

Detonation Transmission Behavior in Stoichiometric Hydrogen-Air Mixtures: Effect of Tube Bundle Structures

Sun X., Li Q., Li C., Lu S.*

State Key Laboratory of Fire Science, University of Science and Technology of China,
Hefei, China

*Corresponding author's email: sxlu@ustc.edu.cn

ABSTRACT

In this study, the effects of bundle geometries and initial pressures on the detonation transmission behaviors were examined systematically in a circular tube with 6 m long and an inner diameter of 90 mm. The tube bundle structures were created by inserting several smaller pipes (20 mm outer diameter, 2 mm wall thickness) into the tube. Three different bundle structures can be obtained by varying the number of smaller pipes n of 3, 4 and 5. The iron probes and pressure transducers were used to determine the average velocity while the smoked foil technique was adopted to register the detonation cellular structures. The experimental results indicate that detonation can propagate at about the theoretical CJ velocity when the initial pressure (P_0) is greater than the critical value (P_c). However, when the initial pressure approaches to the critical value, the average velocity is decayed rapidly causing the failure of detonation. For the cases of $n = 3$ and 4, the phenomenon of detonation re-initiation with clear cellular pattern can be observed. The re-initiation distance is increased remarkably at $P_0 \approx P_c$. In the case of $n = 5$, the detonation velocity experiences a more violent fluctuation, and the value of the critical pressure is increased to 28 kPa sharply. Finally, the critical condition analysis of successful transmission is performed. The critical condition can be quantified as $D_H/\lambda > 1$. However, the critical values of D_H/λ are not uniform among various tube bundles, but in a small range, i.e., from 1.78 to 2.35.

KEYWORDS: Detonation transmission, tube bundle structures, detonation re-initiation, critical condition.

NOMENCLATURE

D inner diameter of big tube (mm)	l length of tube bundle (m)
d outer diameter of small tube (mm)	Greek
D_H hydraulic diameter (mm)	λ detonation cell size (mm)
P_0 initial pressure (kPa)	Subscripts
P_c critical pressure (kPa)	0 initial condition
V_f velocity deficit (-)	c critical condition
V_{CJ} theoretical CJ detonation velocity (m/s)	CJ Chapman-Jouguet

INTRODUCTION

Hydrogen, as a promising energy carrier, has received considerable attention due to its unique characteristics, e.g. faster laminar burning velocity, no greenhouse gas emissions and higher efficiency. However, because of its low ignition energy [1, 2] and wide flammability limit, even a

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weak ignition source may induce a potential flame hazard. As a result, any leakage of hydrogen during the production, transportation and storage stage may cause explosions/detonations accidents, which seriously threatens personal and property security [3-9]. Detonation wave, consisting of a chemical reaction zone coupled to a leading shock wave, travels at a supersonic speed. Across the detonation wave front, the thermodynamic parameters, e.g. initial pressure and temperature, increase sharply. In stoichiometric fuel-air mixtures, detonations can travel at thousands of meters per second and produce a very high overpressure (approximately 15-20 times initial pressure). From above discussions, it can be found that detonation wave has a more seriously destructive effect than other combustion modes. Thus, the detonation behaviors in hydrogen-air mixtures must be investigated in detail prior to its wide utilization.

This work aims to investigate the detonation transmission behaviors downstream of a sudden expansion in stoichiometric hydrogen-air mixture. Three different bundle structures are employed to explore the mechanisms of detonation transmission, re-initiation and failure. The pressure sensors and iron probes are adopted to derive the average velocity evolution. Moreover, smoked foil technique is used to register the detonation cellular structures, and the critical condition analysis of detonation transmission is also performed.

EXPERIMENTAL SET-UP

The experiments are conducted in a shock tube with an inner diameter of 90 mm and 6 m long. The tube consists of the driver section and the test section. The driver section is 4 m long, and the test section is 2 m in length. A sketch of the experimental set-up is shown in Fig. 1a.

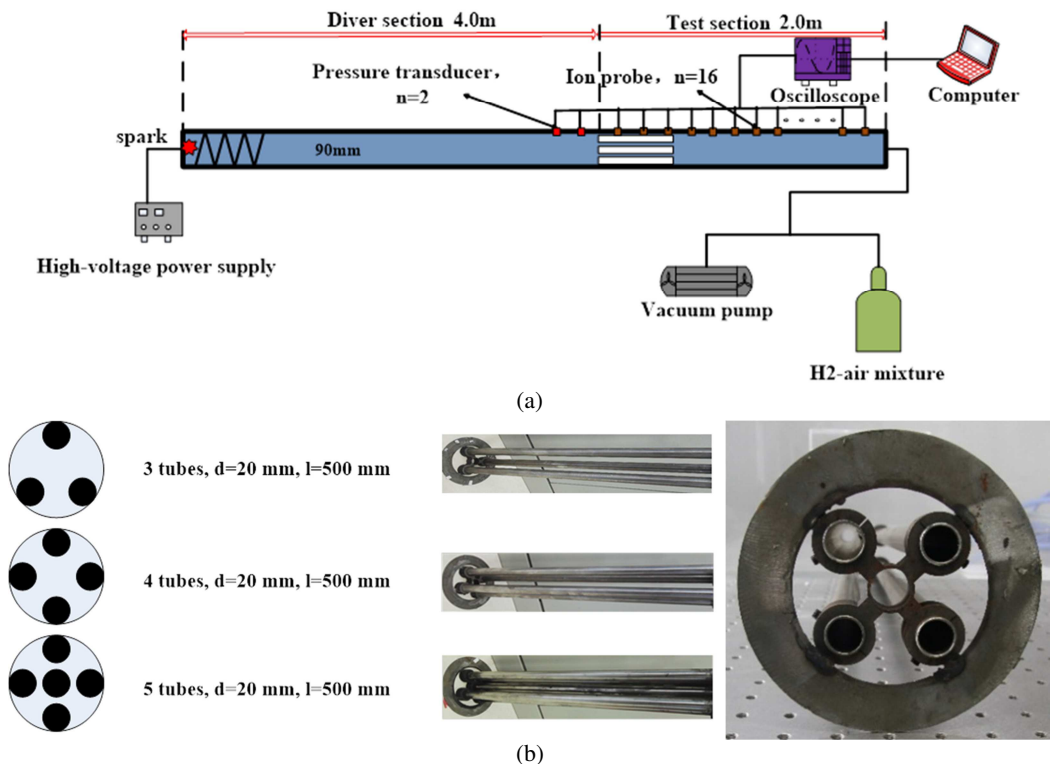


Fig. 1. Experimental set-up for tube experiments (a), tube bundle sections (b).

A 3.5 m long Schelkin spiral with 6 mm outer diameter is inserted into the driver section to accelerate the formation of detonation wave. The tube bundle section consists of multiple smaller pipes with an outer diameter of 20 mm, 2 mm wall thickness and 0.5 m long (see Fig. 1b, the schematic diagram and real picture of the tube bundle structure). It is located at the test section next to the driver section.

Of note is that the smaller pipes are all hollow and the combustion wave front can propagate through them and around them. Here, the interval between the outer wall of bundle structures and the inner wall of big tube is about 6 mm. By varying the number of smaller pipes n of 3, 4 and 5, three different tube bundle structures are obtained. The blockage ratios (BR) of bundle structures are 0.054, 0.072 and 0.09, respectively. In present study, the blockage ratio (BR) can be written as

$$BR = n \left(\frac{\pi d^2}{4} - \frac{\pi (d - 2\delta)^2}{4} \right) \frac{1}{\pi D^2 / 4} = \frac{4n\delta(d - \delta)}{D^2}, \quad (1)$$

where D is the inner diameter of big tube (mm), n is the number of small pipes, d is the outer diameter of small pipes (mm) and δ is the wall thickness of small pipes (mm).

In this study, the stoichiometric hydrogen-air mixtures are considered as the test gas with the initial temperature of 293 K. The mixtures were introduced into a 150 L mixing tank for at least 24 h to ensure homogeneity. The detonation tube is evacuated to smaller than 100 Pa pressure prior to each shot, and then a mixture is prepared by the method of partial pressures. The static pressure in the mixing tank and the tube was monitored by a pressure gauge (SXT-4A, 0-150 kPa) with an accuracy of $\pm 0.06\%$ full scale. The mixtures are ignited after 60 s when the mixtures were guided into the tube by an electric spark from the discharge of a capacitor bank. Sixteen Iron probes were fixed at the test section to record the time-of-arrival (TOA) of the detonation wave, from which the average velocity can be obtained. Two piezoelectric pressure transducers (PCB102B06) were mounted on the driver section to ensure a stable detonation wave has been produced prior to its transmission into the test section. A 0.1 mm thick stainless steel plate covered with uniform soot is inserted into the test section prior to each shot to record the detonation cellular structures.

RESULTS AND DISCUSSION

Smooth tube

Figure 2 shows the normalized detonation velocity by the CJ value as a function of distance in the smooth tube. The theoretical CJ detonation velocity (V_{CJ}) calculated by the CHEMKIN package is also given for comparison. Here, three various propagation mechanisms can be observed, i.e., supercritical condition, critical condition and subcritical condition. Of note is that, in this study, the propagation regimes are defined based on the average velocity. When the initial pressure (P_0) is greater than the critical value (P_c), e.g. $P_0 = 30$ and 28 kPa, the detonation velocity nearly fluctuates between $1.07V_{CJ}$ and $0.78V_{CJ}$. But its averaged value is approximately the theoretical CJ detonation velocity, which is defined as super-critical condition. As the initial pressure progressively decreases to 23 kPa, it can be observed that the average wave velocity continuous decreases to smaller than $0.5V_{CJ}$. It indicates that the detonation fails eventually by decoupling the leading shock wave from the reaction zone. This phenomenon is defined as sub-critical condition. The regime between super-critical condition and sub-critical condition is defined as critical condition, and it will be discussed in detail in the next section. For example, for the case of $P_0 = 25$ kPa, the wave velocity is in the range of $0.5V_{CJ}$ to V_{CJ} , which is often referred to as the quasi-detonation regime [10, 11]. This phenomenon can be explained by the complex interaction between shock waves and chemical reactions [12, 13].

Above results indicate that the velocity behavior of detonation propagation closely depends on the initial pressure. Moreover, the instabilities may also have a significant effect on detonation propagation. Lee [12, 14] claimed that, for an unstable mixture with high irregular cellular structure, the instability play an important role in the process of detonation propagation through sustaining and amplifying transverse wave in the reaction zone [12]. The localized explosion centers can be produced, which leads to the development of detonation. Meanwhile, it is also found that $0.5V_{CJ}$ is a rather universal phenomenon just prior to the failure of detonation, which is similar to the results obtained by Peraldi et al. [15], Zhu et al. [16] and Kuznetsov et al. [17].

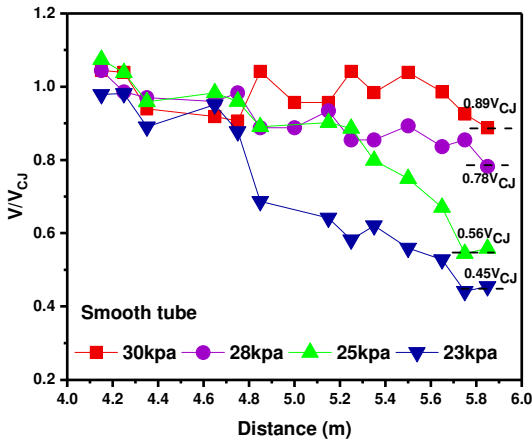


Fig. 2. Averaged velocity as a function of distance in the smooth tube.

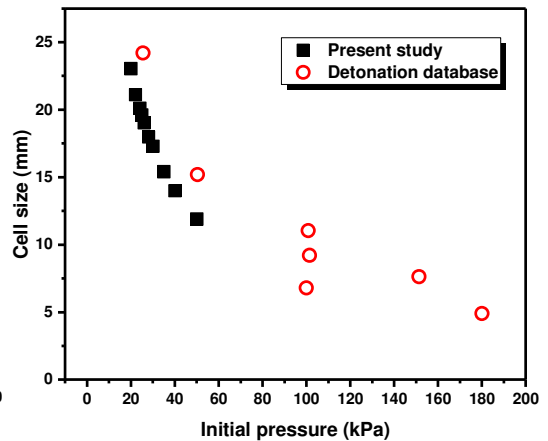


Fig. 3. Cell size for stoichiometric hydrogen-air mixtures at different initial pressures.

Smoked foil technique, as a simple and convenient test method, is widely employed in the study of detonation problems. The detonation cell size is produced from two sets of transverse waves (i.e. one rotating clockwise and another counterclockwise), then the helical paths of these two sets of transverse waves intersect to form a “fish scale” pattern on a smoked foil [12]. The characteristics of detonation in fuel/air and fuel/oxygen mixtures can be reflected by the cell size and regularity. In this study, the cell sizes of stoichiometric hydrogen-air mixtures at different initial pressures are shown in Fig. 3. The data obtained from the detonation database are also given for comparison. It can be found that the cell size is decreased with the increases of initial pressure. The agreement is good between two sets of results if the measurement error is considered.

EFFECT OF TUBE BUNDLES ON DETONATION TRANSMISSION

Figure 4 presents the averaged detonation velocity as a function of initial pressure (P_0) in the tube bundle section. It can be seen that the detonation velocity gradually decreases and deviates from the CJ value with the decreases of initial pressure. When the initial pressure (P_0) approaches to a certain critical value, a sudden velocity drop can be observed. This indicates that the detonation cannot sustain a steady velocity causing the failure of detonation. Therefore, the corresponding pressure value below that no steady velocity can be obtained is referred to as the critical pressure (P_c). For the cases of $n=3, 4,$ and 5 , the critical pressures are 25, 25 and 28 kPa, respectively. What also can be seen from Fig. 1 is that detonation can propagate at about the theoretical CJ velocity with a small deficit at $P_0 > P_c$. As the P_0 further drops, the velocity deficit (V_f) is increased sharply due to the heat and momentum losses by boundary effects [18-21]. The effect of boundary layer on the velocity deficit is firstly proposed by Manson and Guénoche [22], who suggested that the velocity deficit exists in the tube because the chemical reactions are inhibited in a thin layer adjacent to the

tube walls. Moreover, Manson and Guénoche [23] modified the hydrodynamic theory of detonation waves, and concluded that the velocity deficit is increased with the decreases of tube diameter. Here the velocity deficit can be defined as

$$V_f = \frac{\Delta V}{V_{CJ}} = \frac{V_{CJ} - V}{V_{CJ}}, \quad (2)$$

where V_{CJ} is the theoretical CJ velocity (m/s) and V is the experimentally measured velocity (m/s).

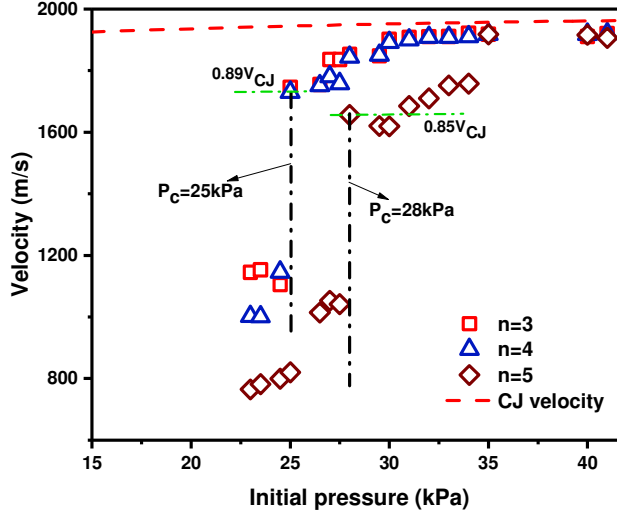


Fig. 4. Averaged velocity as a function of initial pressure in stoichiometric hydrogen-air mixture.

Figure 5 presents the detonation velocity evolution among three different tube bundles at $P_0 = 35, 30, 28$ and 25 kPa. Herein, every point is the experimental measured average velocity from three various shots. At $P_0 = 35$ kPa, the super-critical condition can be observed for three tube bundle structures. The detonation can propagate at about the theoretical CJ velocity with minor local fluctuations, which indicates the sudden expansions nearly have no influence on the detonation propagation. With the initial pressure is decreased to 30 kPa and 28 kPa, the phenomenon of detonation re-initiation can be seen (i.e., critical condition occurrence). Firstly, in the cases of $n = 3$ and 4 , the detonation velocity is rapidly decayed to about $0.5V_{CJ}$ after its propagation through the sudden expansion. However, the decoupled detonation wave is re-initiated with the speed back to over-driven state quickly. Subsequently, the over-driven detonation decays to a self-propagated detonation, similar to that be observed by Wu et al. [24]. This indicates that when the decoupled shock wave reflects from the wall, the shock-wall interaction ignites the detonation re-initiation [25-27]. Secondly, for the case of $n = 5$, the average velocity nearly fluctuates between $0.6V_{CJ}$ and V_{CJ} with a high frequency. This phenomenon is similar to the mode of “rapid fluctuation” observed by Lee et al. [28]. The mechanism of re-acceleration may be caused by the interaction between the flame and the boundary layer effect [29]. The transverse acoustic waves are amplified downstream of the obstacle due to reflections from the walls, which facilitates the re-acceleration of the detonation. As the initial pressure further decreases to 25 kPa, in the cases of $n = 3$ and 4 , the run-up distance of the over-driven state is sharply enhanced to 0.5 m far from the sudden expansion. This indicates that the decoupled detonation may be too weak causing the strength of shock-wall interaction is not enough to ignite the detonation re-initiation after a short distance. Therefore, the detonation re-initiation occurs with some delay. However, for the case of $n = 5$, the average velocity always fluctuates in the vicinity of $0.5V_{CJ}$ leading to the failure of detonation, and the phenomenon of re-initiation is not observed. This indicates that the negative effect (diffraction and wall loss

effect) plays a dominant role in the detonation propagation. Moreover, it is found that the velocity deficit is enhanced obviously with the increases of the number of smaller pipes at the same initial pressure. This phenomenon can be attributed to the boundary layer effect [23].

Above results show that the detonation sensitivity of mixtures is reduced with the decreases of initial pressure. The strength of detonation wave is not enough to survive from the perturbation induced by the obstacle, which causes the detonation fails eventually. Subsequently, detonation re-initiation may occur due to the shock-wall interaction. This is similar to the results obtained by Zhang et al. [30] and Teodorczyk et al. [31].

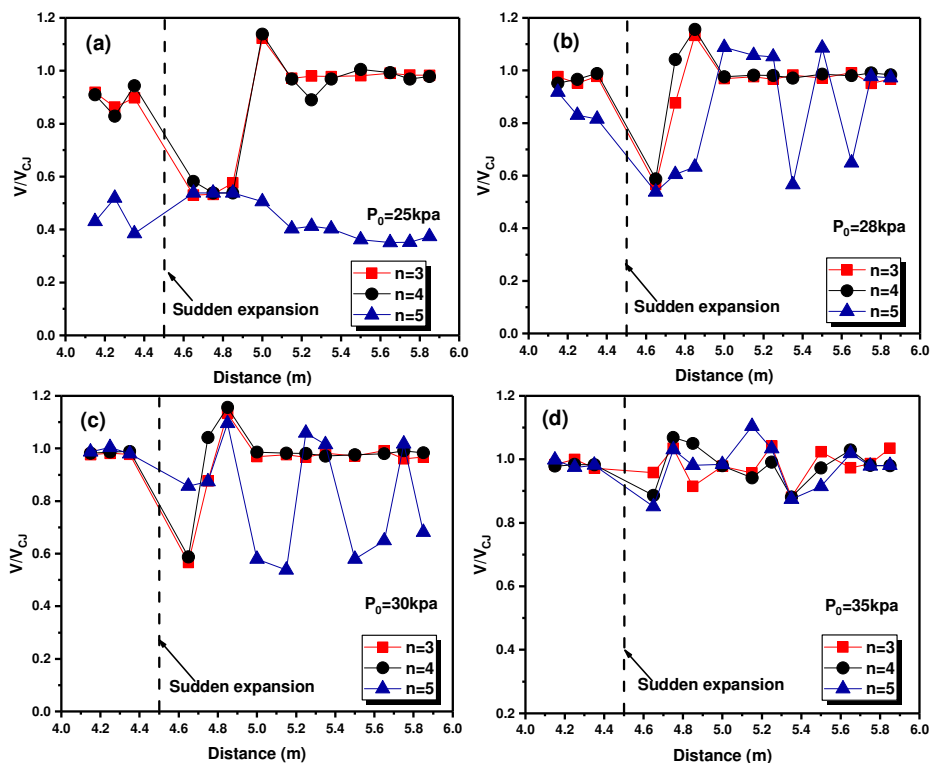


Fig. 5. Averaged velocity as a function of distance for different tube bundle structures.

To further understand the mechanism of the detonation re-initiation, the detonation cellular patterns recorded on the foil downstream of the sudden expansion with $n = 4$ are presented in Fig. 6. For the case of super-critical condition (i.e. $P_0 = 35$ kPa), detonation cell structure is recorded on the foil immediately after the sudden expansion. This indicates that the detonation implodes before the decoupled detonation wave front contacts the tube wall. In the study of Pintgen and Shepherd [32], for the case of super-critical condition, a transverse detonation can be observed when the detonation diffracts from a circular tube, which can trigger the detonation re-initiation.

At $P_0 = 30$ kPa, cellular patterns disappear at first and the cone-shaped boundary line between no cell zone and small cell zone can be seen obviously. Afterwards, the detonation cells gradually grow as its propagation. The over-driven detonation decays to a self-sustained detonation wave. This further indicates that when the decoupled detonation reaches the wall, the shock-wall interaction ignites the detonation re-initiation, similar to that be observed by Wu et al. [24]. At $P_0 = 25$ kPa, the run-up distance of detonation re-initiation is sharply increased to about 520 mm, which indicates

that the shock-wall interaction is too weak when the initial pressure approaches to the critical value of detonation transmission. Thus, the detonation is re-initiated with some delay.

As the initial pressure progressively decreases to 24 kPa, the detonation velocity continuously decreases to about $0.34V_{CR}$, which indicates that the detonation fails eventually and cellular structure cannot be recorded on the smoked foil.

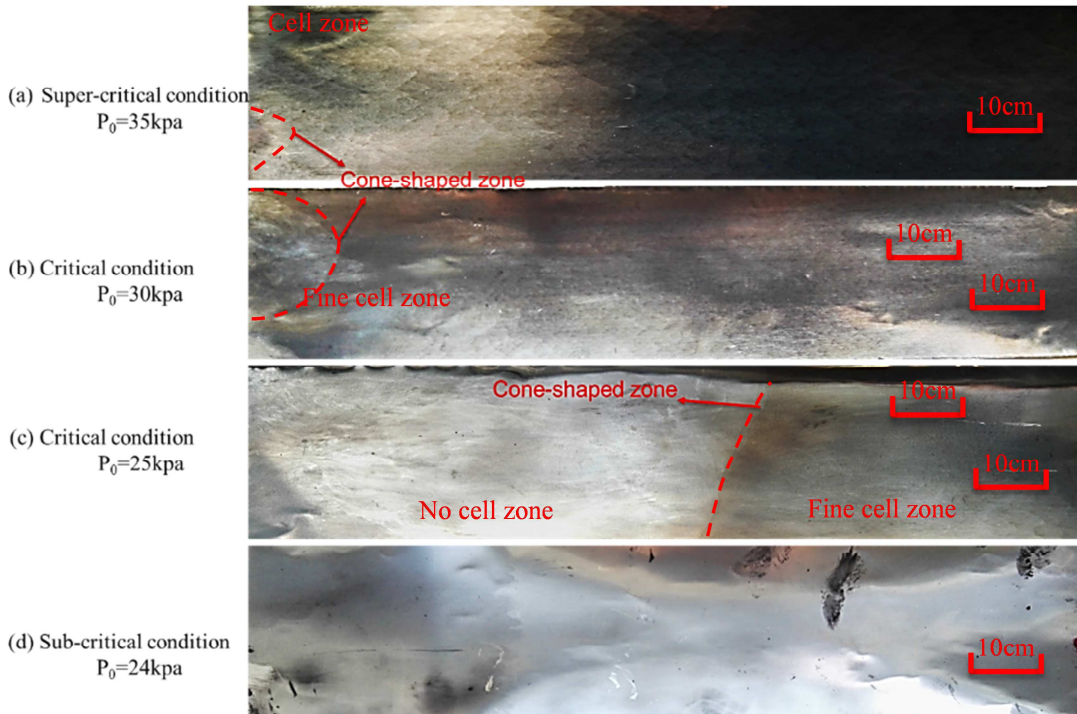


Fig. 6. Detonation cell records at $n = 4$.

The experimental results after the tube bundle section are presented in Table 1, including the critical pressure, the detonation cell size and the values of D_H/λ . Herein, the value of λ is a mean value from five different shots in this study. In previous investigations, d/λ as a proper parameter is often adopted to predict the detonation propagation limits [12, 30, 31]. Lee et al. [34] reported that the influence of boundary condition on the detonation propagation closely depends on the tube dimension and the instability in the near-critical conditions, and the tube diameter (d) should be related to the length scale of the detonation structure itself characterized by λ . For the bundle structures adopted in this paper, it is more reasonable to determine the hydraulic diameter (D_H) as a characteristic dimension to research the propagation of detonation. Because D_H is a common parameter to investigate flow in noncircular tubes or channels. Using this term one can compare the results in round tube and bundle sections at the same standard. In the present study, the corresponding hydraulic diameter is $D_H = 46, 38.2,$ and 32.1 mm, respectively. Figure 7 shows the normalized detonation velocity as a function of D_H/λ at different bundle structures. It can be observed that, for all these mixtures and geometries, the failure condition is similar to the results obtained by Cross and Ciccarelli [10], Peraldi et al. [15] and Knystautas et al. [35], i.e., $D_H/\lambda > 1$, which indicates that the detonation can sustain its propagation only when the number of detonation cells across the hydraulic diameter is larger than 1 at least. Of note is that the values of D_H/λ are not uniform, but in a small range among various tube bundle structures, i.e., from 1.78 to 2.35. The

discrepancy can be explained and the specific reasons are as follows. The logical criterion, $D_H/\lambda > 1$, is mainly related to the global reaction zone thickness, Δ_H [36] and the experimentally measured detonation cell size, λ . Firstly, the experimentally measured reaction zone thickness is defined as the distance between the shock front and an equivalent CJ surface, which is also called as the hydrodynamic thickness [37]. Except for the directly experimental measurement, the value of Δ_H can be replaced by the ratio of the detonation velocity to the rate of transverse shock amplification [38]. Thus, the values of Δ_H remain some deviation. Secondly, the subjectivity of the experimentally measured detonation cell size is inevitable, accompanying large fluctuations, especially near the critical conditions. Therefore, the fluctuation in the values of D_H/λ cannot be avoided. However, the agreement is good if these measured uncertainties are taken into account.

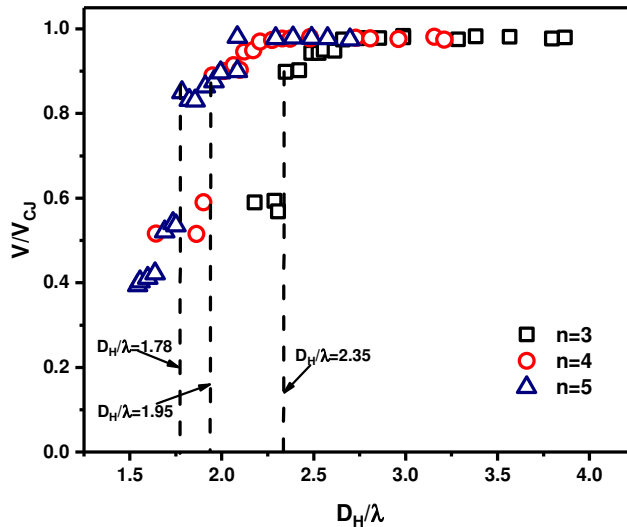


Fig. 7. The normalized detonation velocity as a function of D_H/λ .

Table 1. Experimental results for detonation at the critical condition

n	D_H , mm	P_c , kPa	λ , mm	D_H/λ
3	46	25	19.6	2.35
4	38.2	25	19.6	1.95
5	32.1	28	18	1.78

CONCLUSIONS

Experimental studies of detonation transmissions through finite expansions in bundle geometries are performed comprehensively in stoichiometric hydrogen-air mixture. Three various tube bundle structures can be obtained by varying the number of small pipes n of 3, 4 and 5. The influences of initial pressure and bundle geometries on the detonation transmission behaviors are explored systematically. The results indicate that three various propagation mechanisms can be observed, i.e., supercritical condition, critical condition and subcritical condition. In the tube bundle section, when the initial pressure is larger than P_c , the detonation can propagate at about the theoretical CJ velocity. However, the average velocity is decayed rapidly at $P_0 \approx P_c$.

In the cases of $n = 3$ and 4, the phenomenon of detonation re-initiation can be observed after its propagation through the sudden expansion, and the localized explosion centers are indicated on the smoked foil obviously. For the reactive reactants, detonation re-initiation can be ignited after a short

distance far from the sudden expansion due to the stronger shock-wall interaction. However, as the initial pressure approaches to the critical value, the re-initiation distance is significantly lengthened due to the weaker detonation sensitivity. For the case of $n = 5$, the detonation velocity experiences a more violent fluctuation, and the critical pressure value is also enhanced to 28 kPa sharply. The bundle structures can enhance the critical pressure (P_c) obviously.

Detonation cell sizes are measured at the critical pressure. A dimensionless parameter D_H/λ is introduced to correlate with the normalized detonation velocity (V/V_{C1}). The results indicate that the critical condition of detonation propagation can be quantified as $D_H/\lambda > 1$.

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