

Scaling Analysis of Gaseous Detonation Limits in Tubes

Xinru Zhang^a, Minhui Zeng^a, Ashwin Chinnayya^b, Wei Fan^a, Qiang Xiao^{*,a,c}

^aSchool of Power and Energy, Northwestern Polytechnical University
Xi'an, 710072, PR China

^bInstitut Pprime, UPR 3346 CNRS, ISAE-ENSMA, Université de Poitiers
86961 Futuroscope-Chasseneuil Cedex, France

^cAdvanced Power Research Institute of
Northwestern Polytechnical University in Sichuan Tianfu New Area, Chengdu, PR China

1 Introduction

The detonation limit problem is a classical topic of fundamental detonation research relevant to industrial safety and engine propulsion applications, such as the design of flame arrestors for suppressing explosions in pipelines and of pre-detonators for detonation engines. It generally refers to the minimum tube size (d_c) required for detonations to propagate successfully at specific pressures or the minimum pressure (p_c) for the specific tube dimension, below which detonations would fail. Thus, these critical conditions define the detonation limits [1–4]. While extensive experiments have been conducted by numerous researchers for measuring the limits of gaseous detonations in tubes of different sizes for various mixtures, the inherent stochastic nature of the limiting phenomenon, the considerable measurement uncertainty of near-limit detonations, and moreover the notable detonation cellular instability have posed remarkable challenges for the community to achieve a unified description of the limits, irrespective of mixtures and tube sizes. Even the proposed rule of $d_c \sim \lambda/3$ can break down for different tube dimensions [1, 4], where λ is the detonation cell size, whose measurement could significantly introduce additional uncertainty. Also, these works shed little light on the role of instability in quantitatively impacting the detonation limits.

Recently, Xiao and collaborators [5, 6] employed the well-established instability parameter of $\chi = (E_a/RT_s)(\tau_{ig}/\tau_{re})$ to quantify the effects of cellular instability on detonation dynamics, where E_a/RT_s represents the von Neumann(vN) state reduced effective activation energy (also written as $\theta = E_a/RT_s$) and τ_{ig}/τ_{re} characterizes the system's sensitivity to temperature fluctuations through the ratio of characteristic induction time to exothermic reaction time. By adopting the characteristic length of the effective induction zone length $\Delta_{i,loss}$ (calculated by considering the detonation velocity deficits) to normalize the geometry dimensions, they successfully obtained the universal dynamics of detonations in 23 different gaseous mixtures, covering the instability range from 1 to 2000 [6]. Of noteworthy is that such an attempt did not focus on limiting behaviors, due to the large spread of velocity deficits typically measured for near-limit detonations from experiments, which lead to substantially different induction lengths of $\Delta_{i,loss}$. As a result, the scaled limits can vary up to several orders of magnitude [6]. Therefore, as a follow-up study, the present work aims to unify the propagation limits of gaseous detonations in tubes by analyzing the large pool of the already published experiments data. Particularly, the link of scaled limits with respect to detonation instability would be established for the first time for gaseous detonations in tubes.

2 The Generalized ZND Model Predicted Hydrogen Detonation Limits

The recent works of Xiao and collaborators [5, 8] have demonstrated the good performance of the generalized Zeldovich-von Neumann-Döring (ZND) model in predicting the hydrogen detonation dynamics. Before analyzing the large pool of the experimentally obtained detonation limit data obtained by different researchers, we adopted this well-performed steady model for theoretically calculating the critical detonation propagation limits in terms of the critical tube size with respect to initial pressures. In the shock-attached frame of reference, the extended ZND model with wall losses can be expressed as [2, 9]

$$\frac{dp}{dt} = -\rho u^2 \frac{\dot{\sigma}_{re} - \dot{\sigma}_A}{\eta} \quad (1a)$$

$$\frac{d\rho}{dt} = -\rho \frac{\dot{\sigma}_{re} - M^2 \dot{\sigma}_A}{\eta} \quad (1b)$$

$$\frac{du}{dt} = u \frac{\dot{\sigma}_{re} - \dot{\sigma}_A}{\eta} \quad (1c)$$

$$\frac{dy_i}{dt} = \frac{W_i \dot{\omega}_i}{\rho} \quad (i = 1, \dots, N_s) \quad (1d)$$

$$\frac{dx'}{dt} = u \quad (1e)$$

with

$$\eta = 1 - M^2, \quad \dot{\sigma}_{re} = \sum_{i=1}^{N_s} \left(\frac{W}{W_i} - \frac{h_i}{c_p T} \right) \frac{dy_i}{dt}, \quad \dot{\sigma}_A = \frac{u}{A_{tot}} \frac{dA_{tot}}{dx'} \quad (1f)$$

where $\dot{\sigma}_{re}$ is the thermodynamicity of ideal gases, and $\dot{\sigma}_A$ represents the source term representative of wall losses, which can generally be interpreted by the boundary layer-induced flow divergence. According to Fay's boundary-layer mechanism [7], such boundary-layer-induced flow divergence of detonations in tubes can be modeled as

$$\frac{d \ln(A_{tot})}{dx'} = \frac{2}{r + \delta^*(x')} \frac{d\delta^*(x')}{dx'} \quad (2a)$$

where r is the tube radius, and $\delta^*(x')$ the boundary layer displacement thickness, which can be evaluated by [5, 10]

$$\delta^*(x') = K_M \sqrt{\nu_s \int_0^{x'} \frac{1}{u(x')} dx'} \quad (2b)$$

where ν_s is the post-shock kinetic viscosity, and $u(x')$ is the post-shock particle velocity in the shock-attached frame of reference. K_M is the Mirels' constant, which turns out to be approximately 4.5 for hydrogen-oxygen-argon detonations [8]. By following the ZND computation framework of Xiao & Radulescu [8], we could then evaluate the minimum tube size for detonation propagation at specific initial pressures.

Figure 1 shows the theoretically calculated relationship between the minimum tube radius and the critical initial pressures for the hydrogen-oxygen-argon detonations, made by solving the generalized ZND model with the detailed San Diego reaction mechanism (The effect of reaction mechanisms on the evaluation of the scaled limits will be clarified in detail during the presentation in the conference). It is evident that the minimum tube radius decreases with the increasing initial pressure, which means that higher initial pressures with a higher kinetic sensitivity enable detonations to propagate in much smaller tubes. Also, the addition of argon decreases the mixture sensitivity and thus requires a larger minimum tube size for detonations propagating at the same initial pressure. Moreover, the relation between the minimum tube radius and the critical initial pressure follows the power-law relationship, as can be readily inferred from the linear curves in the log-scale framework in Fig. 1(a). Such finding is consistent with the experimental results of Gao et al. [4] that the experimentally measured minimum tube diameter with respect to initial pressures is also of the power-law relationship. Furthermore, we normalized the critical tube size using the ideal Chapman-Jouguet (CJ) detonation induction zone length ($\Delta_{i,CJ}$), as shown in Fig. 1(b). Clearly, in spite of the argon dilution and initial pressures, the scaled detonation limits tend to collapse well around $r/\Delta_{i,CJ} = 4$, particularly for those above the critical initial pressure of 10 kPa.

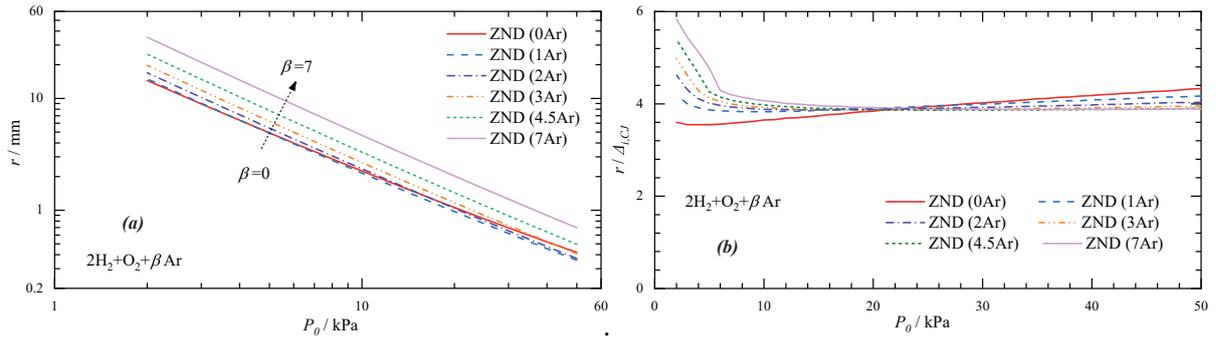


Figure 1: ZND model calculated hydrogen-oxygen-argon detonation limits: (a) the minimum tube radius with respect to the critical initial pressure and (b) the critical tube radius scaled by the ideal CJ detonation induction zone length $\Delta_{i,CJ}$

3 Scaled Detonation Limits from Experiments

As the theoretical results and the experiments of Gao et al. [4] have demonstrated that the minimum tube size with respect to the critical initial pressure followed a power-law relationship, we thus took the same approach, using the same type of relationship, from the large pool of the already published detonation limits data, which were experimentally measured by a large number of researchers [4, 11–31]. Figures 2 and 3 show the experimentally measured minimum tube radius with respect to critical initial pressures for 8 different mixtures, and the corresponding fitted relationships using the least-squares method. It is clear that the experimentally measured minimum tube sizes, obtained by different researchers, are scattered around the fitted relationships. Particularly for the stoichiometric hydrogen-oxygen ($2H_2 + O_2$) in Fig. 2(a), methane-oxygen ($CH_4 + 2O_2$) in Fig. 3(b), and propane-oxygen ($C_3H_8 + 5O_2$) in Fig. 3(c), such scatter is substantial, which shows the large uncertainties in experimentally determining the detonation propagation limits. Causes of these discrepancies can be partly due to the inherently stochastic nature of the complicated limiting phenomenon. As recently shown by Xiao et al. [8], whether detonations near the limit can go or no-go depends on probability, thus leading to different limits measured in experiments. Moreover, the experimental detection techniques of propagation limits, employed by different techniques, could also impact the results. Notably, detonation limits do not have a clear definition, but is arbitrary (e.g., the stability of the detonation velocity, the onset of spinning detonation, etc.), different definitions can also have an impact.

Finally, we scaled the experimentally measured detonation limits with respect to the detonation instability (χ) by the ideal CJ detonation induction zone length $\Delta_{i,CJ}$, as shown in Fig. 4. Note that we resorted to such characteristic length scale for normalization instead of the detonation cell size λ , due to its considerable measurement uncertainty involved in experimentally determining this size (particularly for irregular detonations), which could add to the difficulty in unifying the propagation limits. While for the induction zone length $\Delta_{i,loss}$, whose evaluation requires measuring the velocity deficit, of which the measurement in experiments could vary significantly for the limiting detonations, it is thus also subject to substantial uncertainty. Also of noteworthy is that for other mixtures except those shown in Figs. 2 and 3, the experimental data are quite limited for fitting. As such, we both incorporated the fitted results for the 8 mixtures (as shown in Figs. 2 and 3) and also the discrete data for the rest mixtures (as listed in the left-bottom legend in Fig. 4). From the scaled results in Fig. 4, it can be clearly seen that the detonation limits have almost no dependency on the detonation instability χ , with those of the most mixtures remaining in the range between $r/\Delta_{i,CJ} = 5$ and $r/\Delta_{i,CJ} = 10$. The obvious exception is the methane-oxygen mixtures, whose instability is in the order of 1000, with their limits substantially smaller than the other less unstable mixtures. Such a significant difference also enables us to conclude that methane-oxygen detonations have a potentially very distinct physical mechanism at play for their failure events.

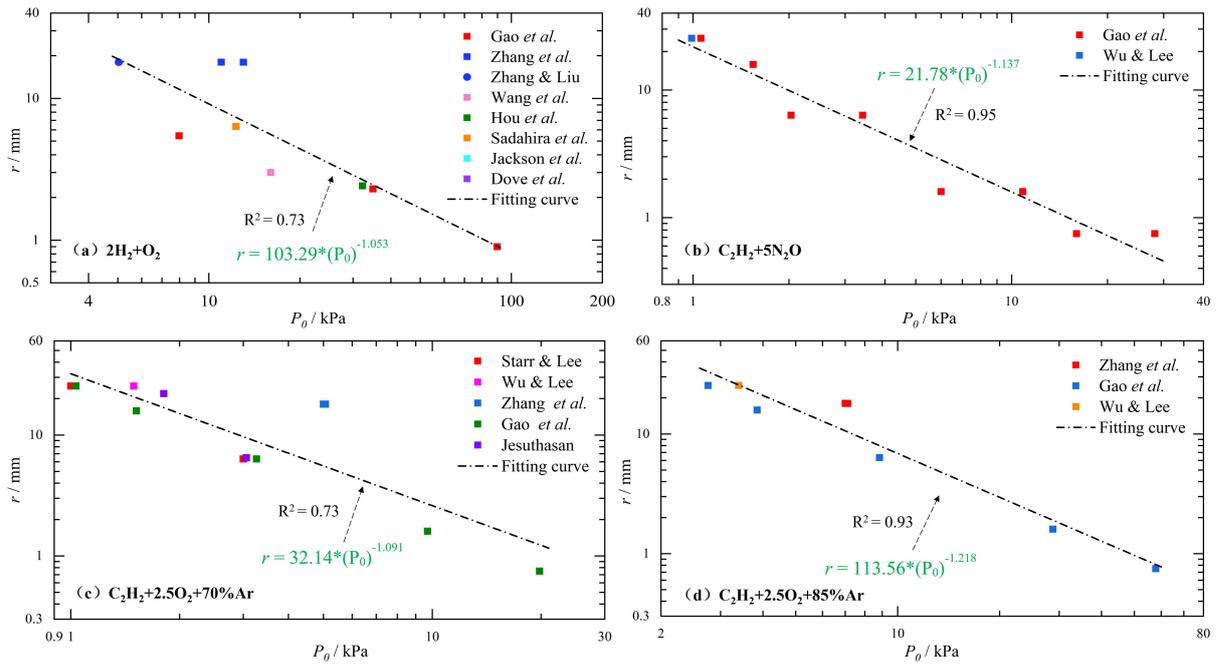


Figure 2: Relationship between the minimum tube radius and the critical initial pressure for four different mixtures, fitted from the experimental works [4, 11–22].

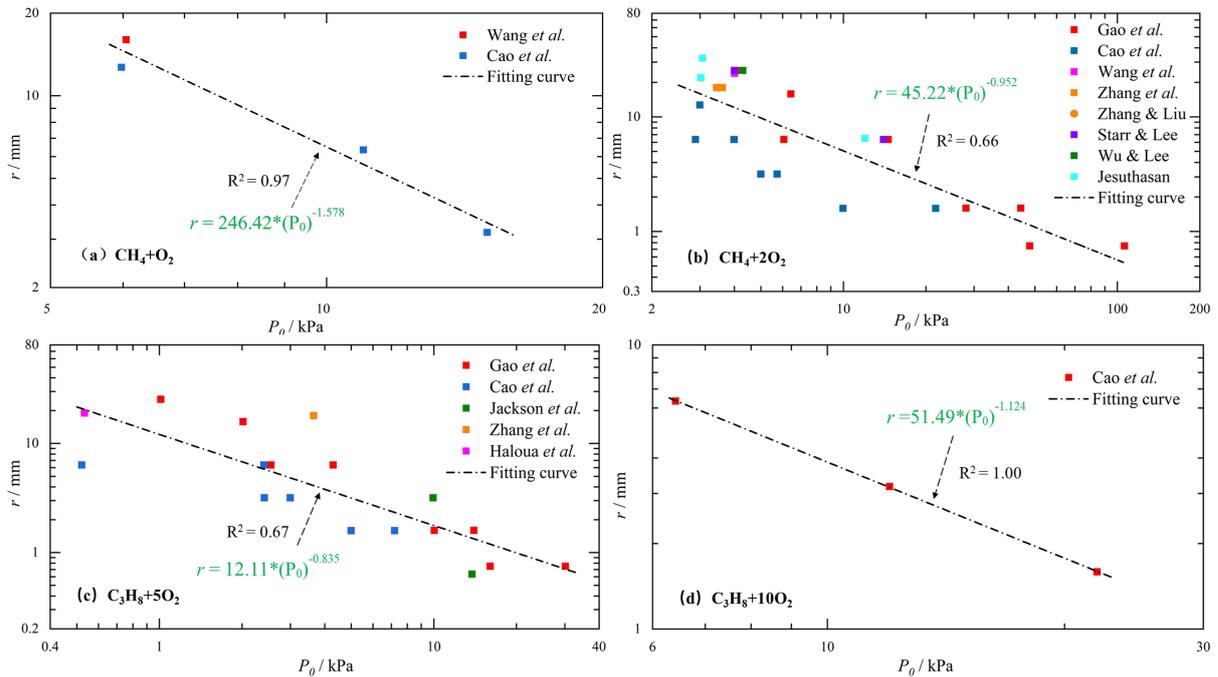


Figure 3: Fitted relationship between the minimum tube radius and the critical initial pressure for four different mixtures, with the experimental data adapted from Refs. [4, 12, 14, 16, 18–20, 22–29].

4 Conclusion

The present work adopted the generalized ZND model for theoretically calculating the critical detonation propagation limits of hydrogen-oxygen-argon mixtures. It is found that the relation between the minimum tube radius and the critical initial pressures follows a power-law relationship. Meanwhile, the scaled detonation limits (with the critical tube radius normalized using the ideal CJ detonation induction zone length) tend to collapse around $r/\Delta_{i,CJ} = 4$. Moreover, we adopted the least-squares

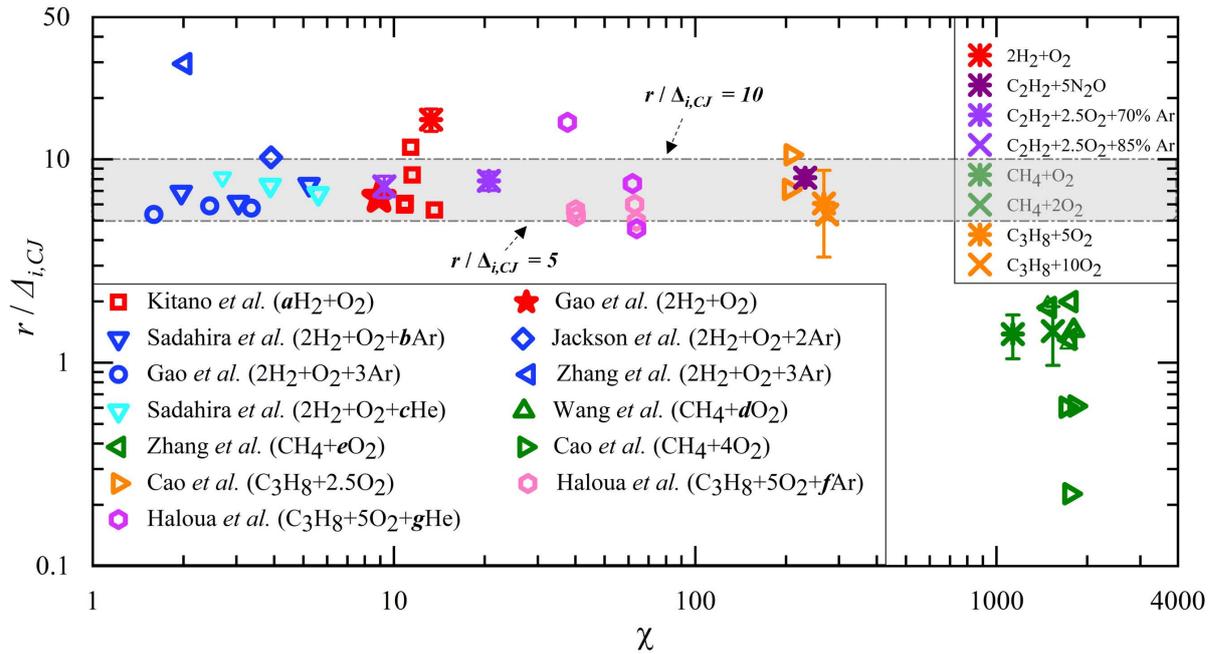


Figure 4: The ideal CJ detonation induction zone length $\Delta_{i,CJ}$ scaled detonation limits with respect to the detonation instability. Note that the results are either directly adapted from the Refs. [11, 13, 15, 16, 23–25, 28–31] (as listed in the left-bottom legend) or evaluated from the fitted relationships in Figs. 2 and 3 (with the mixtures documented in the top-right legend).

method for fitting the characteristic relation from a large number of already published detonation limit data for 8 different mixtures. The results showed that the experimental data were scattered around the fitted relationships. Finally, we scaled the experimentally measured detonation limits (including the fitted results for these 8 different mixtures and also the discrete data for the rest mixtures) by the ideal CJ detonation induction zone length $\Delta_{i,CJ}$. We found that the scaled detonation limits remain in the range between $r/\Delta_{i,CJ} = 5$ and $r/\Delta_{i,CJ} = 10$, with respect to the detonation instability (χ) except for the methane-oxygen mixtures, due to the potentially very distinct physical mechanism at play for their failure events.

Acknowledgments

The authors acknowledge the National Natural Science Foundation of China (Grant Nos. 52176133 and 52336006). This study is also supported by Sichuan Provincial Natural Science Foundation (NO: 2025ZNSFSC1247) and the Fundamental Research Funds for the Central Universities.

References

- [1] Lee JHS, Jesuthasan A, Ng HD. (2013). Near limit behavior of the detonation velocity. *Proc. Combust. Inst.* 34: 1957-1963.
- [2] Chao J, Ng HD, Lee JHS. (2009). Detonability limits in thin annular channels. *Proc. Combust. Inst.* 32: 2349-2354.
- [3] Lee JHS. (2008). *The Detonation Phenomenon*. Cambridge University Press (ISBN 978-0-521-89723-5).
- [4] Gao Y, Ng HD, Lee JHS. (2014). Minimum tube diameters for steady propagation of gaseous detonations. *Shock Waves*. 24: 447-454.
- [5] Xiao Q. (2023). On the geometrical scaling of hydrocarbon detonation dynamics. *Combust. Flame*. 251: 112714.
- [6] Xiao Q, Zhang Q, Chinnayya A. (2024). The universal gaseous detonation dynamics. *Combust. Flame*. 270: 113757.

- [7] Fay JA. (1959). Two-dimensional gaseous detonations: Velocity deficit. *Phys. Fluids*. 2: 283-289.
- [8] Xiao Q, Radulescu MI. (2020). Dynamics of hydrogen–oxygen–argon cellular detonations with a constant mean lateral strain rate. *Combust. Flame*. 215: 437-457.
- [9] Klein R, Krok JC, Shepherd JE. (1995). Curved quasi-steady detonations: Asymptotic analysis and detailed chemical kinetics. GALCIT Rep. FM 95-04.
- [10] Zangene F, Hong Z, Xiao Q, Radulescu MI. (2021). The Role of the Argon and Helium Bath Gases on the Detonation Structure of H₂/O₂ Mixture. International Conference on Hydrogen Safety, Edinburgh.
- [11] Gao Y, Zhang B, Ng HD, Lee JHS. (2016). An experimental investigation of detonation limits in hydrogen–oxygen–argon mixtures. *Int. J. Hydrogen Energy*. 41: 6076-6083.
- [12] Zhang B, Liu H, Li Y. (2019). The effect of instability of detonation on the propagation modes near the limits in typical combustible mixtures. *Fuel*. 253: 305-310.
- [13] Zhang B, Shen X, Pang L, Gao Y. (2015). Detonation velocity deficits of H₂/O₂/Ar mixture in round tube and annular channels. *Int. J. Hydrogen Energy*. 40: 15078-15087.
- [14] Zhang B, Liu H. (2019). Theoretical prediction model and experimental investigation of detonation limits in combustible gaseous mixtures. *Fuel*. 258: 116132.
- [15] Sadahira K, Kitawaki Y, Inaba T, Susa A, Matsuoka K, Johzaki T, Endo T. (2013). Velocity deficits of Ar and He diluted H₂-O₂ system in small diameter tubes. In Proc. 24th Int. Colloq. Dynamics Expl. Reac. Sys, Taipei.
- [16] Jackson S, Lee BJ, Huang W, Pintgen F, Karnesky J, Liang Z, Shepherd JE. (2009). Experimental detonation propagation under high loss conditions. In Proc. 22nd Int. Colloq. Dynamics Expl. Reac. Sys, Belarus.
- [17] Dove JE, Scroggie BJ, Semerjian H. (1974). Velocity deficits and detonability limits of hydrogen-oxygen detonations. *Acta Astronaut*. 1: 345-359.
- [18] Gao Y, Ng HD, Lee JHS. (2015). Experimental characterization of galloping detonations in unstable mixtures. *Combust. Flame*. 162: 2405-2413.
- [19] Wu Y, Lee JHS. (2015). Stability of spinning detonation waves. *Combust. Flame*. 162: 2660-2669.
- [20] Starr A, Lee JHS, Ng HD. (2015). Detonation limits in rough walled tubes. *Proc. Combust. Inst*. 35: 1989-1996.
- [21] Zhang B, Liu H, Wang C. (2018). Detonation propagation limits in highly argon diluted acetylene-oxygen mixtures in channels. *Exp. Therm. Fluid Sci*. 90: 125-131.
- [22] Jesuthasan A. (2011). Near-limit propagation of detonations in annular channels. McGill University (Canada).
- [23] Wang L, Ma H, Shen Z, Xue B, Cheng Y, Fan Z. (2017). Experimental investigation of methane-oxygen detonation propagation in tubes. *Appl. Therm. Eng*. 123: 1300-1307.
- [24] Cao W, Ng HD, Lee JHS. (2020). Near-limit detonations of methane–oxygen mixtures in long narrow tubes. *Shock Waves*. 30: 713-719.
- [25] Cao W, Gao D, Ng HD, Lee JHS. (2019). Experimental investigation of near-limit gaseous detonations in small diameter spiral tubing. *Proc. Combust. Inst*. 37: 3555-3563.
- [26] Wang LQ, Ma HH, Deng YX, Shen ZW. (2019). On the detonation behavior of methane-oxygen in a round tube filled with orifice plates. *Process Saf and Environ*. 121: 263-270.
- [27] Zhang B, Liu H, Wang C, Yan B. (2017). An experimental study on the detonability of gaseous hydrocarbon fuel–oxygen mixtures in narrow channels. *Aerosp. Sci. Technol*. 69: 193-200.
- [28] Zhang B, Shen X, Pang L, Gao Y. (2016). Methane–oxygen detonation characteristics near their propagation limits in ducts. *Fuel*. 177: 1-7.
- [29] Haloua F, Brouillette M, Lienhart V, Dupré G. (2000). Characteristics of unstable detonations near extinction limits. *Combust. Flame*. 122: 422-438.
- [30] Kitano S, Fukao M, Susa A, Tsuboi N, Hayashi AK, Koshi M. (2009). Spinning detonation and velocity deficit in small diameter tubes. *Proc. Combust. Inst*. 32: 2355-2362.
- [31] Zhang B, Liu H, Yan B. (2019). Investigation on the detonation propagation limit criterion for methane-oxygen mixtures in tubes with different scales. *Fuel*. 23: 617-622.