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Short communication

Measurement and prediction of detonation cell size in binary fuel blends of methane/hydrogen mixtures

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HIGHLIGHTS

- New detonation cell sizes for CH_4–H_2–O_2 are obtained from experimental measurement.
- Cell sizes are predicted from a detailed chemical kinetic model.
- A linear relationship between detonation cell size and the ZND induction zone length is determined.

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ABSTRACT

In this study, detonation cell sizes of binary fuel blends of methane–hydrogen–oxygen mixtures with different compositions (i.e., CH_4–$2H_2$–$3O_2$, CH_4–H_2–$2.5O_2$ and CH_4–$4H_2$–$4O_2$) are experimentally measured. Good agreement is found between the experimental data and predictions based on the chemical length scales obtained from a detailed chemical kinetic model. The results show that detonation structure in methane–hydrogen–oxygen mixtures are irregular and detonation cell size (λ) for CH_4–H_2–$2.5O_2$ mixture is larger than CH_4–$2H_2$–$3O_2$ and CH_4–$4H_2$–$4O_2$ mixtures. A linear relationship is determined by: $\lambda = 34.62\Delta_I$, through scaling the detonation cell size with the ZND induction zone length (Δ_I) for methane–hydrogen–oxygen mixtures, and this scaling function is universal in CH_4–H_2–O_2 mixtures at three compositions.

1. Introduction

Binary fuel blends of methane and hydrogen mixture have many promising combustion performances, e.g., lower the levels of unwanted pollutants (i.e., nitric oxide, polycyclic aromatic hydrocarbons and soot particles), higher thermal efficiency, larger cycle-by-cycle variation, and better lean-burn capability. It thus has a wide application in industry, especially in the internal combustion engines [1,2].

It is known explosions and detonations in fuel/air or fuel/oxygen always happen and result in severe casualty and property loss [3–9]. Hence, before promoting wide use of binary fuel blends of methane and hydrogen as an alternative fuel in industrial applications, related safety issues have to be prioritized. For the detonation hazard assessment, measurement of dynamic detonation parameter such as cell sizes provides fundamental information for the characterization of the explosion properties and the detonation sensitivities [10,11]. The detonation cell size is formed from two sets of transverse waves, i.e., one rotating clockwise and the other counterclockwise, then the helical paths of these two sets of transverse waves intersect to produce a "diamond" or "fish scale" pattern on a smoked foil [12], and the regularity of the cellular structure pattern indicates the degree of detonation stability in fuel/air and fuel/oxygen mixtures. But unfortunately, there is no detonation cell size available for methane–hydrogen–oxygen mixtures as yet.

In this study, detonation cell sizes of methane–hydrogen–oxygen mixtures at different compositions are measured from experiment. A theoretical approach, which is based on the properties obtained from chemical kinetics, is carried out to predict the cell size. The results from two methods are compared. Furthermore,

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the relationship between cell size and characteristic length scale in detonation structure is also analyzed.

2. Experimental section

Experiments were performed in a 1.2 m long, 68 mm inner diameter steel driver section followed by a test section of tube with 2.5 m in length and an inner diameter of 36 mm, the detailed experimental setup can be found in our previous study, and the references therein [13,14]. For completeness, it is briefly described here. The smoked foils with 500 mm in length (i.e., from 2950 mm to 3450 mm to the igniter) and 100 mm in width, were inserted from the end of test tube to record the cellular structure as the detonations propagate with steady velocities. At least three shots were repeated for the mixture at each initial condition. It has been suggested by Jesuthasan [15] that, the structure of the detonation is independent of the geometry as the condition well within the detonation limits. Since all the shots were performed within the limits in this study, therefore, we did not consider the geometry of the tube, but rather focused on the measurement of the detonation cell size.

Optical fibers connected to a photodiode (IF-95OC) were employed to record the time-of-arrival (TOA) of the detonation wave. Twenty fibers with interval distance of 10 cm in the test section were used to measure the TOA, from which it can be determined whether it is a successful detonation. Methane–hydrogen–oxygen mixtures with three different fuel compositions were used in this experiment, the detailed compositions for fuels are the same as those in our previous study [14] to research their near detonation limits behavior, which are tabulated in Table. 1. The equivalence ratio based on the total fuel/oxygen was kept to stoichiometric condition (i.e., $\varphi = 1$). It is noteworthy that # 1 mixture is at stoichiometry both for CH_4–O_2 and H_2–O_2, # 2 mixture has higher content of methane and # 3 mixture has higher content of hydrogen, respectively.

3. Results and discussions

Due to the instability nature of the unstable mixture, the cellular pattern from smoked foil for CH_4–H_2–O_2 mixture detonation has a degree of irregularity. Typical detonation cellular pattern in CH_4–H_2–$2.5O_2$ (# 2) mixture at initial pressure of 20 kPa is shown in Fig. 1. Besides the factor of instability of detonation itself, the different technique and the deviation of the manual measurement would bring the maximum difference of cell sizes up to a factor of two [16]. In Fig. 1, the cell size (width) is 17.89 ± 2.59 mm. Therefore, it is reasonable to conclude there is an associated uncertainty with the corresponding cell size from experimental measurement.

Alternatively, detonation cell size can also be more accurately predicted from chemical kinetic approach using the Zel'dovich–von Neumann–Döring (ZND) model [17] associated with Konnov chemical kinetic mechanism [18]. The version of Konnov mechanism used in this work is Release 0.4. This mechanism was validated by performing explosion and combustion experiments in hydrogencarbon fuels, e.g., ethylene, propane and hydrogen. Furthermore, this mechanism was applied in our previous study to investigate the stability of the same CH_4–H_2–O_2 mixtures [14].

With the availability of the Konnov chemical kinetic mechanism for CH_4–H_2–O_2 mixtures, detonation length scale (i.e., ZND induction length) and chemical kinetic properties can be determined. The induction zone length is determined as the length of the thermally neutral period in the ZND structure. It is defined as the distance from the leading shock to the maximum temperature gradient in the ZND temperature profile, which was also used in previous studies [19–21]. In this study, we use the Ng [22–24] model to predict characteristic cell size for a given mixture and initial conditions. This model was also verified in our previous studies [25–27]. In this model, the cell size is estimated from chemical kinetics by correlating ZND chemical length scales using the linear proportionality relationship, which is given by: $\lambda = A\Delta_I$. Where, Δ_I is the characteristic ZND induction zone length, A is a ratio between cell size and induction length, thus the cell size expression is as following:

$$\lambda = A(\chi)\cdot\Delta_I = \sum_{k=0}^{N}\left(a_k\chi^{-k} + b_k\chi^{k}\right)\cdot\Delta_I \tag{1}$$

$$\begin{aligned}\lambda = A(\chi)\cdot\Delta_I &= \left[(a_0+b_0) + \frac{a_N}{\chi^N} + \ldots + \frac{a_1}{\chi} + b_1\chi + \ldots + b_N\chi^N\right]\cdot\Delta_I \\ &= \left[A_0 + \left(\frac{a_N}{\chi^N} + \ldots + \frac{a_1}{\chi} + b_1\chi + \ldots + b_N\chi^N\right)\right]\cdot\Delta_I\end{aligned} \tag{2}$$

where χ is a non-dimensional stability parameter,

$$\chi = \varepsilon_I\frac{\Delta_I}{\Delta_R} = \varepsilon_I\Delta_I\frac{\dot{\sigma}_{\max}}{u'_{CJ}} \tag{3}$$

ε_I, Δ_R, $\dot{\sigma}_{\max}$ and u'_{CJ} denote the activation energy of the induction process, main heat release zone length, maximum thermicity and CJ particle velocity in shock-attached frame, respectively. A_0, $a_1 - a_N$ and $b_1 - b_N$ are fit coefficients, one can find the values in Refs. [22–24]. The theoretical predicted cell sizes of CH_4–H_2–O_2 mixtures are also compared with experimental results, which are shown in Fig. 2. Good agreement is found by comparing those two sets of data, and the maximum difference is within 10%. It can also be observed detonation cell size (λ) for # 2 mixture is larger than # 1 and # 3 mixtures by comparing three mixtures at the same initial pressure. It also can be seen the detonation cell sizes are larger at lower initial pressures, and there are fewer cells available to be measured for each foil, those factors render the error is larger at the lower initial pressure.

By scaling the detonation cell size (λ) with the ZND induction zone length (Δ_I) for methane–hydrogen–oxygen mixtures (shown in Fig. 3), a fit function of those two lengths is given by:

$$\lambda = 34.62\cdot\Delta_I \tag{4}$$

The above analysis confirms the linearly relationship between detonation cell size with the ZND Induction zone length, with the linear factor and coefficient of determination R^2 equal to 34.62 and 0.9948. It is noteworthy that Eq. (4) is universal in all methane–hydrogen–oxygen mixtures with different compositions that used in this study, this behavior is unlike pure methane–oxygen and hydrogen–oxygen mixtures, in which the proportionality

Table 1
CH_4–H_2–O_2 mixtures with different fuel compositions used in the experiment.

Mixture	Molecular formula	Methane (vol.%)	Hydrogen (vol.%)	Oxygen (vol.%)	Equivalence ratio, φ	Note
# 1	CH_4–$2H_2$–$3O_2$	16.67	33.33	50.00	1	Stoichiometry
# 2	CH_4–H_2–$2.5O_2$	22.22	22.22	55.56	1	Higher content of methane
# 3	CH_4–$4H_2$–$4O_2$	11.11	44.44	44.44	1	Higher content of hydrogen