Three-Dimensional Parallel Simulation of Cornstarch-Oxygen Two-Phase Detonation

Nobuyuki. Tsuboi,[*] A.Koichi Hayashi,[**] and Yoichiro Matsumoto[†]

[*]Dept. of Mech. Eng., The University of Tokyo, E-mail:tsuboi@fel.t.u-tokyo.ac.jp
[**]Dept. of Mech. Eng., Aoyama Gakuin Univ., E-mail:hayashi@me.aoyama.ac.jp
[†]Dept. of Mech. Eng., The University of Tokyo, E-mail:ymats@mech.t.u-tokyo.ac.jp

Abstract

Numerical simulation with a parallel computer is conducted to solve three-dimensional gas-solid two-phase detonation. The numerical flux applies a second-order modified Harten-Yee TVD upwind method and time integration uses Euler integration. Reaction model adopts a 2-step chemical reaction model for cornstarch-particles. The numerical results show that the periodic two-headed detonation with a complicated flow structure is obtained. The comparison between the numerical and experimental results reveals that the detonation velocity of numerical results agrees well with that of experimental results.

Introduction

Recently, there have been many studies related with gas-solid two-phase detonations in order to obtain the detail of structure of the detonation, mechanism of Deflagration-to-Detonation Transition (DDT) and so on. In experimental studies, velocity and pressure profiles have been measured to clarify DDT by using the tube where particles are dispersed or layered [1]-[2]. In numerical studies, structures and DDT have been analyzed by one- and two-dimensional numerical simulations [3]-[4]. The gas-solid two-phase detonation has some different characteristics from the gas-phase detonation, although the gas-phase reaction still has an important role on the propagation of detonation in two-phase detonation. Thus, the rates of gasification and diffusion of gaseous fuel result in an increase of the induction time of the two-phase reaction. Besides, the thermal relaxation of the solid phase behind a shock front also retards the ignition. A large induction time corresponds to a large cell size, so that a sufficient length is required for transition to a self-sustained dust detonation wave with a large diamond structure in a tube.

The purpose of the present study is to investigate the detonation cell structure and the mechanism of propagation of cornstarch particle-oxygen two-phase detonation in a circular tube performing unsteady three-dimensional numerical simulations. Especially, the unsteady three-dimensional two-phase simulation requires a large amount of computational time so that the present simulation code is improved to have a superior parallel efficiency.

Modeling

The Euler equations are used for both gas and solid phases with assumptions that both phases can be taken as continuous. The gas mixture is assumed to consist of O_2, H_2O, CO_2 and N_2, and gaseous volatility emitted from cornstarch particles. The particles are treated as rigid spheres with a constant specific heat and uniform internal temperature, and particle collisions are considered.

The governing equations have an unsteady three-dimensional conservative form in order to apply for a TVD(Total Variation Diminishing) scheme, therefore a solid-phase stress term is introduced in the momentum and energy equations. External forces are neglected. The constant pressure specific heat of species is provided by the polynomial function of temperature where their coefficients are obtained from JANAF table. The molecular viscosity, thermal conductivity, and diffusion as well as the drag force and heat conduction between two phase are considered.

A two-step chemical reaction model for cornstarch particles is employed since the actual combustion process of a cornstarch particle which consists of liquidizing, gasifying, and providing ashes is too complex to solve with the elementary reaction model.

Numerical method

The governing equations are solved using the second-order Harten-Yee non-MUSCL modified-flux type TVD-upwind scheme for the convective terms and the second-order central difference method for the diffusion terms. Euler explicit integration is used for the time integration. The interaction and production terms are calculated explicitly. The averaged state on a cell boundary is given by the generalized Roe's average to evaluate the numerical flux in the convective terms.

In order to simulate a two-phase detonation wave in a circular tube using a moving grid coordinate system, a computational grid system of 161 points in the propagating direction (Δx=1 mm), 26 points in the radial direction and 40 points in the circular direction is applied. The tube diameter is 141 mm. Also, in order to obtain the numerical smoked foil record, a laboratory coordinate system of 6002 points in the propagating direction (Δx=1 mm) is set to calculate the maximum pressure for "scratching" the smoked foil on each grid point.

The adiabatic condition is applied for the wall of the circular tube. The inflow condition provides the unburned mixture flow. In the outflow condition, the zeroth-order extrapolation is used for the subsonic case and the second-order extrapolation for the supersonic cases.

The initial condition is given that an artificial perturbation is set by sifting the only gaseous data toward the propagating direction, considering that the one-dimensional steady solution obtained from the Rankine-Hugoniot relation can be arranged uniformly in the three-dimensional space since the experimental C-J detonation velocity is quite consistent with the one-dimensional C-J values [5]. The present one-dimensional solutions are calculated using the initial conditions at the pressure of 1.0 atm, temperature of 293.15 K, incident shock Mach number of 3.5, cornstarch particle radius of 5.0 μm and stoichiometric ratios of 0.45 with oxygen as an oxidizer.

The parallel implementation is based on the computational domain decomposition in order to reduce the calculation time. The radial and circular directions are divided to allocate to each processor. Flow quantities and numerical flux that locate in the subdomain boundaries are sent to the appropriate processor using MPI(Message Passing Interface) message passing scheme. The performance parallel computing of the code was measured on IBM SP2. A linear speed performance is attained at the various number of processors and the speed performance with 16 CPUs is 12.38.

Results and discussions

The pressure contours on $\theta = 0 + 180$ degs. plane in the tube at the various time during one

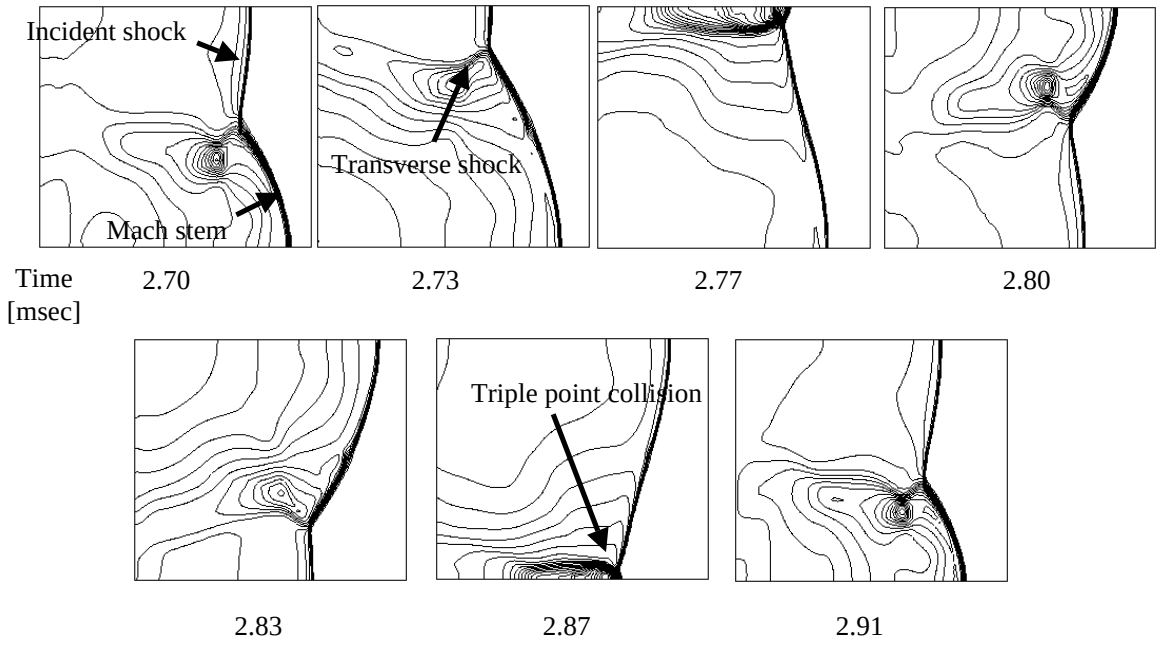

Figure 1: Pressure contours at various time on $\theta = 0 + 180$ degs. plane in the tube.

period of detonation are shown in Fig. 1. As discussed later, the numerical results for detonation show a steady state mode. It is shown that Mach stem, incident shock, and transverse shock are captured clearly. Triple point movements in the tube and triple point collisions on the wall are also simulated. When the triple point collides on the wall at time=2.77 and 2.87 msec., high pressure region appears between the transverse shock and the wall.

Figure 2 shows the pressure contours on the wall at various time during one cellular cycle of det-

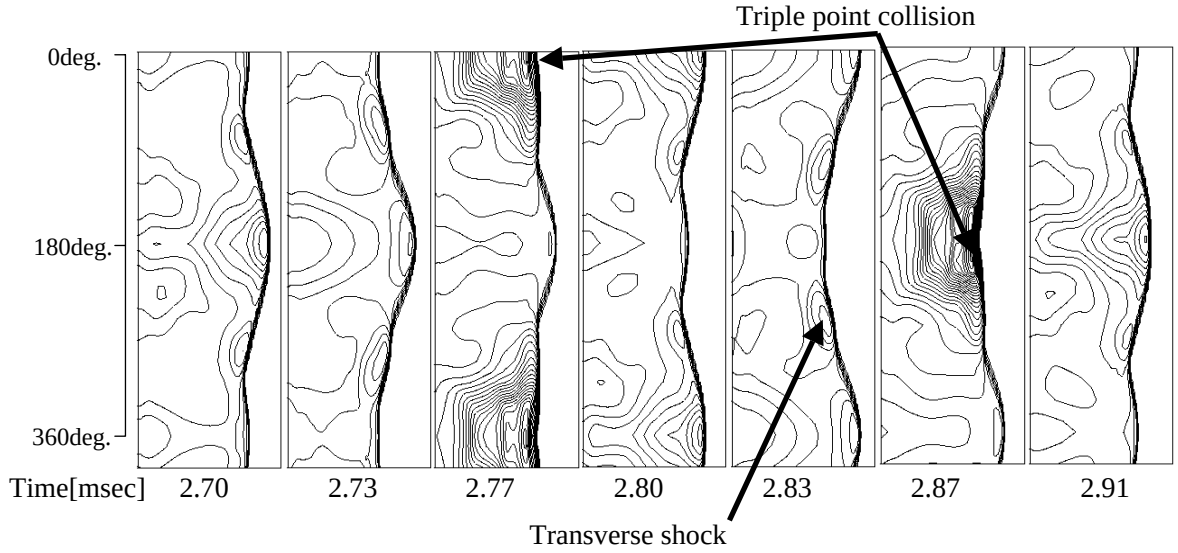

Figure 2: Pressure contours at various time on the tube wall.

onation. The figure shows that the transverse shock and triple point collisions are captured in spite of less grid points(40 points) at circular direction on the wall. From Figs. 1 and 2 the three-dimensional transverse shock propagation and shock focusing phenomena exist in the tube.

Maximum pressure history contours on the wall(Fig. 3) shows that the two-headed detonation

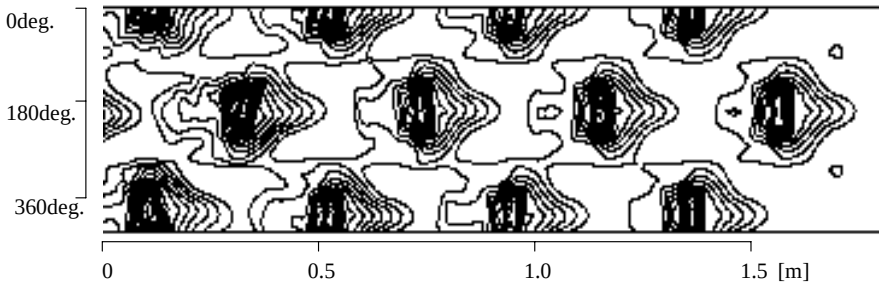

Figure 3: Maximum pressure history contours on the wall(the detonation propagates from left to right).

including triple point collision appears, however the experiment conducted by Zhang *et al.* [1] shows the existence of single spin detonation at the same unburned inflow conditions. The discrepancy between the experimental and numerical results is considered to be the effects of computational space size. When the number of grid points in the propagation direction is 81 points($\Delta x = 1mm$), the detonation pattern forms a four-headed detonation. However, the detonation pattern forms a two-headed detonation with 161 or 200 points in the propagation direction. In the simulation, the stable detonation can be usually obtained at the time of 2 msec. after starting the calculation. This implies that the sufficient grid points in the flow direction are required to simulate in present conditions.

The instantaneous detonation velocity on the wall and at symmetric line of the tube during two cellular cycles is shown in Fig. 4(a). The detonation velocity is calculated from the shock front location and its averaged detonation velocity D_{avg} is 1882 m/sec. The detonation velocity decays almost exponentially in the first half of a cellular cycle and more gradually decays in the latter half of a cellular

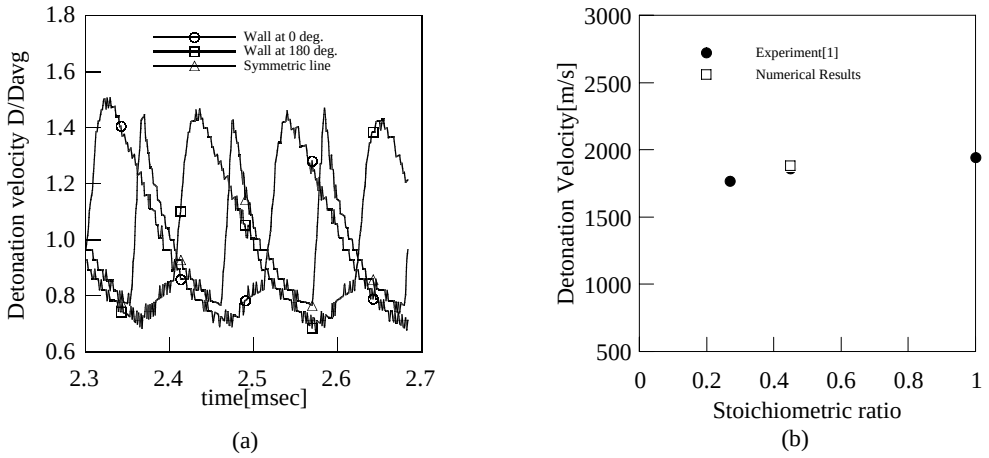

Figure 4: Detonation velocity ((a):the history of normalized instantaneous detonation velocity, (b):the comparison between experimental and numerical results).

cycle. The detonation characteristics in the two-phase media is as same as that in the single-phase reported by Oran *et al.* [6]. The variation of detonation velocity at the center line of detonation cell in the experiment [1] shows from 1.4 D_{avg} to $0.87D_{avg}$ for the two-headed detonation (the stoichiometric coefficient of 1.0 and initial pressure of 1.15 atm). In the case of numerical results, the detonation velocity on the wall at 0 deg(center of detonation cell) decreases from about $1.4D_{avg}$ to $0.7D_{avg}$, and the numerical results agrees well with the experimental results. A comparison between the experimental results [1] and numerical results with respect to the detonation velocity is shown in Fig. 4(b). The result shows that the detonation velocity agrees well with that of the experimental value.

Conclusions

The three-dimensional cornstarch/oxygen two-phase detonation is simulated using a parallel computer to show that the stable two-headed detonation is obtained. The detonation structure of the numerical simulation does not agree with that of the experimental results of a single spin detonation. However, with respect to the detonation velocity, the numerical results agree well with the experimental results. Furthermore, the detailed three-dimensional detonation structure with the propagating transverse shock, triple point collision, and so on are revealed. It is shown that the calculation region affects significantly on the detonation structure, so that a large computation region will be required to obtain a single-spin detonation.

References

[1] Zhang, F. and Grönig, H., "Spin detonation in reactive particles-oxidizing gas flow," Physics Fluids A Vol.3(8), August, p.1983-1990, 1991.

[2] Wolański, P., "Dust explosion research in Poland," Powder Technology Vol.71, p.197-206, 1992.

[3] Korobeinikov, V. P., "Numerical method for unsteady two-phase flows," 5th International Symposium on Computational Fluid Dynamics, 1993.

[4] Gonthier, K. A. and Powers, J. M., "A numerical investigation of transient detonation in granulated material," 15th International Colloquium on the Dynamics of Explosions and Reactive Systems, 1993.

[5] Kuo, K. K., Principles of combustion, A Wiley-Interscience Publication, pp 231-284, 1986.

[6] Oran, E.S. *et al.*, "A numerical study of a two-dimensional $H_2 - O_2 - Ar$ detonation using a detailed chemical reaction model," Combustion and Flame Vol.113, p.147-163, 1998.