Self-acceleration of Propagating Cylindrical Hydrogen/air Flames at Normal and Cryogenic Temperatures

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1 Introduction

As a carbon-free fuel, hydrogen has received great interest since it helps to achieve decarbonization. However, the volumetric energy density of gaseous hydrogen is very low. One common solution to overcome this shortage is to compress or liquify gaseous hydrogen at cryogenic temperature. Since hydrogen has very low minimum ignition energy and very broad flammability range, accidental hydrogen release may lead to severe safety issues such as fire and explosion even in an open space. Besides, large-scale hydrogen/air flame is subjected to hydrodynamic instability (Darrieus-Landau instability, DLI) [1] when the flame radius is much larger than the flame thickness, which wrinkles the flame front and further accelerates the combustion process. Sometimes the strong flame acceleration caused by instability may lead to deflagration-to-detonation transition (DDT) [2], which has severe damage. Therefore, it is necessary to investigate the self-acceleration of propagating hydrogen/air flames at cryogenic temperature in an open space.

In the literature, the self-acceleration of premixed flame propagation at normal and elevated pressures has been studied by several groups [3–5]. Gostintsev et al. [3] proposed a power-law relation between flame radius R and time t with a constant exponent (α=1.5, $R \sim t^{\alpha}$) to describe the self-acceleration of spherical flame. Later on the experiments under elevated pressures by Kwon at al. [4] found that the unstable cellular flames are self-accelerating with the power-lawer exponent α smaller than 1.5. Wu et al. [5] conducted extensive experiments at elevated pressures for spherical hydrogen/air flame and they confirmed the existence of flame self-acceleration with α<1.5. However, previous studies mainly considered the self-acceleration of hydrogen/air flame at normal temperature while there is little work on hydrogen/air flame propagation at cryogenic temperature. The experiments by Kuznetsov et al. [6] and our simulations [7] both demonstrated that for hydrogen/air flame propagation in a tube, the flame acceleration and DDT become faster at cryogenic temperature than at normal temperature. Nevertheless, it is not clear whether this trend remains for hydrogen/air flame propagation in an open space. According to the linear theory [1], DLI is substantially promoted at cryogenic temperature since the expansion ratio (i.e., the density ratio of unburned gas to burned gas) increases greatly as the temperature of unburned gas decreases. Therefore, the self-acceleration of hydrogen/air flame propagating in an open space at cryogenic temperature is different from that at normal temperature, which motivates this study.

In this study, we conduct two-dimensional simulations considering detailed chemistry and transport for propagating cylindrical hydrogen/air flames at normal and cryogenic temperatures. The objective is to

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assess the effect of cryogenic temperature on the self-acceleration process of premixed hydrogen/air flames. The reminder of this paper is organized as follows. Section 2 introduces the model and numerical method of this work. Then the results and discussion are presented in section 3. Finally, section 4 summarizes the conclusions of this work.

2 Model and Numerical method

We consider an outwardly propagating cylindrical flame in an initially static hydrogen/air mixture. Due to symmetry, in the simulation we only consider a quarter of the domain as shown in Fig. 1, in which the boundary conditions are depicted. The computational domain is a square with the side length of 10 cm. To access the effects of cryogenic temperature, we consider stoichiometric hydrogen/air mixtures at the same atmospheric pressure but different initial temperatures of T_0=100 K and T_0=300 K. The mixture is ignited by a hot-spot with the radius of r_H=0.4 mm and temperature of T_H=1500 K. As shown in Fig. 1, the hot spot is located at the left bottom of the computational domain. After ignition, the highly curved flame front is smooth in its early stage of propagation. Then wrinkles appear on the flame front due to the onset of DLI and flame acceleration occurs.

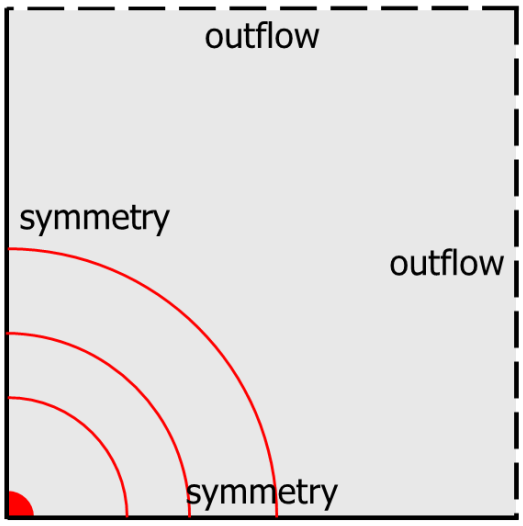

Figure 1: Schematic of the two-dimensional computational domain and boundary conditions.

The transient flame propagation process is simulated by using PeleC [8], which solves the fully compressible equations for a multi-component reactive flows. Detailed chemistry and transport are considered in PeleC. The detailed chemistry mechanism for hydrogen oxidation developed by Konnov [9] is used in all simulations. The reliability of the chemical mechanism for flame propagation in a cryogenic hydrogen/air mixture was demonstrated in the supplementary document of our recent work [7]. To accurately and efficiently resolve the flame propagation and acceleration, adaptive mesh refinement is used and the minimum grid size is 12.5 μm, which is fine enough to resolve the zone.

Note that here we only consider stoichiometric hydrogen/air mixture, whose effective Lewis number is slightly above unity [10]. This ensures that diffusional-thermal instability has little influence on flame propagation. Consequently, the flame propagation and acceleration are mainly affected by DLI.

According to the linear theory of DLI for planar flame [1], the normalized growth rate, ω can be expressed as a function of expansion ratio σ

$$\omega = \frac{\omega^*}{kS_L} = \frac{\sigma}{\sigma+1}\left(\sqrt{\sigma+1-1/\sigma}-1\right) \quad (1)$$

where k is the wave number and S_L is the laminar flame speed. The expansion ratio is σ=6.8 for T_0=300 K and σ=19.5 for T_0=100 K. According to Eq. (1), the normalized growth rate at cryogenic temperature is about two times larger than that at normal temperature. Therefore, it is expected that the self-acceleration caused by DLI is stronger at lower temperature.

3 Results and Discussion

The evolution of the expanding flame front at several consecutive instants forT_0=100 K and 300 K is plotted in Fig. 2. It is seen that the flame front is smooth shortly after the ignition. Then wrinkles on the flame front are formed at about t=3 ms for T_0=100 K and t=2 ms for T_0=300 K. This is reasonable since for higher initial temperature the laminar flame speed is larger and so is the flame radius at the same time. It is noted that the stabilization effect of positive stretch is weakened as the expanding cylindrical flame radius increases [4]. For both T_0=100 K and 300 K, the wrinkles start to appear over the flame front when the flame radius is about R = 3 cm and consequently the DLI occurs.

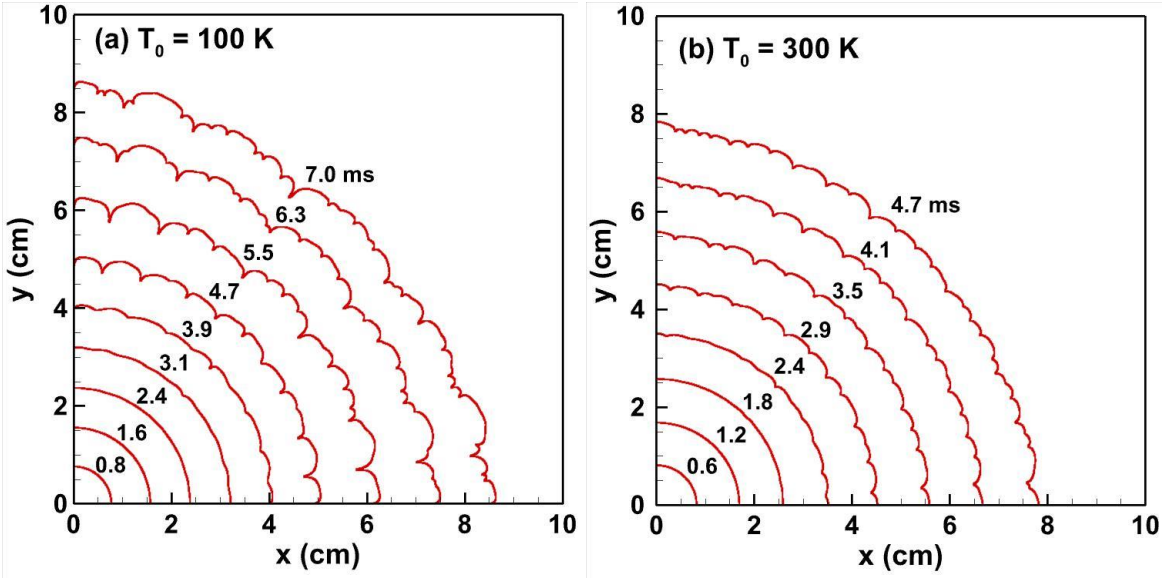

Figure 2: The shape of the unstable expanding flame front at several consecutive instants for (a) T_0=100 K and (b) T_0=300 K.

Figure 2 also shows that at the same flame radius, the cusps on flame front at cryogenic temperature is much sharper that that at normal temperature. This indicates that flame wrinkling is more significant at lower temperature. The appearance of sharp cusps can greatly increase the flame surface area and thereby promote flame acceleration. To quantify the self-acceleration process at normal and cryogenic temperatures, the evolution of mean flame radius R is fitted in Fig. 3 to obtain the acceleration factor. Here the mean flame radius R shown in Fig. 3 is defined as the radius of a smooth front with the same area of burned gas inside it. The fitting formula is in power-law [10]

$$R = R_0 + At^{\alpha} \tag{2}$$

where R_0 is the virtual ignition radius and the power-law exponent α is the self-acceleration exponent. The fitting results forT_0=100 K and 300 K are:

$$R_{T_0=100\,\mathrm{K}} = 0.22600 + 0.7182 \cdot t^{1.235} \tag{3}$$

$$R_{T_0=300\,\mathrm{K}} = 0.07581 + 1.3220 \cdot t^{1.118} \tag{4}$$

Therefore, the self-acceleration exponent α=1.235 for T_0=100 K is higher than α=1.118 for T_0=300 K. According to the work of Xin et al. [10], the relation between fractal excess d and the self-acceleration exponent α for two-dimensional cylindrical flame is

$$d = 1 - \frac{1}{\alpha} \tag{5}$$

Therefore, the fractal excess for is d=0.19 for T_0=100 K and d=0.11 for T_0=300 K. This indicates that the impact of flame wrinkling caused by DLI on the flame surface area growth is stronger for the cryogenic flame.

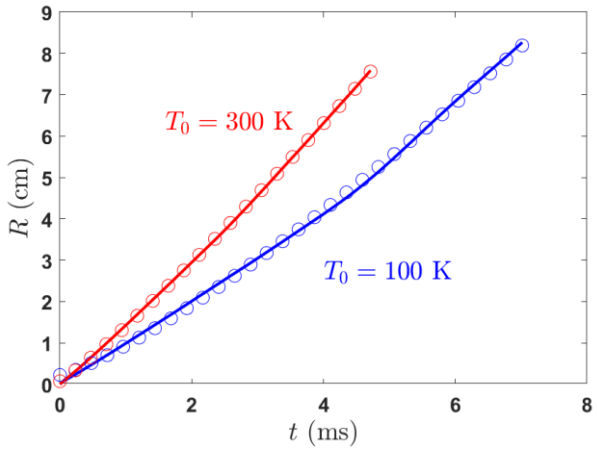

Figure 3: Temporal evolution of mean flame radius R. The solid lines denote simulation results, and the symbles represent curve fitting based on the power-lawer in Eq. (2).

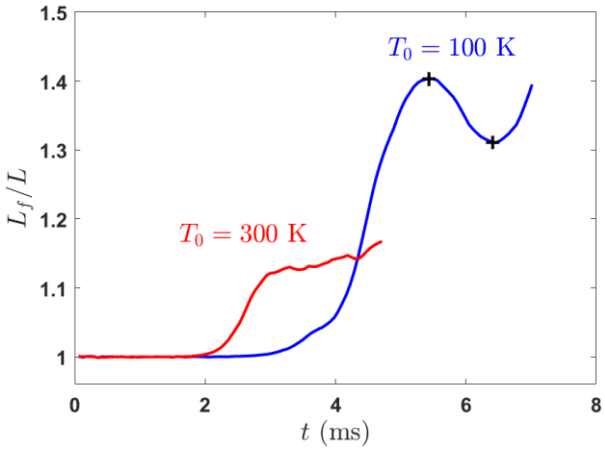

Figure 4: Temporal evolution of the wrinkling factor. The symbols '+' denote the local maximum and mininmum values.

The acceleration characteristics can be quantified by the wrinkling factor (L_f/L), which is defined as the ratio of the length of wrinkled flame front (L_f) to the length of smooth flame front (L) covering the same area of burned gas. Figure 4 compares the evolution of the wrinkling factor for T_0=100 K and 300 K. It is seen that the wrinkling factor is about 1 in the early stage of flame propagation, which corresponds to the smooth flame front shortly after ignition. Then the wrinkling factor increases rapidly. This is the stage of wrinke growth. After this transition, the wrinkling factor evolves non-monotonically, especially for the cryogenic flame of T_0=100 K. It is observed that wrinkling factor at cryogenic temperature reaches much larger value though the onset of DLI is later. This indicates that the DLI more strongly increases the flame surface area at lower initial temperature. The stronger flame wrinkling caused by

DLI helps to explain the self-acceleration exponent observed at cryogenic temperature. Therefore, hydrogen/air flame at cryogenic temperature exhibits stronger flame wrinkling and self-acceleration.

Furthermore, Fig. 4 shows that the wrinkling factor changes non-monotonically at cryogenic temperarture. To explain this phenomenon, the flame shapes corresponding to the local maximum and mininmum values of wrinkling factor are presented in Fig. 5. It is seen that from t=4.7 ms to t=5.5 ms, the cusps is sharpened and new cusps are formed on the flame front. Then from t=5.5 ms to t=6.3 ms, the depth of the large cusp decreases. Therewith, the wrinkling factor exhibits a downward trend.

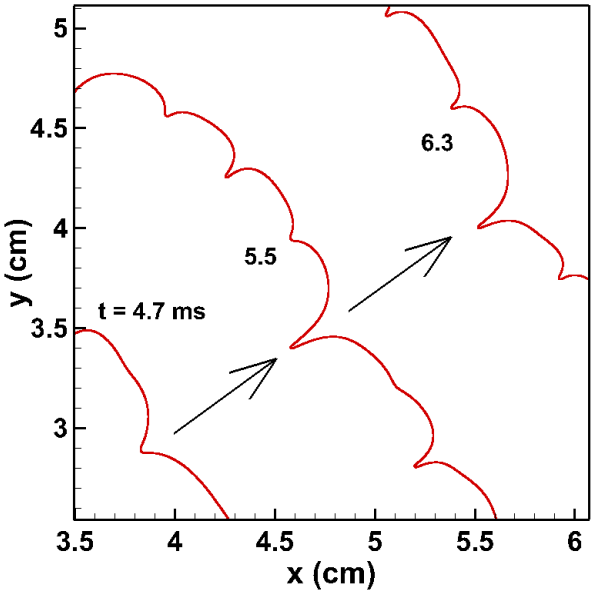

Figure 5: The evolution of a sharp flame cusp for T_0=100 K. The instant of t=5.5 ms corresponds to the local maximum value of wrinkling factor and t=6.3 ms corresponds to the local minumum value of wrinkling factor.

4 Conclusions

The propagation and self-acceleration of cylindrical hydrogen/air flame in an open space are studied via two-dimensional numerical simulations. It is found that expanding hydrogen/air flame is smooth after ignition and then it is strongly affected and accelerated by flame front wrinkling caused by Darrieus-Landau instability (DLI). Compared to normal temperature, the flame cusp is sharper at cryogenic temperature. The self-acceleration exponent and the wrinkling factor at cryogenic temperature are both larger than those at normal temperature.

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