



Laminar burning velocity of 2-methylfuran-air mixtures at elevated pressures and temperatures: Experimental and modeling studies

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ABSTRACT

2-Methylfuran (MF), a promising biofuel candidate catalytically produced from biomass-based fructose, has attracted the attention of fuel researchers. However, there is limited data available for the laminar burning velocity, especially at high initial pressure conditions. In this work, the laminar burning velocity of MF-air mixtures at elevated initial pressures ($T_0 = 363$ K; $p_0 = 0.1$ – 0.4 MPa) was experimentally determined in a spherical outwardly expanding flame. Numerical simulation was also conducted in Chemkin using two detailed chemical kinetic mechanisms at elevated pressures (similar to the experiment condition: $T_0 = 363$ K; $p_0 = 0.1$ – 0.4 MPa) and elevated temperatures ($T_0 = 363$ – 563 K; $p_0 = 0.1$ MPa). Data from experimental and modelling studies were compared and discussed. The experimental results showed that at a given T_0 and p_0 the laminar burning velocity of MF-air mixtures reached peak values at equivalence ratios $\phi = 1.1$ – 1.2 , and it slowed down dramatically when the MF-air mixture was too rich or lean. Laminar burning velocity decreased with the increase in p_0 . The laminar flame speed of MF-air mixture from two chemical kinetic mechanisms exhibited a similar trend with experimental data; however, both the two mechanisms led to overestimation at the most initial conditions. Compared to the Galway mechanism, the Tianjin mechanism better predicted the laminar burning velocity of MF-air mixtures, especially at initial pressures of 0.1 and 0.2 MPa. The current MF mechanism needs further improvement to better predict the combustion of MF at high-pressure conditions.

1. Introduction

Due to the pressures of greenhouse gas emission and limited fossil fuel resources, it is essential to find alternative fuels. Over the past decade, researchers have paid attention to biofuels, such as bioethanol [1,2], biobutanol [3,4] and biodiesel [5,6]. Bioethanol is widely used as a gasoline blending stock because of its renewability, high-octane rating, low carbon footprint and regulation mandatory [7,8]. However, bioethanol has its limitation, such as low calorific value and water solubility [9].

Román-Leshkov et al. [10] proposed a method of producing furan-based fuel, 2-methylfuran (MF), from biomass-based fructose via acid-catalyzed dehydration and hydrogenolysis processes. The properties of MF are listed in Table 1. Compared to bioethanol and gasoline, MF has several advantages [9]: (1) research octane number (RON) of MF is higher than that of gasoline; (2) the low heating value of MF is much higher than that of bioethanol; (3) unlike ethanol, MF is water-

insoluble; (4) the enthalpy of vaporization of MF is lower than that of ethanol, indicating less cold start issues than ethanol.

MF has attracted the attention of engine researchers worldwide. Thewes et al. [13] experimentally investigated the influence of MF on spray, evaporation and engine performance in a direct-injection spark-ignition engine. They concluded that MF had quicker vaporisation compared to ethanol, and it had lower hydrocarbon emissions and better knock resistance compared to gasoline. Wang et al. [12] studied the combustion performance and emissions of MF in a direct-injection spark-ignition engine, and they compared the results with those of ethanol and gasoline. The results showed that MF had a better knock suppression ability and a higher indicated thermal efficiency than gasoline had. The particulate emissions from MF were less than gasoline due to its high oxygen contents. However, NO_x emissions of MF were the highest among the four examined fuels because of its high combustion temperature.

Apart from pure MF, MF-gasoline blends were used as fuels in

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Nomenclature

MF	2-Methylfuran
p_0	Initial pressure
T_0	Initial temperature
A	Area of flame front
t	Time after ignition event
R_0	Radius of window
r_f	Flame radius
N	Number of pixels inside the flame front

N_{all}	Number of pixels of the entire window
α	Stretch rate
L_b	Markstein length
u_L	Laminar burning velocity
ρ_u	Density of unburned gas
ρ_b	Density of burned gas
ϕ	Equivalence ratio
S_b	Stretched flame propagation speed
S_u	Unstretched flame propagation speed

engines. Wei et al. [14] compared a MF-gasoline blend (M10), ethanol-gasoline (E10) and gasoline in a port-fuel-injection spark ignition engine. With less brake specific fuel consumption, the output torque and brake power of M10 were slightly higher than those of E10. Hydrocarbon and carbon monoxide emissions of M10 were lower than gasoline. Studies go beyond the application of SI engines. Xiao et al. [15] studied combustion performance and emissions of MF-diesel blend fuels in a diesel engine and they concluded that a low MF-diesel blend exhibited a longer ignition delay, a shorter combustion duration and lower soot emissions than pure diesel.

In addition to engine researches, fundamental combustion investigations of MF have been conducted. Somers et al. [16] established a detailed kinetic model of MF oxidation and validated it by experimental ignition delay times and laminar burning velocities. The model highlighted the reactions of the H atom with the fuel. Tran et al. [17] used electron-ionization molecular-beam mass spectrometry and gas chromatography techniques to detect the intermediate species of MF combustion under stoichiometric and fuel-rich premixed low-pressure flames conditions. They developed a detailed kinetic model consisting of 305 species and 1472 reactions. In addition, Cheng et al. [18] analysed the reaction pathway of MF and revised the former MF mechanism under fuel-lean, stoichiometric and fuel-rich conditions. Their mechanism was validated experimentally by detecting the mole fractions of major species in MF flames.

Laminar burning velocity is an important physiochemical parameter of a fuel-air mixture at given temperature and pressure conditions. The knowledge of laminar burning velocity is fundamental to the understanding of other more complicated flame behaviours such as flame extinction, flashback and turbulence combustion. Laminar burning velocity determined in experiments is also used to validate chemical kinetic mechanisms [19]. Laminar burning characteristics of MF and its blends with isooctane have been investigated at the atmospheric pressure, using an outwardly spherical flame method [20,21]. The results revealed that the laminar burning velocity of MF was faster than that of isooctane.

The laminar burning velocity of MF-air mixtures at high initial pressures is not available in the previous literature. In this work, the laminar burning velocity of MF-air mixtures at elevated initial pressure ($T_0 = 363$ K; $p_0 = 0.1$ – 0.4 MPa) was experimentally determined with a spherical outwardly expanding flame method. In addition to the

experimental study, laminar burning velocity was also simulated by using two chemical kinetic mechanisms at elevated temperatures ($T_0 = 363$ – 563 K; $p_0 = 0.1$ MPa) and elevated pressures ($T_0 = 363$ K; $p_0 = 0.1$ – 0.4 MPa). Data from experimental and modelling studies were compared and discussed. In the next section, experimental and numerical methods will be introduced.

2. Experimental and numerical methods

2.1. Experimental setup

Fig. 1 presents the experimental setup. The system includes a constant-volume combustion chamber, a Schlieren photography system, an ignition system, an intake and exhaust system, and a data acquisition system.

The combustion vessel has a cubical shape, and it is equipped with a pair of quartz windows for the optical access. At each side, there were six cartridge heaters for temperature control. A K-type thermocouple and a pressure gauge were installed to measure the initial mixture temperature and pressure, respectively. Two opposing-electrodes with diameters of 0.4 mm were used for ignition along with an ignition coil and an ignition control module. Flame images were captured by a camera (speed = 6000 fps; resolution = 512×512). More details about these experimental apparatus and procedures are available in ref. [22,23].

2.2. Data processing

In this study, flame fronts of Schlieren images were determined via the Adobe Photoshop software. The radius (r_f) of spherical flame is calculated via:

$$r_f = \sqrt{\frac{N}{N_{\text{all}}}} R_w \quad (1)$$

where N , N_{all} and R_w are the pixels inside the flame front, the pixels of the optical window, and the actual radius of the optical window, respectively.

The stretched flame propagation speed (S_b) is calculated via:

$$S_b = \frac{dr_f}{dt} \quad (2)$$

where t is the elapsed time after ignition.

In spherical expanding flames, the stretch rate (α) is defined as [24]:

$$\alpha = \frac{2S_b}{r_f} \quad (3)$$

According to [25], during the quasi-steady period stretched propagation speed and stretch rate have linear relationship:

$$S_b = S_u - L_b \alpha \quad (4)$$

where S_u is the unstretched flame propagation speed; L_b is the Markstein length relative to the burned gas.

With the assumption of a quasi-steady and quasi-planar flame,

Table 1

Properties of MF, bioethanol and gasoline [11,12].

	Gasoline*	Bioethanol	MF
Molecular formula	C ₄ -C ₁₂	C ₂ H ₆ O	C ₅ H ₆ O
Density @ 20 °C (kg/m ³)	744.6	790.9	913.2
Initial boiling point (°C)	33	78	64
Research Octane Number	96.8	108	103
Lower heating value (MJ/kg)	42.9	26.8	31.2
Oxygen content (wt%)	0	34.78	19.51
Enthalpy of vaporization (kJ/kg)	351	919.6	389
Stoichiometric air-fuel ratio (gravimetric)	14.46	8.95	10.05

* Typical main-grade EU gasoline that meets the EN228 regulation.

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