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Experimental and theoretical investigation on cellular instability of methanol/air flames

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ABSTRACT

Cellular instability of spherically expanding methanol/air flames was investigated in a constant-volume single-chamber cylindrical combustion vessel at initial temperatures of 373–423 K, initial pressures of 1–10 atm and equivalence ratios of 0.7–2.1. Flame morphology shows that the methanol/air flames suffer from cellular instability, especially at 5–10 atm. Stability analysis was performed to determine the logarithmic growth rate of disturbance, the critical Peclet number and the critical flame radius. The influences of initial temperature, initial pressure and equivalence ratio on cellular instability were analyzed to identify the influential factors. Both experimental results and stability analysis indicate cellular instability monotonically increases with increasing temperature or pressure and non-monotonically varies with increasing equivalence ratio. The reduced critical Peclet number and flame thickness slightly destabilize the flame surface as temperature increases. The almost unchanged critical Peclet number and the greatly reduced flame thickness with increasing pressure make the critical flame radius smaller and the flame surface more unstable at high pressures. The monotonically decreased critical Peclet number and the non-monotonically varied flame thickness result in the non-monotonic variation of cellular instability in methanol/air flames versus equivalence ratio. The critical flame radius consequently increases with increasing equivalence ratio under very rich conditions, while the corresponding flame surface becomes more smooth. The non-monotonic variation of cellular instability versus equivalence ratio is anticipated to exist widely in combustion of heavy fuels.

1. Introduction

Cellular instability is one of the intrinsic characteristics of laminar premixed flames. Cellular instability can change the local flame morphology and stretch, and the unstable structures can accordingly influence the local heat release rate, combustion efficiency and the extent of the pollutant emissions. Dynamically, it can lead to the self-acceleration of laminar flames, the phenomena of deflagration-to-detonation transition, the flame-vortex interaction and the turbulent flame speed [1–8]. Many studies have been performed for the cellular instability of hydrocarbon/air and oxygenated fuel/air flames [6,7,9–11], exhibiting one or both of hydrodynamic instability and diffusive-thermal instability, most frequently observed in flat flames and spherically expanding flames [12–14]. The equivalence ratio (ϕ) of the mixture has been found to be a critical factor for the cellular instability as it tends to form in mixtures that are deficient in the light reactants, such as rich heavy fuel/air mixtures (e.g. propane/air and *iso*-octane/air) and lean methane/air or hydrogen/air mixtures [15]. Most of previous studies focused on the cellular instability in flames with equivalence ratios smaller than 1.6 [2,16–20]. It should be noted that very rich conditions (e.g. $\phi > 1.6$) happen frequently in laboratory flames and real combustion. For example, localized fuel-rich pockets are difficult to be eliminated in many internal combustion engines and gas turbines due to the limited rates of fuel evaporation and fuel–air mixing [21,22]. Studies on the cellular instability of heavy fuel/air mixtures under very rich conditions, especially extremely rich conditions (e.g. $\phi \approx 2.0$), are still deficient.

The main challenges for investigating very rich flames are the concentration limits of flame propagation and buoyancy effect. On the one hand, the premixed fuel/air mixtures should be ignitable under very rich conditions. On the other hand, the burning velocity of flame front should be large enough under very rich conditions to weaken the buoyancy effect [23,24]. According to the existing knowledge of flame propagation of numerous fuels [25–28], methanol is chosen as the target fuel considering its prominent advantages. Methanol is an important alternative for transportation fuels due to its abundant production sources and low cost. It has high research octane number (RON) and has long been used to improve the octane number and knock

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Table 1
Previous measurements of laminar flame propagation of methanol/air mixtures.

P_u (atm)	ϕ	T_u (K)	Year	Reference
1	0.7–1.4	298	1955	Wiser [32]
1	0.7–1.4	298, 373	1959	Gibbs [33]
1	0.7–1.4	298, 358	1982	Metghalchi [34]
1	0.7–1.4	298	1984	Gülder [50]
0.089–0.25	0.7–1.2	323	1991	Bradley [36]
1	0.5–2.0	298–368	1992	Egolfopoulos [37]
1	0.8–1.4	298	2000	Kwon [38]
0.5–6.7	0.7–1.4	298–632	2004	Saeed [39]
1	0.7–1.4	358–480	2006, 2007	Liao [40,41]
1–5	0.7–1.4	373–473	2008	Zhang [42]
1	0.7–1.5	343	2010	Veloo [43]
1	0.7–1.4	373	2010	Wu [44]
1	0.7–1.5	298–358	2012	Vancoillie [45]
10	0.7–1.3	373	2014	Beeckmann [46]
1	0.7–1.5	298–358	2014	Sileghem [47]
1	0.7–1.3	300	2016	Katoch [48]
1	0.7–1.6	363, 393	2016	Li [49]

resistance of SI engine fuels [28]. The flammable range of methanol/air mixtures is 6.7–36% in mole (ϕ = 0.51–4.0) [29]. The laminar burning velocities of methanol/air flames are much larger than those of other hydrocarbon/air and alcohol/air flames [28]. Furthermore, the Markstein numbers of methanol/air flames change similarly to the other heavy fuel/air flames from lean to rich conditions according to the calculation of Bechtold et al. [25]. This indicates the transport properties and the instability characteristics of methanol/air flames are analogous to those of heavy fuel/air flames [15,30,31]. Therefore, methanol can be used as a representative fuel to demonstrate the instability characteristics of heavy fuel/air mixtures under very rich conditions.

In the past decades, numerous studies have been dedicated to laminar flames of methanol as reviewed in [27,28]. Table 1 summarizes the initial pressure (P_u) and ϕ conditions investigated in previous experiments [32–49]. Most of previous studies focused on lean, stoichiometric and moderately rich methanol flames, except the study of Egolfopoulos et al. [37]. However, the study of Egolfopoulos et al. [37] focused on the kinetics of methanol flames at atmospheric pressure and did not analyze the flame instability. In the studies of Kwon et al. [38] and Zhang et al. [42], the flame instability of methanol was analyzed based on the experimental measurements at $\phi \leq 1.4$. Kwon et al. [38] concluded that the negative Markstein number leads to the growth of irregular flame surface disturbance in the flame propagation process. Zhang et al. [42] concluded that the flame instability of methanol/air mixtures increases with increasing ϕ, P_u and initial temperature (T_u). However, the flame instability of very rich methanol/air flames is still not investigated.

The purpose of this study is to investigate the cellular instability of methanol/air flames over a wide range of ϕ, especially under very rich conditions. Firstly, spherically expanding flames of methanol/air mixtures were measured in a high-pressure constant-volume cylindrical combustion vessel. The experiment was performed over the equivalence ratio range of 0.7–2.1 at both atmospheric and high pressures. Differences of the instabilities between very rich flames and other flames were observed. Secondly, stability analysis was performed and onsets of cellular instability were evaluated for the investigated methanol/air flames. The effects of P_u, ϕ and T_u on cellular instability were also investigated. The influential factors for the different characteristics of cellular instability were identified, especially for the very rich flames.

2. Experimental methodology

Detailed description of the experimental apparatus was reported in our recent work [51]. Only a brief introduction is provided here. The experiments were performed in a constant-volume single-chamber cylindrical combustion vessel. The combustion vessel is made of 304 stainless steel and has an inner volume of 2.77 L (inner diameter 150 mm, inner length 152 mm). The vessel was hydrostatically tested to 200 atm. Two quartz windows (diameter 100 mm, thickness 30 mm) are clamped to the vessel flanges, providing an optical access with 75 mm diameter clear apertures.

During the experiment, partial pressure method was used to prepare combustible mixtures in the premixing vessel. Four pressure transducers with different ranges were used to improve the accuracy. All vessels and pipelines were evacuated to about 3 Pa before charging. The liquid fuels were vaporized in an electrically heated vaporizer before the injection to the premixing vessel. The prepared mixtures were stirred by a magnetic stirrer for 10 min to ensure uniform mixing. The volume of the premixing vessel (9.06 L) is more than 3 times as large as the combustion vessel. Each condition was repeated 3–4 times to reduce the random error of the prepared combustible mixture. Relief valves were installed in both the combustion vessel and the premixing vessel to ensure experimental safety. All vessels can be heated up to 500 K by flexible detachable heating jackets. In this work, the combustion vessel, the premixing vessel, the vaporizer, and the pipelines were all heated at 373 K or 423 K using PID temperature controllers and K-type thermocouples. Satisfactory temperature homogeneity was observed in both vessels and the maximum deviation from the target temperature was determined to be ± 1 K.

The combustible mixture in the combustion vessel was ignited by two 500 μm-diameter tungsten electrodes. The gap between the tips of the two electrodes can be adjusted from 0 to 5 mm. Only one discharge occurred in each ignition with a duration less than 10 μs. The ignition energy was minimized by decreasing the voltage and power input of the ignition coil. An outwardly propagating spherically expanding flame was formed after the ignition and a schlieren system was used to record the flame propagation. Schlieren images were recorded by a high speed camera (Phantom V310). The camera was operated at 10,000 frames/s. The spatial resolution was set at 480 × 480 pixels to map a region of 75 × 75 mm^2. In this work, the experiments of methanol were performed at T_u = 373–423 K, P_u = 1–10 atm and ϕ = 0.7–2.1. Methanol (≥99.5%) were purchased from Aladdin Reagent. Synthetic air consisting of 21% O_2 and 79% N_2 provided by Nanjing Special Gas Factory was used as the oxidizer.

3. Stability analysis and numerical simulation

For a spherically expanding flame, the instant flame surface can be expressed by $r = R_f(t)$. When the flame suffers from cellular instability, the perturbed flame surface can be expressed in the form of $r = R_f(t)[1 + A(t)\$_n(\theta,\varphi)]$, where A is the amplitude of disturbance, $\$_n$ is the surface harmonics with wavenumber (n), θ and φ are the polar angle and azimuth angle in spherical coordinate system, respectively [14]. In previous studies, Istratov and Librovich [52] reported the first theoretical description of the onset of instability in a spherically expanding flame by considering the hydrodynamic instability with a Markstein correction. Bechtold and Matalon [30] extended the stability analysis and systematically incorporated the hydrodynamic and diffusive-thermal effects. This stability analysis was applied by Bradley et al. [53,54] to investigate the development of cellular instability in spherically expanding flame. Addabbo et al. [55] further improved the stability analysis by considering temperature-dependent transport coefficients. Accurate stability analysis of spherically expanding flames depends on properly extracted flame thickness, overall activation energy, Lewis number and so on [56]. Based on the stability analysis, the growth rate of cellular instability can be calculated and the transition from stable to unstable flames can be determined. The logarithmic growth rate of disturbance ($\overline{\mathscr{T}}$) can be calculated by Eq. (1) according to the stability analysis in [30,55]. A negative value of $\overline{\mathscr{T}}$ indicates a stable flame while a positive value indicates an unstable one. Detailed flow chart for $\overline{\mathscr{T}}$ calculation can be found in Fig. S1 in the