Numerical Investigation of DDT Mechanism in Cross-Section Abrupt Detonation Tube

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1 Introduction

Detonation, as a special combustion mode, has recently attracted more and more attention due to its pressure gain characteristic and high thermal efficiency [1]. The key of detonation research lies in its initiation. Up to now, there are two methods of ignition to trigger detonation: direct initiation and indirect initiation. Compared with direct detonation, indirect initiation based on deflagration-to-detonation transition (DDT) has the advantage of small energy-consuming [2] and good engineering application value [3], becoming the research hotspot. However, there are still defects urgently to be solved in indirect detonation, such as large randomness, complicated mechanism, long DDT distance, energy loss due to obstacle addition. Among them, forming a stable detonation wave of self-sustainingly propagation in a relatively short distance is deemed to be the most critical issue. In the last few decades, many experiments and numerical simulations have been conducted and lots of achievements have been accomplished to explore the mechanism of DDT and search for the best way to reduce the DDT time and distance [4-5]. Even so, the substantial mechanism of DDT is still not well known and there are not unified theories to quantitatively predict and control DDT, which seriously restricts the development of detonation technology in engineering application [6]. Therefore, it is necessary to further study the DDT phenomenon and find other ways to shorten DDT time and distance.

In this paper, a cross-section abrupt detonation tube which could realize fast detonation initiation is proposed. Based on this, an attempt has been made to further investigate the DDT mechanism by discussing the temperature field and pressure field in detail. Furthermore, DDT features of the cross-section detonation tube is analyzed comparing with that of conventional detonation tube.

2 Numerical model and methods

2.1 computational domain

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Figure 1 presents the schematic diagram of the cross-section abrupt detonation tube. It mainly consists of two components, the inner part is a short solid cylinder, coaxial to the long outer tube which is close at left end and open at right end. The laminar flame is triggered by a high temperature ignition source at the left corner of annular gap and accelerates towards the outlet due to interaction with the boundary layers and effect of instabilities. The accelerated flame further destabilizes when passing through the annular gap exit under the effects of diffraction of flames and collision of pressure waves, ultimately developing into detonation wave.

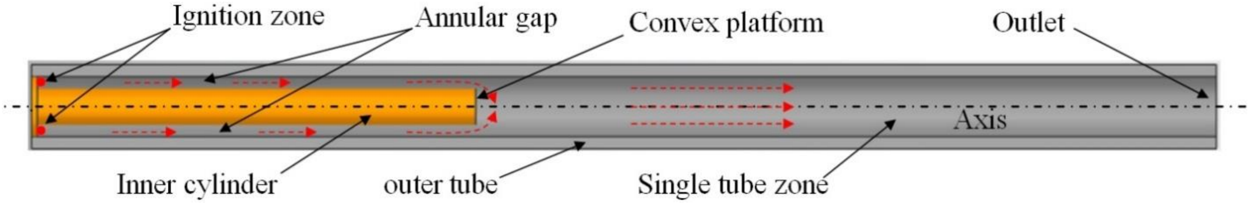


Figure 1. Schematic diagram of cross-section abrupt detonation tube

Considering the high geometric symmetry of the cross-section abrupt tube, the two-dimensional computational domain of the upper half of the symmetry axis is chosen to simulate the model to improve the efficiency of calculation, as displayed in Figure 2. The length l and radius R of the outer cylinder are 200mm and 5mm respectively, the length l_a and radius r of the inner cylinder are 75mm and 3mm respectively, the annular gap ε is 2mm, the ignition zone is a semi-circle with radius of 1mm located at the left end of annular gap.

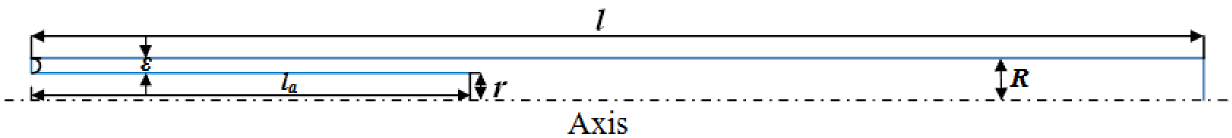


Figure 2. Computational domain of cross-section abrupt detonation tube

2.2 numerical strategy and initial conditions

The simulation in this study is conducted by ANSYS Fluent. One-step reaction kinetics model with 4 species is employed to describe the reaction model in stoichiometric hydrogen/air mixtures [7]. The single-step reaction follows Arrhenius equation:

$$k = Ae^{-E_a/RT} \tag{1}$$

Where k is rate constant, A is pre-exponential factor, E_a is apparent activation energy, R is molar gas constant, T is thermodynamic temperature.

Besides, The Navier-Stokes equation is used to investigate the DDT characteristic for a viscous compressible ideal gas, and the advection upstream splitting method (AUSM) is used to calculate the convection flux term [8]. The standard k-ε model is employed to predict the turbulent flow with high Reynolds number [8-9]. Non-equilibrium wall functions are employed to resolve the flow near the wall.

Stoichiometric hydrogen-air mixture is filled homogeneously in the detonator at temperature of 300K and pressure of 0.1MPa initially, the flame is ignited by a semicircle region of 3000K temperature. Outlet boundary is set as pressure-outlet of 0.1MPa. The remaining boundaries are no-slip boundary condition [5].

In addition, The detonation parameters calculated by numerical simulation of annular jet detonation tube in this study are compared with the theoretical C-J values computed by CEA code from NASA-Glen and data obtained from experiment [10], the conclusions are displayed in Table 1, which shows that the maximum error is 3.8%, validating the feasibility of the numerical model.

Table 1: Comparisons of detonation parameters

Parameters	Numerical results	Theoretical C-J value	Error (%)	Experimental data [10]	Error (%)
P_{CJ}/P_0	15.882	15.460	2.73	15.3	3.8
V_D/(m/s)	2031	1971	3.04	2003	1.4

Note: P_{CJ} is detonation wave C-J pressure, T_{CJ} is detonation wave C-J temperature, P_0 is initial gas pressure, V_D is detonation wave propagation velocity.

3 Results analysis and discussion

3.1 superiority of cross-section abrupt detonation tube

In order to explore the effect of the cross-section of jet flame on DDT, the DDT features of cross-section abrupt detonation tube is compared with those of long annular tube (same annular gap size with the annular gap of cross-section abrupt tube) and long smooth tube (same inner diameter with the single tube zone of the cross-section abrupt tube) under the same numerical strategy and condition firstly. It is worth noting that the ignition position is located at the upper left corner of long smooth tube, which is consistent with the case of the corresponding cross-section abrupt tube, as displayed in Figure 3.

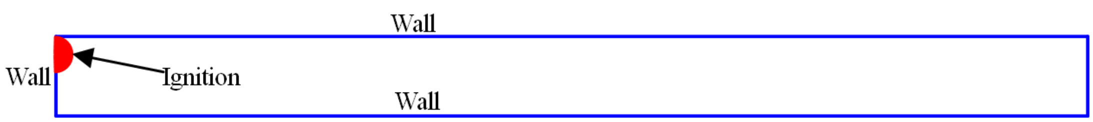


Figure 3. Computational domain of long smooth tube

In fact, there is a little pressure variation in radial direction in front of pressure wave, for convenience, we choose the maximum pressure of pressure front, which could clearly marks the pressure wave intensity and its arriving location, to indicate the one-dimensional distributions of property along the tube of 3 diff-

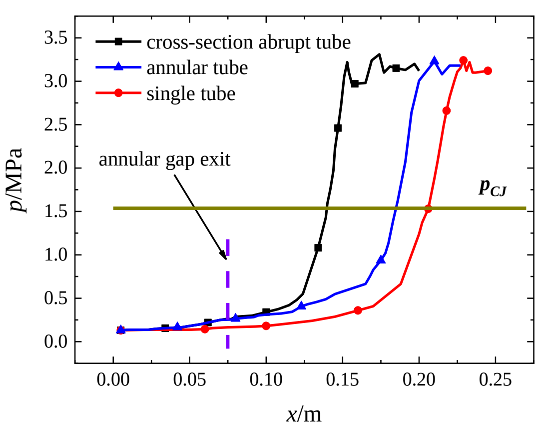


Figure 4. Variations of pressure peak

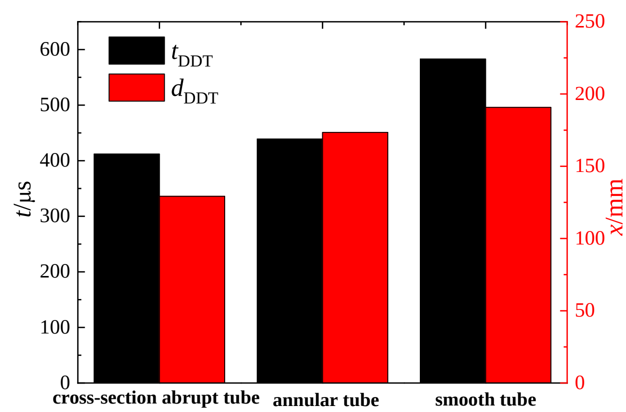


Figure 5. DDT time and distance

erent cases, just as displayed in Figure 4. After propagating across the annular gap exit, the jet flame of cross-section abrupt tube experiences the shortest acceleration process and develops into detonation state compared with annular tube and single tube. In order to present more clearly the superiority of cross-section abrupt tube, we introduce two important features: DDT distance defined as the distance between the ignition position and the position where the pressure first rises to the C-J theoretical value, and its corresponding DDT time. As presented in Figure 5, the cross-section abrupt tube has the most advantage in DDT time and distance over the other cases. Therefore, it is significant to analyze the detonation formation process of cross-section abrupt tube in detail.

3.2 flow field analysis

The flame induced by a soft ignition source propagates in the annular gap in laminar state at the beginning. The travel velocity of the pressure wave is much faster than that of the jet flame behind it, thus the maximum pressure value of the pressure front can't increase fast and keeps a relative low level without the energy supply of combustion, as showed in Figure 6, 62μs (upper half of temperature distribution, lower half of pressure distribution). At 308μs, due to the interaction with the boundary layer and Rayleigh–Taylor (RT) Instabilities [11], the velocity of flame near the boundary accelerates quickly and the shape of flame front changes from the convex of laminar flame to concave of turbulent tulip flame [12] because of the drag of the wall. At the same time, the leading pressure wave continuously increase under the expansion of the combustion products near the boundary layer.

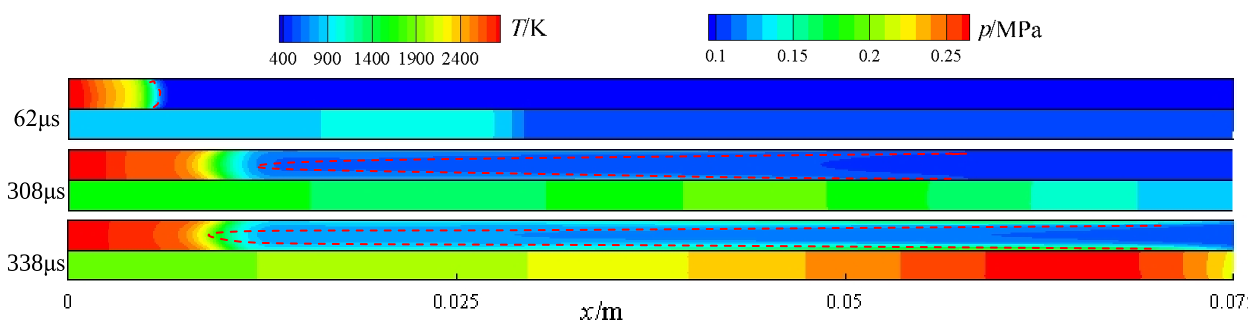


Figure 6. Temperature and pressure distribution

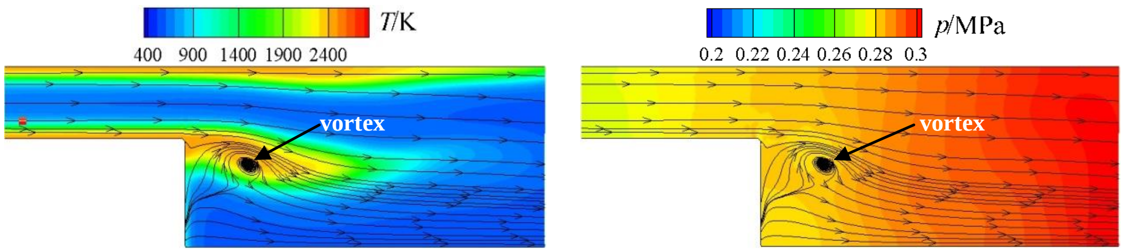
At t=338μs, the pressure front propagates to the exit of the annular gap and the flame surface is further stretched. The main parameters of the annular jet are listed in Table 2:

Table 2: parameters of annular jet flame

t	P/P_0	T/T_0	V_p	Ma
338μs	2.53	2.9	500m/s	0.445

Note: t is the time jet flame arriving the exit of annular gap, P is the pressure of jet, V_P is the propagation velocity of leading pressure wave, Ma is the Mach number of jet flame.

At 356μs, when the jet flame passes through the exit of the annular gap and diffracts downstream of the convex platform, a entrainment vortex forms behind the convex platform and moves towards to the symmetry axis due to the increase of radial velocity of the flame jet, as displayed in Figure 7. The temperature of the vortex region is apparently higher than that of the surroundings due to the mixing reinforcement effect of vortex on burned products and unburned gaseous mixtures, which helps to promote combustion. Furthermore, the expansion of the burned products strengthens the superposition of downstream pressure shock waves, as showed in Figure 7 (b), consequently accelerating the formation of detonation.



(a) Temperature contours with velocity streamtraces

(b) Pressure contours with velocity streamtraces

Figure 7: Flow field distribution of 356μs

Figure 8 shows the pressure variations on the centerline of the annular gap and on the axis of the single tube zone respectively at acceleration stage, corresponding time arranging from 290μs to 390μs, each adjacent line has an equal time interval of 20μs. It is easy to find that pressure increase slowly in the annular gap. When jet flame passes across the annular gap exit, although the pressure decreases a little with the increase of surface of pressure front as the jet flame diffracts, the total pressure increase is larger than before due to the turbulence action of cross-section abrupt of jet flame and collisions of pressure waves. In addition, the increasing spacing between adjacent pressure lines indicates the propagation velocity of jet flame becomes faster.

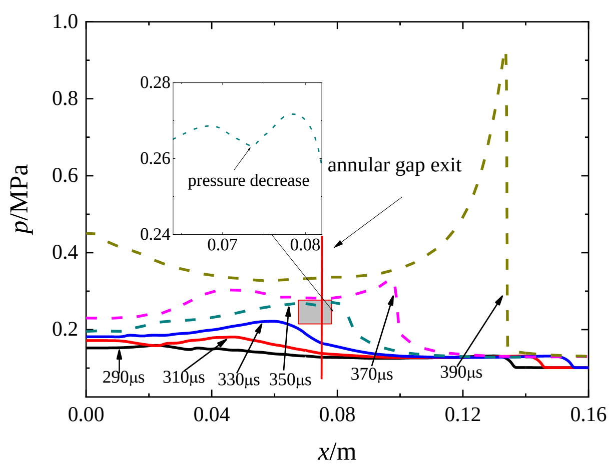


Figure 8. Variations of pressure at acceleration stage

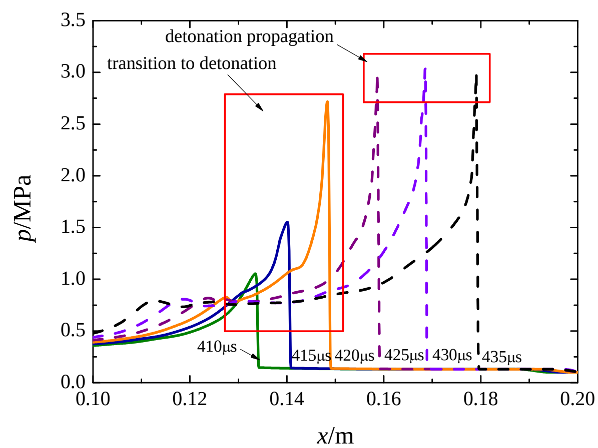


Figure 9. Variations of pressure at detonation stage

Figure 9 gives the pressure variations on the axis at detonation formation and propagation stage, corresponding time arranging from 410μs to 435μs, each adjacent line has an equal time interval of 5μs. The pressure peak of 410μs reaches about 1MPa, meaning that the unburned premixed gas will be highly compressed and well heated when the strong pressure wave passes over. As a result, the hydrogen/air mixtures behind the shock wave are easier to burn. As showed in Figure 10, the flame surface near the boundary starts to extend towards the axis of the tube while chasing the leading shock wave, making the premixed mixture near the axis burn. Furthermore, the quick expansion of products deriving from release of plenty chemical energy strengthen the leading shock wave in return, which constitutes a positive feedback called shock wave amplification by coherent energy release (SWACER) mechanism in the study of J.H. Lee [13]. Therefore, there is a sharp rise of pressure peak (about from 1MPa to 2.7MPa within 20μs) in the region of transition to detonation showed in Figure 8. In addition, the increasing distance between the adjacent pressure lines from 410μs to 420μs means the propagation velocity of pressure front increases dramatically. While from 425μs to 435μs, the distance between the adjacent pressure lines keeps almost invariable and the pressure peaks are almost the same, signifying the formation of stable detonation, of which the calculated detonation velocity is 2031m/s, very close to the theoretical C-J velocity of 1971 m/s.

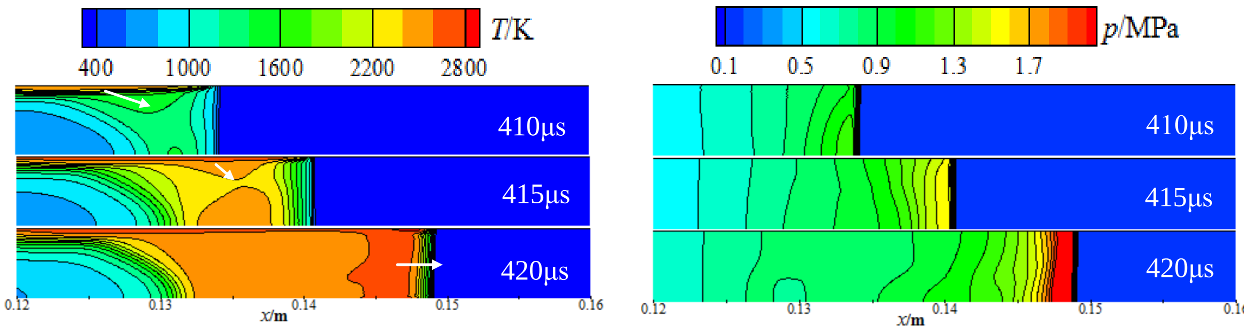


Figure 10. Temperature and pressure distribution

4 Conclusions

Two-dimensional numerical simulation is conducted to investigate the flow field characteristics and DDT mechanism in a cross-section abrupt tube for stoichiometric hydrogen/air mixtures in this study. The variation regulations of pressure and temperature distribution are analyzed in detail from three stages (flame acceleration, transition to detonation and detonation propagation). It is concluded that the existence of convex platform is helpful to DDT, which is validated comparing with the cases of annular tube and single tube: The DDT time and distance of cross-section abrupt tube are both shortest.

Acknowledgments

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