Three-dimensional Numerical Simulation of Detonation Initiation in Supersonic Flows

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1 Introduction

The high thermodynamic efficiency greatly motivates detonation investigation for the application of advanced propulsion systems [1]. Adopting the detonation combustion in the supersonic flow in scramjet may be an alternative choice for advanced propulsion systems. It is more practical to adopt the circular tube for detonation based engine, while some researchers [2, 3] adopted rectangular channels for better observations in detonation experiments with high speed combustible mixtures. However, the detailed three-dimensional initiation process between rectangular tube and circular tube in supersonic flow have not been compared and analyzed much and remain unclear.

Detonation initiation is one of the most important issues in detonation application. In supersonic premixed flows, a hot jet could initiate the combustible mixtures with little energy very fast. Detonation initiation using a hot jet has been investigated numerously in quiescent or low-speed combustible mixtures [4, 5], but rather few studies have been carried out in supersonic combustible mixtures in rectangular tubes or circular tubes. In rectangular channels, Hanana et al. [6] firstly presented rectangular mode and diagonal mode of the detonation front in experiments. Deiterding [7] efficiently simulated three-dimensional detonations using adaptive mesh refinement code AMROC (Adaptive Mesh Refinement in Object-oriented C++). In circular tubes, a few propagation modes of detonation front have been observed in quiescent mixtures: spinning, two-headed, and multi-headed mode [8]. Tsuboi et al. [9] presented spinning detonations in both a circular and a square tube and revealed characteristics of spinning modes by using three-dimensional simulations with detailed chemical reaction model. Cai et al. [10] found that the side walls in three-dimensional rectangular channel make an impact on detonation initiation in supersonic combustible mixtures. However, the different shapes of wall surface in rectangular channel and circular tube may make different impact on detonation initiation. The three-dimensional wave dynamics of detonation initiation using hot jet in rectangular tube and circular tube in supersonic mixtures still need more investigations.

Here, detonation initiation and propagation in both a square tube and a circular tube are investigated by injecting a hot jet into supersonic combustible mixtures. The aim of this work is to providing fundamental

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understanding of the detailed initiation process in square tube and circular tube in supersonic combustible mixtures for the future detonation application on supersonic combustor chamber.

2 Numerical modeling

The three-dimensional Euler equations with an irreversible one-step two-species chemistry model is considered. Here, the simplified chemistry model is selected and fitted to physical parameters of a H2/O2 detonation. Table 1 shows the thermodynamic parameters of the chemistry model adopted in the present simulations.

Table 1: Thermodynamic parameters of the chemistry model

Parameters	Values	Unit
T_∞	300	K
P_∞	6670	Pa
ρ_∞	0.077552	kg/m^3
γ	1.29499	-
W	0.029	kg/mol
q	54000	J/mol
q/RT_∞	21.65	-
Ea	30000	J/mol
Ea/RT_∞	12.028	-
A	6×10^5	s^{-1}

The second-order accurate MUSCL-TVD finite volume method is adopted for the convective flux discretization. The hydrodynamic solution is separated into the flux calculation step and reconstruction step. Dimensional splitting is employed for the three-dimensional simulation. The first-order Godunov splitting is adopted for the reactive source term. The standard one-dimensional Roe-type Riemann solver is applied and then is extended to three dimensions. A hybrid Roe-HLL Riemann solver is adopted to circumvent the intrinsic problem of unphysical total densities and internal energies near vacuum due to the Roe linearization, ensuring positive mass fractions and preventing the disastrous carbuncle phenomenon. The Van Albada limiter is adopted with the MUSCL reconstruction to structure a second-order accurate TVD-type method in space. As for time integration, second order accurate MUSCL-Hancock technique is used. The dynamic time step adjustment with the constant CFL number 0.9 is used for the following simulations. It is more efficient to adopt the high-order shock-capturing finite volume method on rectangular Cartesian grids. In order to construct the circular wall within the old frame, the Ghost Fluid Method (GFM) is adopted, which uses some finite volume cells inserting in the boundary condition as ghost cells.

As shown in Figure 1, in the present study the height, width and length of the square tube is 25 mm, 25 mm, 75 mm respectively. The diameter and length of the circular tube is 25 mm, 75 mm respectively. A hot jet hole with 2 mm height is placed on the symmetry position of upper wall, and the diameter of the hot jet hole is 4 mm. The initial base grid for both computational domains have 150 (x direction or axial direction) $\times$ 54 (y direction or vertical direction) $\times$ 50 (z direction or horizontal direction) (405 thousand) cells. Three additional mesh refinement is set for the simulation. The refinement factor is 2, 2, 2. The corresponding uniform mesh number to the present adaptive mesh resolution is 20.736 million. The 3D computations are conducted on Tianhe-2 with 480 Intel E5-2692 2.20 GHz (Ivy Bridge) processors.

In order to focus the present study just on the jet ignition process in the tube, we have adopted the slip boundary conditions in our investigations for not having to deal with boundary layers produced in the inflow section. Thus reflecting boundary with slip wall conditions are used on the square wall or circular wall. The inflow of the hot jet is adopted on the upper jet channel. When the hot jet is shut down, the inflow condition switches to the reflecting condition immediately. The supersonic flow of the reactive mixture is from right to left throughout the paper. The right boundary adopts the inflow condition and an ideal outflow condition is imposed on the left boundary. A mixture of H_2/O_2 at T = 300 K and P = 6670 Pa flows at V_{CJ} (V_{CJ} = 1587.84 m/s). The inflow parameters of the hot jet in square tube are set to the values of the ZND state of a detonation in H_2/O_2 under the condition of the inflow pressure 60,000 Pa and the temperature 300 K. While the inflow parameters of the hot jet in circular cases are set to the values of the ZND state of a detonation in H_2/O_2 under the condition of the inflow pressure 40,000 Pa and the temperature 300 K. The detail inflow parameters of the hot jets are shown in Table 2. The injection velocity are specified as the sonic speed to make it a chocked hot jet with velocity of 722.73 m/s. The hot jets are shut down when the detonation is initiated successfully.

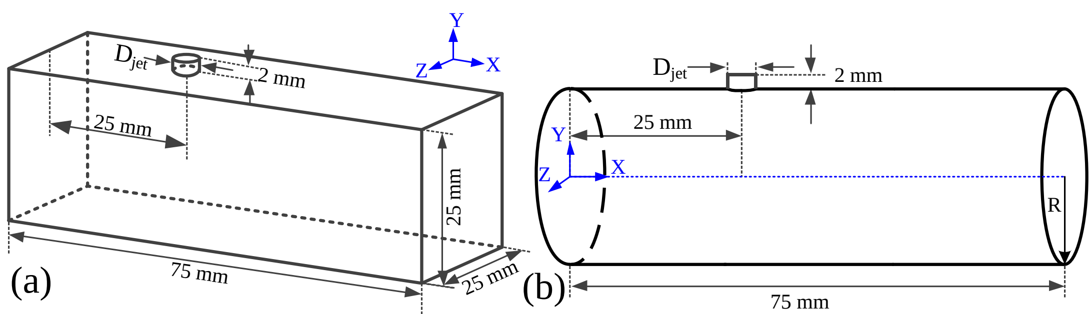


Figure 1. Schematic of computational domain, (a) square tube, (b) circular tube.

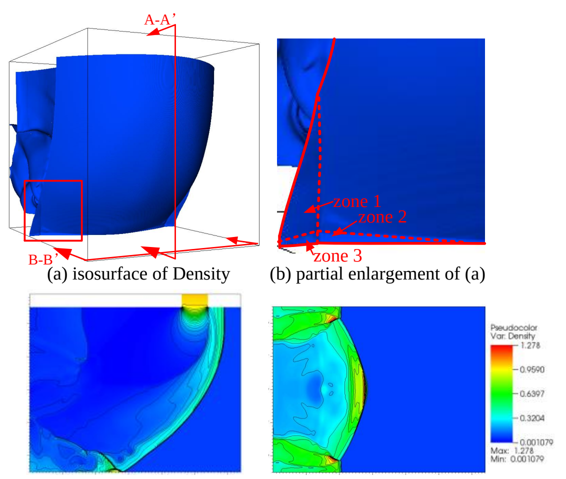
Table 2: Inflow parameters of the hot jets in square tube and circular tube

Parameters	Square tube	Circular tube
Pressure/(Pa)	894501	596334
Temperature/(K)	2519.54	2519.54
Density/(kg/m^3)	1.23836	0.825574
Velocity/(m/s)	722.73	722.73
Energy/(J/mol)	3.36032×10^6	2.24021×10^6
mass fraction of Y1 (reactant)	0.00198911	0.00198911
mass fraction of Y2 (product)	0.998011	0.998011

3 Results and discussions

Figure 2 and Figure 3 show different reflection structure of jet induced bow shock between square tube and circular tube. As shown in Figure 2, the hot jet induced bow shock causes a reflection structure in the square tube. The isosurface view in Figures 2(a) and (b) is a density isosurface of 0.09 kg/m^3. The bow shock caused by the hot jet is reflected on the wall of the square tube, forming a complex wave front structure. As shown in Figures 2(b), in addition to the main curved bow shock surface, there are more complex local Mach reflection surfaces. The local Mach reflection surface can be divided into three sub-regions. Zones 1 and 2 are Mach reflections formed by the bow shock that directly reflects on the wall. Since the walls are vertical, the two Mach reflection regions intersect and focus to form the Mach reflection region 3. The Mach reflection region 3 is much stronger which plays a key role in the formation of the detonation initiation. Regular reflection is formed on the lower wall and most of the sides. For example, as shown in Figures 2 (c), it is a regular reflection structure formed on the central portion. In the region near the corners of the side walls and the lower wall, the bow shock becomes a Mach reflection. The bottom cross-section view shown in Figures 2 (d) clearly shows the Mach reflection structure formed by the bow shock.

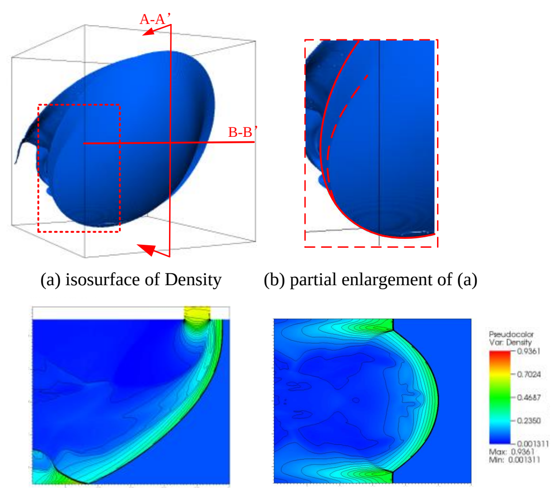
Figure 3 is a diagram showing the reflection structure of the bow shock induced by a hot jet in a circular tube. In contrast to the reflection structure in the square tube, at the initial stage, the bow shock reflection in the circular tube is also mostly an bow shock surface, and the wave surface is also a symmetric structure. The reflection in the circular tube is totally different from that in the square tube. As shown in Figure 3(b), the bow shock surface does not form a distinct triple-line at this time in the lower region, where there is a regular reflection structure. On the side surface, a triple-line is formed from the bottom to the top, and the width of the Mach reflection region gradually becomes wider. At the position near the exit of the jet, the triple-line disappears and the Mach stem structure cannot be clearly distinguished. The density contour and density isolines of the center section in Figure 3(c) clearly show the typical regular reflection structure formed by the bow shock surface on the down wall of the circular tube. And Figure 3(d) clearly show the Mach reflection structure formed by the bow shock surface at the center cross section. When the wave front is further developed, the bow shock at the bottom forms a Mach reflection, and then intersects the Mach face on the side to form a structure as shown in figure 4(c).



(a) isosurface of Density (b) partial enlargement of (a)

(c) Central cross-section A-A' (d) Bottom cross-section B-B'

Figure 2. Initial reflection structure of jet induced bow shock in the square tube



(a) isosurface of Density (b) partial enlargement of (a)

(c) Central cross-section A-A' (d) Central cross-section B-B'

Figure 3. Initial reflection structure of jet induced bow shock in the circular tube

The difference of the wave front structure between the circular tube and the square tube is mainly due to the difference in the shape of the wall surface. The difference in the shape of the wall of the pipe changes the position when the bow shock surface reflects on the wall and, so that the reflection form of the shock surface changes. In addition, the difference in the shape of the tubes also causes the effect of the interaction between the formed shock surfaces to change. When the pipe is square, at the corners of the two pipe faces intersect, the reflected shock surface interacts, so that the shock intensity is further increased. But the other regions do not interact with the shock surface. On the other hand, when the pipe is circular, the shock reflection intensity is larger at the bottom region where the bow shock surface is the strongest, the shock wave interaction is the strongest, and the bottom region is the region where strong shock waves induce combustion forms.

The instantaneous structure comparison of the hot jet induced detonation in the square tube and the circular tube are shown in figure 4. Similar to the hot jet initiated detonation in the circular tube, the hot jet in the square tube also induces a bow shock surface, a Mach stem, a hot jet induced combustion surface, an unburned channel, and a Mach stem induced combustion surface structure. Both in the circular tube and the square tube, the hot jet detonation form a Mach stem by the reflection of the bow shock surface on the wall, inducing the formation of a detonation wave. However, in the square tube, the bow shock surface forms a Mach reflection in the region where the side wall surface and the bottom wall surface intersect. But in the circular tube, the hot jet induced bow shock reflects at the center of the sides and bottom. Therefore, the Mach stem induced detonation zone in the square tube is first formed in the corner area of the lower part, and the Mach stem induced detonation area in the circular tube is formed in the central area of the lower side of the circular tube. There are two detonation zones in the square tube, but only one detonation zone exists in the circular tube. In addition, since the intensity of the jet is not the same, the jet intensity in the square tube is greater, so that the position of the hot jet combustion surface in the square tube is closer to the lower wall surface.

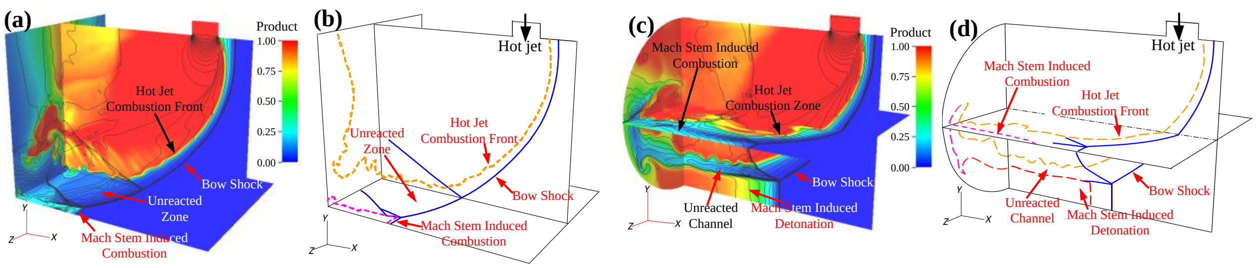


Figure 4. The instantaneous structure diagram of the hot tube jet detonation of square tube and circular tube, (a) the three-dimensional cross-sectional view of the product contour and density isolines in the square tube, (b) the schematic diagram of the detonation flow field structure of the square tube, (c) the three-dimensional cross-sectional view of the product contour and density isolines in circular tube, (d) the schematic diagram of the detonation flow field structure of the circular tube.

It can be seen from figure 4 that the hot jet initiation process in the square tube and in the circular tube have great differences. In the square tube, only a small area on both sides of the wall forms the Mach stem surface, and is quickly engulfed by the Mach face intersecting at the corner area, developing into a Mach stem induced detonation surface. In the circular tube, the hot jet induced bow shock not only forms Mach stem induced combustion on both side walls, but also forms Mach stem induced detonation on the low wall. After the Mach stem induces the formation of the detonation wave, the Mach stem on both sides can be completely engulfed when the entire detonation wave surface is formed. On the other hand, results show that the detonation formation in the square tube exists in the corner areas, and finally the two Mach stem induced detonation areas converge into a Mach stem induced detonation area. In the circular tube, there is only one Mach stem induced detonation zone during the detonation process, and the two Mach stem induce combustion zones cannot form detonation front.

4 Conclusions

In this study, three-dimensional reactive Euler equations with one-step two-species chemistry model are solved using adaptive mesh refinement method to investigate the detonation initiation in both square tube and circular tube in supersonic combustible mixtures. The different shape of the tubes cause the different reflection effects of the shock waves, resulting in different effects of the hot jet detonation. In square tube, the corner regions where the two tube faces intersect, the reflected shock surfaces interact, so that the shock wave strength is further increased, and the detonation occurs in the corner region. In the circular tube, the bow surface of the bottom of the tube has the strongest reflection, and the Mach stem near the bottom region first induces detonation, initiating the combustible mixtures.

Acknowledgments

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References

[1] Kailasanath K. (2003). Recent developments in the research on pulse detonation engines. AIAA J. 41:145.

[2] Ishii K, Kataoka H, Kojima T. (2009). Initiation and propagation of detonation waves in combustible high speed flows. Proc. Combust. Inst. 32:2323.

[3] Han X, Zhou J, Lin Z-Y. (2012). Experimental investigations of detonation initiation by hot jets in supersonic premixed flows. Chin. Phys. B. 21:124702.

[4] Lin W, Zhou J, Liu S-j, Lin Z-y, Zhuang F-c. (2015). Experimental study on propagation mode of H_2/Air continuously rotating detonation wave. Int. J. Hydrogen Energy. 40:1980.

[5] Carpio J, Iglesias I, Vera M, Sánchez AL, Liñán A. (2013). Critical radius for hot-jet ignition of hydrogen–air mixtures. Int. J Hydrogen Energy. 38:3105.

[6] Hanana M, Lefebvre MH. (2001). Pressure profiles in detonation cells with rectangular and diagonal structures. Shock Waves. 11:77.

[7] Deiterding R, Bader G. High-resolution simulation of detonations with detailed chemistry. Analysis and Numerics for Conservation Laws: Springer Berlin Heidelberg; 2005.

[8] Voitsekhovskii BV, Mitrofanov VV, Topchiyan MY. (1966). Structure of the detonation front in gases. (FTD-MT-64-527).

[9] Tsuboi N, Koichi Hayashi A. (2007). Numerical study on spinning detonations. Proc. Combust. Inst. 31:2389.

[10] Cai X, Liang J, Deiterding R, Che Y, Lin Z. (2016). Adaptive mesh refinement based simulations of three-dimensional detonation combustion in supersonic combustible mixtures with a detailed reaction model. Int. J. Hydrogen Energy. 41:3222.