ detonation velocity. The detonation velocities for p_0 = 0.01 MPa become approximately 0.85 D_{CJ} and finaly the detonation disappears.

Evolution of pressure ratios behind the head of the spinning detonation on the tube wall during one quarter cycle is plotted in Fig. 5. The locations of these pressures are also shown in this figure. The pressure ratio behind the incident shock, $p_1 \cdot p_0^{-1}$, is approximately 20 except the beginning of one quarter cycle because the angle of the incident shock is not normal to the side wall. The averaged

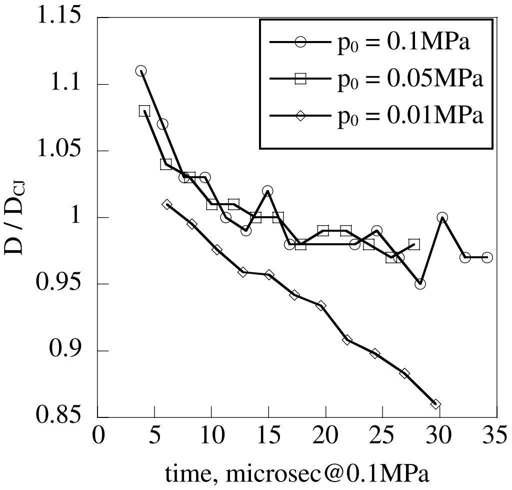

Fig. 4 Initial pressure effects on detonation velocity along the tube corner.

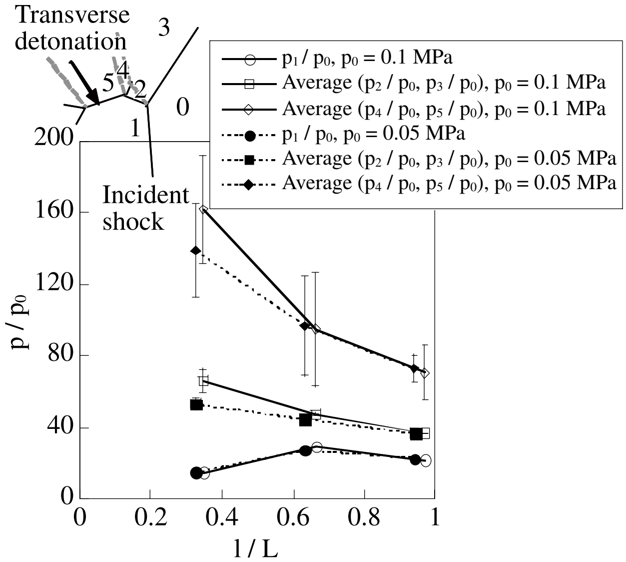

Fig. 5 Evolution of pressure ratio behind the head of the spinning detonation on the tube wall during one quarter cycle.

values between the pressure ratio behind the Mach stem, $p_3 \cdot p_0^{-1}$, and that near the reflected shock, $p_2 \cdot p_0^{-1}$, are plotted in this figure. They decrease to become approximately 40 after the averaged value is equal to 70 at $l \cdot L^{-1}$ = 0.95 due to the explosion of the transverse detonation with the wall. The average value between the maximum pressure ratio near the transverse detonation, $p_4 \cdot p_0^{-1}$ and $p_5 \cdot p_0^{-1}$, is equal to 160 and it decreases to be 80 asymptotically. This means that the strength of the transverse detonation changes during the on quarter cycle. The pressure ratios around the transverse detoination and that behind the Mach stem for p_0 = 0.1 MPa are 10 % lower than those for p_0 = 0.05 MPa because the release energy depends on the initial pressure.

4. Conclusion

Unsteady three-dimensional simulations with a detailed reaction model were performed for the stoichiometric hydrogen/air mixture in the square tube in order to understand the effects of the initial pressure on the detonation structure. The instantaneous shock structures in all cases have similar pattern; however, the track angle and the band width on the maximum pressure history on the wall depend on the initial pressure because the release energy also depends on the initial pressure.

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References

1) C.Campbell, D.W.Woodhead, J. Chem. Soc., 3010 (1926).
2) C.Campbell, D.W.Woodhead, J. Chem. Soc., 1572 (1927).
3) C.Campbell, A.C. Finch, J. Chem. Soc., 2094 (1928).
4) J.H. Lee, R.I. Soloukhin, A.K. Oppenheim, Astron. Acta. 14, 565 - 584 (1969).
5) D.N. Williams, L. Bauwens, and E.S. Oran, Proc. Comb. Inst. 26: 2991 - 2998 (1996).
6) D.N. Williams, L. Bauwens, and E. S. Oran, 16th ICDERS, pp. 374 - 376 (1997).
7) N. Tsuboi, S. Katoh, and A.K. Hayashi, Proc. Comb. Inst. 29: 2783 - 2788 (2002).
8) K. Eto, N. Tsuboi, and A.K. Hayashi, Proc. Comb. Inst. 30: 1907 - 1913 (2005).
9) K. Eto, N. Tsuboi, and A. K. Hayashi, AIAA paper, 2004-0311 (2004).
10) A.K. Hayashi, K. Eto, N. Tsuboi, 20th ICDERS No. 85 (2005).
11) N. Tsuboi, and A. K. Hayashi, Proc. Comb. Inst. 31: 2389 - 2396 (2006).
12) H. C. Yee, NASA Technical Memorandum 89464 (1987).
13) R. L. Petersen, and R. K. Hanson, J. Propulsion Power 15: 591 - 600 (1999).
14) V. N. Gamezo, D. Desbordes, and E. S. Oran, Shock Waves 9: 11 - 17 (1999).