Combustion and Flame 191 (2018) 213–225

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Laminar flame characteristics and chemical kinetics of 2-methyltetrahydrofuran and the effect of blending with isooctane

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ARTICLE INFO

Article history:
Received 15 June 2017
Revised 10 August 2017
Accepted 23 December 2017

Keywords:
2-methyltetrahydrofuran
Flame propagation
Laminar burning velocity
Flame instability
Isooctane
Mixing rule

ABSTRACT

2-methyltetrahydrofuran (MTHF) has been considered as a potential biofuel candidate for the renewable feedstock and attractive properties. In this study, the spherically propagating flames of the MTHF/isooctane-air mixtures in different blending ratios were investigated at elevated temperatures and pressures over equivalence ratios of 0.8–1.5 in a constant volume chamber using high-speed photography technique. Laminar burning velocities were calculated through nonlinear method and correlated by mixing rules as a function of initial temperature, pressure, equivalence ratio, and blending ratio. To investigate the influence of the potential interaction between MTHF and isooctane, a detailed model was established by merging the models of the two fuels and validated against laminar burning velocity, ignition delay times and flame structure.

The laminar flame velocities of MTHF were observed to increase with initial temperature while the flame velocities decrease with increase in pressure. Kinetic analysis indicates that the major consumption pathways for MTHF are through H abstraction reactions at 2 and 5 sites. The H abstraction reactions at methyl group are less competitive. Unsaturated hydrocarbons and aldehydes are produced in high concentration and are the main stable intermediates of MTHF combustion. The laminar burning velocity is sensitive to the reactions of small radicals and some intermediates such as propylene and ethylene.

The laminar burning velocities of MTHF/isooctane blends increase with MTHF blending ratio. The influence of blending ratio on laminar burning velocity should attribute to the chemical factors, rather than thermal or diffusion factors. MTHF oxidation generates less proportion of propylene and higher fractions of H, OH than isooctane, reflecting positive chemical effects on laminar burning velocity as MTHF blended. According to the instability analysis, the Markstein length and critical radius shows similar flame instability among different blending ratios.

1. Introduction

As traditional fossil fuels are largely responsible for energy crisis and atmospheric degradations, there is an increasing attention to biofuels. 2-methyltetrahydrofuran (MTHF) is considered as a promising biofuel for its attractive properties. MTHF could be produced from agricultural and forestry wastes using furfural [1] and levulinic acid [2] as platform molecules. As an important component of P-series fuels which are a series of renewable, non-petroleum fuels providing significant emissions benefits, MTHF plays an important role in reducing fuel volatility and promoting environmental quality [3,4]. In "Tailor-Made Fuels from Biomass" project of RWTH Aachen University [5], MTHF was also selected as a promising candidate for alternative transportation fuels.

MTHF has been studied experimentally [5–11] to understand the engine performances and emissions. García et al. [5] studied fundamental spray characteristics related to fuel vaporization and fuel/air mixing for MTHF and reported extremely low soot emissions in a single-cylinder CI engine indicating that MTHF is very suitable for mixing-controlled combustion. MTHF shown higher enleanment potential and ignition prone than RON 95 fuel in a study on a direct injection single cylinder research engine [6]. Thewes et al. [7] compared the knock resistance and required compress ratios of MTHF with several other bio-fuel candidates on homogeneous engine combustion systems. They concluded pure MTHF is knock restricted and requires a low compression ratio as its low RON. Autoignition characteristics and derived cetane numbers (DCN) of pure MTHF was also investigated experimentally using motored-engine technique [8] and ignition quality tester [9].

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https://doi.org/10.1016/j.combustflame.2017.12.028
0010-2180/

Fuel design provides an innovative and sustainable way for the development of internal combustion engines. As a bio-derived oxygenated fuel of low octane number, MTHF exhibited excellent performance through blending with other fuels in new concept combustion modes. Janssen et al. [10] reported that the blending of MTHF and dibutylether used in homogeneous low-temperature combustion is a potential way to realize ultra-low soot emissions. Heuser et al. [11] reported the low PM, HC, CO emissions and noise of the blend fuels of dibutylethe and MTHF on a single-cylinder diesel research engine.

Gasoline direct injection (GDI) engine is notorious for its much higher particulate emissions than traditional gasoline engine, and it is a great challenge to meet the increasingly stringent emission standards. As MTHF is known to reduce particulate emissions, the blending with gasoline are considered could reduce the particulate emission on GDI engines, and the optimal blending ratios will depend on the trade-off with the engine efficiency [12]. There are some studies about the performances and emissions of engines fueled with MTHF/gasoline mixtures. Rudolph et al. [13] reported the SI engine fueled with gasoline/MTHF blend containing 10% MTHF has comparable power outputs and CO, NO_x, and NMHC emissions to unleaded gasoline. Lucas et al. [14] reported the HC, CO and benzene emission decrease evidently in a field trial using fuel blend consisting of 60% MTHF and 40% gasoline in volume.

Many studies were carried out to explore the combustion characteristics of MTHF. Simmie [15] conducted theoretic study at CBS-QB3 and G3 level for bond dissociation energies (BDE) of MTHF, barrier heights, and reaction enthalpies of all possible H abstraction reactions by H atoms and methyl radicals. The ignition delay times of MTHF at low to high temperature were investigated in shock tubes and rapid compression machines [6,9,16–20]. The structures and intermediates of laminar premixed low-pressure MTHF flames were measured using gas chromatographs (GC) and mass spectrometry (MS) technique [21–23]. The laminar burning velocities of MTHF/air mixtures at atmosphere pressure were measured in flat flames at 298–398 K [21] and spherically propagating flames at 333–393 K [24]. Moreover, the reactivity of MTHF with OH [25] and HO_2 [26] were also studied. Based on experiments and calculations, pyrolysis and combustion chemistries of MTHF were developed [18,21,22].

Laminar burning characteristics at elevated pressures and temperatures which resemble to the conditions in internal combustion engines are essential for the design and optimization of combustion chamber as well as combustion simulation in engines. Although the above studies have significantly improved the understanding into the combustion chemistry of MTHF, the laminar burning characteristics at elevated pressures are still not studied yet. Besides, the excellent emission characteristics of MTHF blend fuels on engine studies suggest that it is necessary to study the combustion characteristics of MTHF blends.

In this paper, the spherically propagating flames of the mixtures of MTHF–air and MTHF/isooctane–air were explored in a constant volume chamber using high-speed photography technique. The experiment was performed at the temperatures of 373, 423 and 453 K, the pressures of 1, 2 and 4 bar, the equivalence ratios of 0.7–1.6 with MTHF blending ratios of 0%, 20%, 40%, 60% and 100%. The laminar burning velocity, Markstein length and flame instability were discussed. To understand the combustion chemistry of MTHF and the kinetic interaction with isooctane, a detailed model for MTHF/isooctane high-temperature oxidation was developed based on the work of Bruycker et al. [21] and Chaos et al. [27], and adopted to analyze the combustion process.

Table 1
Operating conditions for MTHF/isooctane–air mixtures in this experiment.

Temperature (K)	Pressure (bar)	Equivalence ratio	MTHF blending ratio (in mole)
373	1	0.7–1.5	0, 20%, 40%, 60%, 100%
423	1, 2, 4	0.7–1.5	0, 20%, 40%, 60%, 100%
453	1	0.8–1.5	0, 20%, 40%, 60%, 100%

2. Experimental and computational methods

2.1. Experiment setup

The present facility has been specified in detail in previous works [28] and will be described here briefly. The experimental apparatus consists of a cylinder chamber of 0.0055 m^3 in volume, a gas supply system, a schlieren optical system, an ignition system and a timing control system. Heating tapes wrapped around the apparatus aid in modifying the initial temperature. Pressure transducer with the deviation of 1% and thermocouples with the accuracy of ± 2 K are installed inside the chamber to monitor the initial temperature and pressure. Each component of the fuel/air mixtures is induced into the chamber individually with the amount controlled by Dalton's law. Before every ignition, the mixture was mixed by molecular diffusion for at least 5 min to guarantee homogeneousness. Two horizontal tungsten electrodes with the radius of 0.5 mm are utilized to ignite the mixtures. After each ignition, fresh air is induced to scavenge the residual gas for at least 3 times. Two circular quartz windows of 80 mm in diameter on each side of the chamber supply the optical path for the schlieren system. A high speed camera (Phantom V611) is utilized to capture the ignition and flame propagation at a sample rate of 10 kHz and a resolution of 752×752 pixels. Raw data of the combustion characteristics would be obtained from the schlieren images.

The MTHF and isooctane used for current experiment are from Aladdin Industrial Corporation with the purity of 99%. N_2 and O_2 of ultra-high purity (99.999%) were induced in the ratio of 3.76 to simulate the composition of dry air. The MTHF blending ratios of 20%, 40% and 60% in mole are marked as M20, M40 and M60 in this study. The experiment conditions are listed in Table 1. For each operating condition, the experiment repeated at least 3 times to reduce the random uncertainty.

2.2. Data processing

The flame radius could be obtained from the schlieren pictures of flame propagation. In order to avoid the effect of ignition and cylindrical confinement on the flame propagation, the data with flame radius of 8–22 mm was selected for subsequent processing.

The stretched flame speed (S_b) could be derived from the relation between flame radius (r_f) and time (t):

$$S_b = dr_f/dt \tag{1}$$

The stretch rate, κ, of the spherical flame surface (A_f) could be deduced.

$$\kappa = \frac{dA_f}{A_f \cdot dt} = 2S_b/r_f \tag{2}$$

The flame speeds of most fuels can be considered to vary linearly with the stretch rate and the unstretched flame speeds could be extrapolated according to $S_b = S_b^0 - L_b \cdot \kappa$, where S_b^0 is the unstretched flame speed, L_b is the Markstein length. However, strong nonlinearity was found for heavy fuels at fuel-rich conditions, casting considerable uncertainty on the conventional method of linearly extrapolating. As a consequence, the nonlinear model [29] was employed for the calculation of unstretched flame speed