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Laminar burning characteristics of 2-MTHF compared with ethanol and isooctane

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HIGHLIGHTS

- Laminar flame characteristics of 2-MTHF were studied.
- Laminar flame speed of 2-MTHF was compared with ethanol and isooctane.
- The peaks of un-stretched flame speeds occur in a range of Φ 1.1–1.2.
- Laminar burning velocity of 2-MTHF is ~0.56 m/s at stoichiometric ratio, 393 K.

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ABSTRACT

2-Methyl tetrahydrofuran (2-MTHF) is one of the promising second-generation biofuel candidates, raising increasing interest because of the recent breakthrough in producing 2-MTHF from biomass. As a potential gasoline extender and renewable oxygenate, its high energy density and avoidance of competing with food make it attractive compared with ethanol. In the current work, the laminar burning characteristics of 2-MTHF-air mixtures are studied with varying equivalent ratios (0.88–1.43) and initial temperatures (333 K, 363 K and 393 K) at ambient pressure in a constant-volume vessel. The results are compared with ethanol and isooctane, a representative component in gasoline. The stretched flame speed, un-stretched flame speed, Markstein length, flame thickness, Markstein number, laminar burning velocity and burning flux are calculated and analyzed. The result shows that for most tests, the ranking of un-stretched flame propagation speed is ethanol, 2-MTHF and isooctane. The peaks of un-stretched flame speeds against varying equivalent ratios appear at Φ = 1.1–1.2 for three tested fuels. The Markstein length indicates that generally isooctane has the most diffusion-thermal stable flame than 2-MTHF and ethanol when Φ < 1.2 at 393 K. Ethanol shows the smallest flame thickness in most of the test points. The laminar burning velocity of 2-MTHF is much faster than isooctane and is comparative with ethanol, indicating its fast-burning property and potential of improving engine thermal efficiency.

1. Introduction

Nowadays, alternative biofuels are raising increasing interest as they are an important solution to reduce the reliance on fossil fuels. Moreover, the use of biofuels helps to limit the greenhouse gases in the atmosphere, which contribute to global warming. Fuels of the furan family, i.e. 2-methylfuran (MF) and 2,5-dimethylfuran (DMF), have been regarded as promising second-generation biofuel candidates [1], for their potential of mass production from non-food biomass [2–4]. The authors‘ group and many other researchers have carried out wide ranging research on MF and DMF [5–10] for their application as alternative fuels. Recently, 2-methyl tetrahydrofuran (2-MTHF), a novel biofuel candidate which is similar to furan type fuels, is receiving more attention.

Geilen et al. [11] have reported a new pathway to synthesize 2-MTHF from levulinic acid, which is accessible from biomass via molecular transformation to γ-valerolactone and 1,4-pentanediol. The pathway from cellulose to 2-MTHF and its potential to large-scale production have been analyzed by Marquardt et al. [12]. Table 1 shows the properties of 2-MTHF, gasoline and two other test fuels used in this work, ethanol and isooctane [13–15]. The

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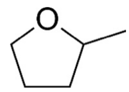
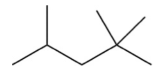
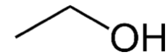
Table 1
Properties of tested fuels and gasoline [13–15].

	2-MTHF	Isooctane	Ethanol	Gasoline
Molecular formula				C2–C14
H/C ratio	2	2.25	3	1.795
O/C ratio	0.2	0	0.5	0
Gravimetric oxygen content (%)	18.60	0	34.78	0
Density @ 20 °C (kg/m^3)	863.0	691.9	791.9	744.6
Research Octane Number (RON)	86	100	109	97
Motor Octane Number (MON)	73	100	90	86
Stoichiometric air/fuel ratio	11.23	15.13	9.00	14.46
LHV (MJ/kg)	32.7	44.3	26.8	42.9
LHV (MJ/L)	28.2	30.7	21.2	31.9
Heat of vaporization (kJ/kg)	375	308	912	373
Initial boiling point (°C)	78	99	78	33

lower heating value (LHV) of 2-MTHF (~28.2 MJ/L), which is close to that of gasoline (~31.9 MJ/L), is much higher than that of ethanol (~21.2 MJ/L). The Research Octane Number (RON) of 2-MTHF is 86, which means that the blending of 2-MTHF with gasoline produces a decrease in the octane rating, as noted in a previous work [13]. However as [14] suggests, 2-MTHF may perform well as a low-concentration blend with gasoline in standard vehicles as well as in higher concentrations in flex fuel vehicles (FFVs). Besides, as a low octane number gasoline fuel, 2-MTHF also has the potential to be used in some new concept combustion modes, such as partially premixed compression ignition (PPCI) [16] and multiple premixed compression ignition (MPCI) [17]. Early in 1988, Rudolph and Thomas [18] studied the feasibility of using 2-MTHF in an SI engine as a fuel extender. Hülser et al. [19] studied the pre-ignition characteristics of 2-MTHF with an optical SI engine. Janssen et al. [20] pointed out that 2-MTHF blended with di-*n*-butylether complies with the desired fuel properties and investigated its use in a single-cylinder diesel engine.

The main interest with 2-MTHF as potential candidate is it can be biomass derived by the recently developed new production technology and thus can become a renewable energy supply [4]. Another main advantage is due to the potential of the oxygenated fuel for reducing soot emissions of combustion engines. Adding shares of up to 30% to standard diesel fuel may have a significant positive effect, especially on soot emissions while still allowing a stable combustion in the complete operating range. 2-MTHF has a lower octane number rating and thus can only be used in low blending ratio in spark ignition engines for its negative effect on engine anti-knock resistance. For gasoline direct injection engines, there is a great challenge to reduce particulate emissions for meeting more and more stringent emission standards and therefore the optimal blending ratios will depend on the trade-off with the engine efficiency [21]. Brassat et al. [22] studied the effect of 2-MTHF on controlled auto ignition. However, experimental studies on the 2-MTHF flames are scarce.

Laminar flame propagation characteristics are very important fundamental physicochemical properties of a fuel-air mixture. They could be used to validate the chemical reaction mechanisms and provide insight into their combustion process [23]. The laminar burning characteristics of 2-MTHF are hardly seen in previous work. In the current work, propagating spherical flame method was applied to study the laminar flame speed, Markstein length, Markstein number and laminar burning velocity in a constant-volume vessel. Ethanol, the market leading gasoline alternative, and isooctane, which is a representative component of gasoline [14,24,25], were used for comparison to 2-MTHF.

2. Experimental setup

The system of the shadowgraph method used in this study is shown in Fig. 1. It should be noted that compared to the schlieren method used in previous work [8,9,26], the knife edge was removed in order to get better flame boundary detection in the image processing. A constant-volume bomb equipped with two fused silica windows (100 mm in diameter visible area) on opposite sides was used for the experiment. The volume of the vessel is approximately 4.048 L. The vessel was heated by eight heating rods, which were mounted in eight corners of the vessel, using an electric heating system. In the top of the vessel, a gasoline direct injection (GDI) injector driven by an ECU system was mounted for fuel injection. Two electrode needles were mounted in opposite side covers of the vessel, to ignite the mixture in the center of the vessel. These electrode needles were driven by a high-voltage unit for the power supply.

In this test, a pointolite was generated using a 500 W xenon lamp combined with a focusing lens and a pin-hole. Light from the pin-hole was collected and transformed into parallel light by the following concave mirror. The parallel light travelled across the test field and was focused by the second concave mirror before being collected by a Phantom V710 ultra-high speed camera. The camera was synchronized with the spark plug electrodes and worked with a 10,000 fps sampling rate and an 800 × 800 pixels resolution for all conditions.

For each test, the vessel was scavenged by a plenty of compressed air and then extracted to 10 kPa absolute pressure using a vacuum air pump. The fuel was injected into the vessel using a GDI injector with an injection pressure of 15 MPa. Calibration work on fuel mass against injection duration time curve under this fuel pressure was carried out in the preparation phase, in order to calculate injection durations required by different tests. The fitting curve of fuel injection mass against different injection durations was calibrated by measuring the injected fuel volume of 1000 injections which was repeated by three times and then averaged. Three minutes after injection, for vaporization consideration, the intake valve was opened and then closed at the instant when the pressure inside the vessel reached ambient pressure (0.1 MPa). After that, the mixture was left still for five more minutes to gain uniformity. Finally, the mixture was ignited by electrodes and the camera was triggered simultaneously to record the flame propagation images with one synchronized triggering signal. During the whole process, the temperature inside the vessel was controlled and monitored to ensure an accurate initial temperature. The accuracies of temperature and pressure in the vessel were within 1% and 0.5% respectively.