**Numerical analysis on acoustic coupling of spinning detonation in a square tube**

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Abstract
We investigate spinning detonations propagating in a square tube using numerical simulations based on three-dimensional compressible Euler equations and the two-step-reaction model proposed by Korobeinikov et al. The dynamics of the simulation results is used to understand how spinning detonations propagate. The track angles calculated from soot-track images of the square-tube walls are numerically reproduced for various initial pressures and channel length. The results show that the numerically obtained track angles are consistent with those of the previous reports. The spinning detonation maintains its propagation when the rotating transverse detonation completely consumes any unburned gas. Transverse detonation is important for the propagation of spinning detonations. We also discuss acoustic coupling between the transverse detonation and the acoustic wave that propagates along the wall. The rotating transverse detonation propagates with successive reflections off the walls, and acoustic waves are generated at the reflections. When the spinning detonation maintains its propagation, the rotating transverse detonation couples with the acoustic wave traveling between the walls. We analyze the maximum and minimum track angles that allow the coupling and propagation of a spinning detonation in a square tube to be maintained and find that the simulated track angles fall within the estimated maximum and minimum track angles. This result indicates that acoustic coupling is important for maintaining propagation of a spinning detonation in a square tube.

Key words: Spinning detonation, Propagation mechanism, Detonation limit, Acoustic coupling, CFD

1. Introduction

Detonations are supersonic flow phenomena with leading shock waves that ignite premixed gas. Many researchers have used experimental, theoretical, and numerical approaches to investigate the structure and properties of detonations. Detonation has experimentally shown to propagate both longitudinally and transversely and contain an unstable three-dimensional structure. The detonation shock structure comprises an incident shock wave, a Mach stem, and transverse waves that propagate perpendicular to the shock front. A few modes have been observed in detonation in circular and square tubes, such as the spinning mode (single-headed) and multi-headed modes, which are classified according to the number of transverse waves. Spinning detonations in circular tubes, discovered experimentally by Campbell and Woodhead (1926, 1927) and Campbell and Finch (1928), occur near the detonation limit and the lowest mode has only one transverse wave in the circumferential direction. Edwards et al. (1966) studied how spinning detonations propagate in a square tube.

Over the last two decades, many researchers have investigated multidimensional detonation, and numerical studies have led to remarkable insights into their propagation and physics. For example, Williams et al. (1996) studied the two-headed mode in a square tube. Deledicque and Papalexandris (2006) studied the multiheaded mode in a rectangular tube using the one-step chemical-reaction model based on the Arrhenius form. Using a detailed reaction model, Eto et al. (2005) and Tsuboi et al. (2008) investigated the shock structures in a rectangular tube containing two- and
single-headed modes. Tsuboi et al. (2007a, 2007b), Virot et al. (2007), and Sugiyama and Matsuo (2009) investigated spinning detonations in circular tubes, and their simulation results are consistent with experimental data. Sugiyama and Matsuo (2013) studied pulsating detonations in circular and square tubes and showed that owing to the lack of a transverse wave, the longitudinal instability dominates in pulsating detonations.

From acoustic theory for a spinning detonation in a circular tube, Fay (1952) derived the ratio 3.13 of spin pitch to tube diameter. Acoustic theory can explain the spinning property of the detonation but not its structure. Later, Sugiyama and Matsuo (2012) studied the acoustic coupling of spinning detonations propagating in a circular tube. The results of all these studies indicate that the coupling between the transverse detonation and an acoustic wave is an important mechanism for the propagation of spinning detonation in a circular tube. Herein, we discuss (from the viewpoint of acoustic coupling) how spinning detonations propagate in a square tube. On the basis of the simulated dynamics, we discuss in detail the unsteady propagation and shock structure of spinning detonations.

2. Numerical setup

The governing equations consist of the compressible and reactive three-dimensional Euler equations from the two-step-reaction model of Korobeinikov et al. (1972). The actual fluid mechanics may involve three-dimensional mixing and turbulent effect. The present paper is the first attempt to discuss the failure mechanism of the spinning detonation in a square tube. Our study focuses on the fundamental behavior of the reaction mechanism as having two periods—induction and exothermic periods—whose reaction rates \( \omega_a \) and \( \omega_b \) are given as

\[
\frac{d\alpha}{dt} = -k_1 \rho \exp\left(-\frac{E_1}{RT}\right)
\]

and

\[
\frac{d\beta}{dt} = \begin{cases} 
-k_2 \rho \left[ \beta^3 \exp\left(-\frac{E_2}{RT}\right) - (1-\beta)^3 \exp\left(-\frac{E_2 + Q}{RT}\right) \right] & (\alpha \leq 0) \\
0 & (\alpha > 0)
\end{cases}
\]

(1)

(2)

In this model, the induction-progress variable \( \alpha \) varies from 1 to 0 (the exothermic-progress variable \( \beta = 1 \) is constant) in the induction period, whereas the exothermic progress variable \( \beta \) varies from 1 to \( \beta_{eq} \) (the induction-progress variable \( \alpha \) is below 0) in the exothermic period. The fluid is an ideal gas with a constant specific heat ratio \( \gamma = 1.4 \). The parameters of this model for this study are listed in Table 1. The premixed gas is modeled as a stoichiometric hydrogen–air mixture. The system is parametrized by initial pressure \( (P_i = 0.2, 0.6, \text{ and } 1.0 \text{ atm}) \), and the initial temperature is \( T_i = 293 \text{ K} \).

Table 1 Chemical parameters of two-step reaction model.

| \( Q \) | 2.33 MJ/kg |
|---|---|
| \( E_1/R \) | 9850 K |
| \( E_2/R \) | 2000 K |
| \( k_1 \) | \( 3.0 \times 10^8 \text{ m}^3/\text{kg/s} \) |
| \( k_2 \) | \( 4.185 \times 10^5 \text{ m}^4/\text{N}^2/\text{s} \) |

For the spatial integration, Yee’s Non-MUSCL Type 2nd-Order Upwind Scheme (Yee, 1987) is used. For temporal integration, we use the point-implicit method, which treats only the source term implicitly. Grid resolution is defined as the number of grid points in the induction length \( L_{ind} \) as calculated by a one-dimensional steady solution. Thirty-three grid points are in the induction reaction length \( L_{ind} \) and are set in all directions. The incoming flow velocity of the premixed gas is 2000 m/s, which is slightly (~3%) overdriven with respect to the Chapman–Jouguet (CJ) velocity \( D_{CJ} \) of 1940 m/s. To avoid disturbance from the outflow boundary, we use the rarefaction boundary condition proposed by Gamezo et al. (1999), and the axial length in the computational grid is greater than 500 \( L_{ind} \). The results of a one-dimensional steady simulation are used as initial conditions. To create initial disturbances, sheets of a three-dimensional unburned-gas mixture are artificially added behind the detonation front. The wall boundaries on a square tube are adapted to adiabatic and slip conditions.
3. Results

Because the propagation of a spinning detonation in a square tube is essentially the same in all details as described in previous study by Tsuboi et al. (2008), we focus herein on the acoustic coupling between a transverse detonation and the acoustic waves between the walls.

3.1 Effect of initial pressure, tube size, and cell width

Figure 1 shows the initial conditions for the calculation and for the different propagation modes [spinning (○) and pulsating (×)] for detonations in a square tube. As the channel width decreases, the spinning detonation shifts toward the pulsating detonation, as shown in Fig. 1. In the pulsating mode, since the channel width is small, the spinning detonation cannot maintain its propagation. Then, a detonation shows strong oscillation in the longitudinal direction and periodic behavior including reignition, propagation and decay. The details of a pulsating detonation are described by Sugiyama and Matsuo (2012). Vasil’ev (1987) demonstrated that an empirical critical channel width \( L_{cr*} \) exists and is given by \( 4L_{cr*} = \lambda \), where \( \lambda \) is the cell width. To discuss how the channel width \( L \) affects the results, we obtain the empirical channel width \( L_{cr*} \) from a two-dimensional simulation with several initial pressures \( P_1 \) and cell widths \( \lambda \) (see results in Table 2). Cell width \( \lambda \) is obtained by grid convergence study. The red circles (●) show the result for \( L_{cr*} = \lambda/4 \). Taylor et al. (2013) showed that a cell width by numerical simulation tends to be smaller than that by an experiment even if a detailed chemical reaction model is adopted. Cell widths listed in Table 2 by the present study are also a factor of 4 – 6 times smaller than those from the detonation database (Kaneshige and Shepherd, 1997), but they are proper values in our numerical method. It is because that, in our paper, spinning detonation observes at conditions of \( 4L \sim \lambda \) (\( \lambda \); cell width, \( L \); channel width) as well as those by a previous experiment. Therefore, the present numerical simulations using a simplified chemical reaction model are properly conducted for spinning detonation in a square tube.

Table 2 Initial conditions for simulation: initial pressures \( P_1 \), cell widths \( \lambda \) by Sugiyama and Matsuo (2013) and, empirical channel width \( L_{cr*} = \lambda/4 \).

| Initial pressure \( P_1 \) [atm] | Cell width \( \lambda \) [mm] | Empirical channel width \( L_{cr*} \) [mm] |
|-----------------------------|-----------------|-----------------|
| 1.0                         | 1.62            | 0.405           |
| 0.60                        | 3.33            | 0.833           |
| 0.20                        | 10.2            | 2.55            |

Fig. 1 Initial conditions for simulation (initial pressure and channel width) for spinning (○), and pulsating (×) modes of a spinning detonation in a square tube. Red circles (●) show the empirical critical channel \( L_{cr*} = \lambda/4 \), where \( \lambda \) is the simulated cell width.

Fig. 2 Soot-track image and the definition of track angle \( \alpha \). Acoustic wave is generated at the corner B and travels along the wall BC. The labels A–D indicate the corners of a square tube. \( P_1 = 1 \) atm and \( L = 0.8 \) mm.
Figure 2 shows the maximum-pressure history for $P_1 = 1$ atm and $L = 0.8$ mm, and corresponds to the soot-track images obtained experimentally. The labels A–D indicate the corners of a square tube. The black sloped lines show the trajectory of the transverse detonation over the maximum-pressure history. The track angle $\alpha$ is defined as the arctangent of the perimeter $4L$ divided by the pitch of the spin. The transverse detonation undergoes successive reflections, and the soot-track image seems to spin on the wall.

We now focus on the reflection of the transverse detonation from the corner D, which is identified by the blue-dashed region in Fig. 2. The transverse detonation maintains its propagation with reflections from the corner D and rotations along the subsequent wall DA. At the reflection, an acoustic wave is generated that travels along the wall CD. We discuss in the next section the coupling between the rotating transverse detonation and the traveling acoustic wave. We assume the burned-gas region is in a CJ state, so the sonic velocity $a_{CJ}$ is calculated by

$$a_{CJ} = \frac{\gamma M_{CJ}^2 + 1}{\gamma + 1}$$

(3)

where $M_{CJ}$ denotes the CJ Mach number (= 4.87) for a stoichiometric hydrogen-air mixture. Here, we define an “acoustic wave” propagating through the burned-gas region as a wave with the velocity of 1.05 $a_{CJ}$ and is actually a weak shock wave.

Table 3 shows the initial conditions for the simulation and the resulting track angles $\alpha$ and propagation modes. Pulsating detonations pulse strongly and undergo intermittent local explosions in a cycle consisting sequentially of reignition, multtheaded mode, spinning mode, and decay. Track angles are obtained when the spinning detonation is transient. The simulation track angles are consistent with those of previous reports [49.5° from Bone et al. (1936), 49.0° from Lee et al. (1969), and 47.0° from Tsuboi et al. (2008)]. As the channel narrows, the track angle decreases, and the transverse detonation weakens. When the channel length drops below the critical value, the transverse detonation cannot consume the unburned gas behind the shock wave; thus the spinning detonation ceases.

Table 3 Initial conditions for simulation (two left columns) and resulting track angle and propagation modes (two right columns) for detonations in a square tube.

| Initial pressure $P_1$ [atm] | Channel width $L$ [mm] | Track angle $\alpha$ [º] | Propagation |
|-----------------------------|------------------------|--------------------------|-------------|
| 1.0                         | 0.32                   | 44.3                     | pulsating   |
| 1.0                         | 0.40                   | 47.3                     | spinning    |
| 1.0                         | 0.50                   | 47.5                     | spinning    |
| 1.0                         | 0.80                   | 49.4                     | spinning    |
| 0.60                        | 0.60                   | 44.3                     | pulsating   |
| 0.60                        | 0.75                   | 47.2                     | spinning    |
| 0.60                        | 0.90                   | 47.5                     | spinning    |
| 0.20                        | 2.48                   | 44.6                     | pulsating   |
| 0.20                        | 2.80                   | 47.5                     | spinning    |

3.2 Propagation behavior

Simulation results for spinning detonations show that the propagation mechanism is almost independent of the initial conditions. Therefore, we show the propagation by using the following initial conditions: initial pressure $P_1 = 1.0$ atm and channel width $L = 0.40$ mm for a spinning detonation and $L = 0.32$ mm for a pulsating detonation. The dynamics of the simulation results is used to reveal the propagation of the spinning detonation. The results for the spinning detonation are shown in Figs. 3–5.

In a spinning detonation in a circular tube, as acoustic coupling is not satisfied, the shock structure of spinning detonation is disturbed by the acoustic wave. Chemical reaction is decelerated by the acoustic wave, and transverse detonation fails (Sugiyama and Matsuo, 2013). This is to say that changes of physical values by the acoustic wave are very sensitive to the propagation of transverse detonation, and that acoustic coupling should be satisfied in order to maintain the propagation of spinning detonation in a circular tube. Here, we focus on the propagation behavior of the transverse detonation and the acoustic wave in a square tube. Figure 3(a) shows a quarter cycle of the shock fronts and Fig. 3(b) shows the pressure distribution at the isosurface of the induction-progress variable $\alpha = 0$ from the front side.
for $L = 0.40$ mm. The spinning detonation interacts in a complicated way with the reaction zones. The images show the instantaneous distributions before and after the intersection wave of the two triple lines reflects off wall DA. In Fig. 3(a), two triple lines that are respectively parallel and orthogonal to the sidewalls emanate from the shock front and move partially out of phase. The intersection wave of two triple lines reflects from the walls at an angle of $45^\circ$ and seems to rotate on the shock front. Therefore, the spinning detonation in a square tube shows that the transverse detonation repeatedly collides with the wall and that the intersection wave between two triple lines creates a spinning detonation. At the reflection, an acoustic wave is generated, which travels back along wall CD. In Fig. 3(b), the new chemical-reaction front is only generated at the transverse detonation. No unburned gas pocket forms behind the detonation front because the rotating transverse detonation completely consumes any unburned gas.

Fig. 3 Quarter cycle of (a) shock fronts and (b) pressure distribution at the isosurface of the induction-progress variable $\alpha = 0$ from the front side of the spinning detonation in a square tube at $L = 0.40$ m.

Fig. 4 Density distribution on the wall over one cycle for spinning mode with $L = 0.40$ mm.

Fig. 5 Density distribution on the wall over one cycle for pulsating mode. The spinning detonation begins to appear at $L = 0.32$ mm.

Figures 4 and 5 show one cycle of the density distribution on the wall during the spinning and pulsating modes, respectively. These images capture the moments at which the transverse detonation collides with (a) wall AB, (b) wall BC, (c) wall CD, and (d) wall DA for $L = 0.40$ and 0.32 mm, respectively. For $L = 0.32$ mm during the pulsating mode, spinning detonation does not maintain the propagation but transiently appears, as shown in Fig. 5. The white lines in Figs. 4 and 5 indicate the corners of the square tube and the white arrows show the position of the acoustic wave that is generated by the collision of the transverse detonation with corner A in Figs. 4(a) and 5(a). Here, we use the flow
features at wall DA. The transverse detonation rotates on the wall and undergoes successive reflections off the walls. Once generated in Fig. 5(a), the acoustic wave travels between corners D and A. The moment that the rotating transverse detonation collides with wall AD [Fig. 4(d)], the acoustic wave and the transverse detonation couple together and propagate to corner A. This occurs repeatedly at each wall, and the rotating transverse detonation always couples with one of the acoustic waves propagating between corners. For the pulsating mode, the acoustic wave in Fig. 5(d) is located at corner A and will propagate to corner D, where it will collide with the transverse detonation. At this point, they are not coupled together, which indicates that the conditions for the transverse detonation to couple with the acoustic wave are not satisfied. The shock structure of the spinning detonation is disturbed, which causes the spinning detonation to fail. Because the conditions for the rotating transverse detonation to couple with the traveling acoustic wave are always satisfied on the walls (between the corners), the spinning detonation can maintain stable propagation as well it does in a circular tube (Sugiyama and Matsuo, 2013).

3.3 Acoustic coupling on walls

The present study shows that between corners, the interaction of the traveling acoustic wave with the rotating transverse detonation is important for maintaining propagation of the spinning detonation in a square tube. Therefore, we now discuss the propagation of a transverse detonation and an acoustic wave along the walls. Figure 6 shows a schematic diagram of an acoustic wave fully coupled [Fig. 6(a)], weak coupled [Fig. 6(b)], and uncoupled [Fig. 6(c)] with a rotating transverse detonation and its projection on the walls. The blue, red, and black arrows represent the trajectories of the intersection point of two triple lines, the transverse detonation projected onto the walls, and the acoustic wave at wall AD, respectively. Figures 6(a) and 6(c) correspond to Figs. 4 and 5, respectively. The instant that the transverse detonation collides with wall AB is used as the reference time, and the black circles (●) show the initial point of the trajectory of the transverse detonation and the acoustic wave. The acoustic wave created by the reflection from wall AB is generated at the reference time and propagates back and forth between corners A and D. For Fig. 6(a), the acoustic wave immediately couples with the transverse detonation at the moment it collides with wall AD. After that, the transverse detonation propagates with the acoustic wave along wall AD. Because the transverse detonation is always faster than the acoustic wave, the case described in Fig. 6(b) is referred to as “weak coupled.” The acoustic wave couples with the transverse detonation just before the collision with transverse detonation and the wall AB. In this case, the transverse detonation catches up with the acoustic wave at corner A. This represents the limiting case for which acoustic coupling is possible. In Fig. 6(c), the acoustic wave traveling from corner A to corner D collides with the transverse detonation at wall AD.

![Schematic illustration of transverse detonation](image)

*Fig. 6 Schematic illustration of transverse detonation (a) fully coupled, (b) weak coupled, and (c) uncoupled with an acoustic wave. Blue, red, and black lines show the trajectories of the intersection point of two triple lines, the transverse detonation projected onto the walls, and the acoustic wave at wall AD, respectively. The black circles (●) show the initial point of the trajectory of the transverse detonation and the acoustic wave.*

We assume that, in a square tube, an acoustic wave behind the transverse wave propagates at the speed of sound of the CJ state [see Eq. (3)]. In Figs. 6(a) and 6(b), the propagation distances of transverse detonation projected onto the
wall are 2 and 1.75 times greater than that of the acoustic wave at wall AD, respectively. Therefore, to maintain the acoustic coupling, the velocity of the transverse detonation projected onto the walls must satisfy the inequality

\[ 1.75 \leq \frac{V_{\text{tran}}}{C_J} \leq 2. \tag{4} \]

From Eqs. (3) and (4), the range for track angle \( \alpha = \tan^{-1}(V_{\text{tran}}/D_{CJ}) \) is found to be

\[ 45.6^\circ \leq \alpha \leq 49.4^\circ \tag{5} \]

These results show that the simulation track angles fall between the maximum and minimum track angles. From Table 3, we see that the maximum track angle is 49.4°, and that the spinning detonation cannot continue to propagate if the track angle is less than 45.6°. This result indicates that acoustic coupling between the rotating transverse detonation and the traveling acoustic wave on the wall determines whether the spinning detonation in a square tube maintains propagation as well it does in a circular tube.

4. Conclusion

We numerically investigate spinning detonations in square tubes at various initial pressures by using the three-dimensional Euler equations combined with a two-step chemical-reaction model proposed by Korobeinikov et al. (1972). We discuss the propagation mechanism of a spinning detonation in a square tube based on coupling of the transverse detonation with the acoustic wave.

Because the transverse detonation reflects off successive walls, it appears to spin in a square tube. Similarly, the acoustic wave is generated by successive reflections and travels back and forth between walls. When the spinning detonation continues to propagate, the conditions are always satisfied for the acoustic wave traveling along the walls to couple to the rotating transverse detonation. The maximum and minimum track angles that allow the spinning detonation in a square tube to continue to propagate are analyzed from the viewpoint of the coupling between these waves. The results show that the track angles always fall within the estimated maximum and minimum, which indicates that acoustic coupling is important for a spinning detonation in a square tube to continue to propagate as well as it does in a circular tube.

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