Numerical Investigations of Spinning Detonations in a Circular Tube by One-step Reaction Model

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1 Introduction

Spinning detonation in circular tube, discovered experimentally in 1926 by Campbell and Woodhead [1–3], is observed near detonation limit and the lowest mode that has only one transverse wave in a circumference direction. The spinning detonation propagates helically on the wall and rotates around the tube axis. Schott [4] tried to understand the shock structure of spinning detonation, and he concluded that the wave front contains a complex Mach interaction. Voitekhovskii [5] and his co-workers measured the Mach configuration by examining smoked disks attached to the end plate of the detonation tube. Their experimental observation says that it consists of a "leg" and one or two "whiskers." They also used the term "leg" as in "Mach leg." Tsuboi et al. [6] numerically studied the structure of spinning detonation using detailed reaction model. Our group [7] also studied the influence of activation energy by one-step reaction model.

Many researchers studied one-dimensional detonation using one-step reaction model by Arrhenius's form, and activation energy is chosen as a parameter. Lee and Stewart [8] reported the critical activation energy based on the stability analysis of one-dimensional detonation, where the shock pressure history oscillates when the activation energy is greater than the critical value.

The aim of this work is to clarify the effect of the diameter and activation energy to propagation of spinning detonation in a circular tube using one-step reaction model governed by Arrhenius's form. The detailed discussion is carried out to explain the influence of diameter and activation energy.

2 Numerical setup

The governing equations are the compressible and reactive two- and three-dimensional Euler equations for the calculations of channel flow and spinning detonation, respectively. The fluid is an ideal gas with constant specific heat ratio, and all diffusive are neglected. Chemistry is modeled by a one-step Arrhenius kinetics whose parameters are specific heat ratio, heat release and activation energy [7]. As discretization methods, Yee's Non-MUSCL Type 2nd-Order Upwind Scheme [9] is used for the spatial integration, and Point-Implicit Method that treats only source term implicitly is used for the time integration. Governing equations are normalized by values of standard region and half-reaction length, $L_{1/2}$, which is the distance required for mass fraction of reactant reducing to 0.5 in one-dimensional steady CJ detonation analysis. Grid resolution is defined as the number of grid points in half-reaction length. In our simulations, heat release and specific heat ratio are fixed as 50 and 1.2,

respectively. Diameter and activation energy are chosen as parameters. In this paper, we used activation energy of 10, 20, 27, 35, and 50.

The computational grid is an orthogonal system for two-dimensional calculations whose channel length is fixed as 200L1/2, and cylindrical system for spinning detonation, whose diameter is changed from 2.5L1/2 to 7.1L1/2, respectively. Previous study showed that a high grid resolution is needed for the calculation in the case of high activation energy. In all calculations, at least, 32 grid points in half reaction length L1/2 are set in all direction. The axial length in the computational grid is more than $100L_{1/2}$ to avoid disturbance from the outflow boundary which is the non-reflected boundary proposed by Gamezo et al. [10]. The present computational grid has a singular point in the tube center, where physical values are an average around it for three-dimensional calculations. The results of one-dimensional steady simulation are used as an initial condition. Sheets of two- and three-dimensional unburned gas mixture behind detonation front are artificially added in order to create initial three-dimensional disturbances.

3 Results

Previous experiments revealed the existence of critical diameter, which is empirically obtained as $D_{cr}=\lambda/\pi$ (λ : cell width). In order to discuss the effect of diameter, critical diameter Dcr is calculated by two-dimensional calculation. Figure 1 shows the smoked foil images of (a) Ea=10 and (b) Ea=27. Figure 1a shows regular cell pattern, whereas Fig. 1b shows irregular one. Because it is difficult to decide the cell width at irregular cell, the averaged value is used for it. Table 1 shows the relationship between activation energy Ea, cell width $\lambda/L_{1/2}$ and critical diameter Dcr/L_{1/2} obtained at various activation energy.

activation enegy Ea	cell width $\lambda/L_{1/2}$	critical diameter Dcr/L1/2
10	11.8	3.76
20	15.4	4.90
27	17.4	5.54
35	16.7	5.32
50	9.09	2.89

Table 1. The relationship between activation energy and critical diameter

Figure 2 shows propagation modes of spinning detonation as functions of activation energy and diameter. Circles denote that spinning detonation propagates in a stable mode, whereas cross marks denote that the spinning detonation propagates in an unstable mode. These propagation modes are discussed at our report [7]. We reported that an increase of activation energy in the cases of Ea=10, 20 and 27 at D= $3.5L_{1/2}$ makes the simulated spinning detonation unstable, but Fig. 2 shows that spinning detonation becomes stable at D= $3.5L_{1/2}$ and Ea=50. It says that the stability of spinning detonation depends not only on activation energy but also on the diameter.

The soot tracks on the tube wall were recorded in previous experimental studies [4]. A track angle, which is defined as arctangent of the spin pitch divided by the length in circumference, is derived from the experimental observation. The track angle is about 45 degrees under various experimental conditions. The simulated track angle is 33 - 42 degrees depending on the calculation condition and smaller than those of the previous experimental [4] and numerical studies [6]. It is because, in our calculations, the simulated longitudinal velocities are almost the same as CJ velocity, but simulated circumferential velocities are lower than CJ velocity. In order to clarify this reason, instantaneous distributions of pressure and mass fraction of reactant on the tube wall are used in Fig. 3, (a) Ea=10, D=5.0L1/2 and (b) Ea=50, D=3.5L1/2. The distributions on the tube wall always show a unique profile and move upward at a constant speed. Figure 3 shows the transverse wave. Previous experiments and

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numerical simulation results showed that transverse wave of spinning detonation is always transverse detonation. Because unreacted region behind transverse wave exists in Fig. 3, simulated transverse wave is not transverse detonation, and the track angle bocomes smaller than the experimental values. Difference between experiments and our calculations comes from the reaction model used in the present study.

Figure 4 shows the propagation mode, stable and unstable, of spinning detonation as functions of activation energy and diameter normalized by the critical diameter Dcr as shown in Table 1. Solid line shows empirical limit D/Dcr=1. Because spinning detonation propagates in stable mode in spite of 0.9 < D/Dcr < 1 in the case of Ea=27 and 35, empirical limit D/Dcr=1 cannot be used as a criterion for the stability of spinning detonation. As mentioned above, track angle α is smaller than 45 degrees, and then experimental limit D/Dcr=1 is modified to D/Dcr=tan α . Table 2 denotes the relationship between the activation energy and track angle at D=5.0L1/2. Dashed line in Fig. 4 shows proposed limit D/Dcr=tan α in Table 2. Figure 4 shows that D/Dcr=tan α must be the good criterion for the stability of spinning detonation. This indicates that track angle is also important parameter to determine the stability.

4 Conclusion

Spinning detonations at various activation energies and diameters were numerically investigated using three-dimensional Euler equations with a one-step chemical reaction model governed by Arrhenius kinetics. The simulated track angle was smaller than the experimental values because of the existence of unburned region behind transverse wave. Stability of spinning detonation depended not only on the activation energy but also on diameter. Critical diameter D/Dcr=tan α (Dcr= λ/π) was newly proposed, which was a good criterions for the stability of spinning detonation. In the case of D/Dcr<tan α , spinning detonation kept its propagation, but unstable mode appeared. In the case of D/Dcr>tan α , spinning detonation kept its propagation in a stable mode.

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Figure 1. Trajectory of triple points in case of (a) Ea=10 and (b) Ea=27 at two-dimensional detonation





Figure 2. The propagation mode of spinning detonation as a function of activation energy and diameter. \bigcirc : stable mode, \times : unstable mode



Figure 3. Instantaneous distribution on the wall of pressure (left) and mass fraction of reactant (right) at (a) Ea=10, $D=5.0L_{1/2}$ and (b) Ea=50, $D=3.5L_{1/2}$



Figure 4. The propagation mode of spinning detonation as a function of activation energy and normalized diameter. \bigcirc : stable mode, \times : unstable mode. Solid and dashed lines denotes D/Dcr=1 and D/Dcr=tan α , respectively.

Table 2. The relationship between the activation energy and track angle when propagation mode is stable mode at $D=5.0L_{1/2}$.

activation energy	track angle α	$tan\alpha$
10	37.4	0.765
20	39.6	0.827
27	40.8	0.863
35	41.2	0.875
50	42.5	0.916