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A high pressure ignition delay time study of 2-methylfuran and tetrahydrofuran in shock tubes

Yasar Uygun *, Sakiko Ishihara, Herbert Olivier

Shock Wave Laboratory, RWTH Aachen University, Templergraben 55, D-52056 Aachen, Germany

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ABSTRACT

Ignition delay time studies for tetrahydrofuran (THF) and 2-methylfuran (2MF) as well as optical investigations of combustion for 2MF have been carried out using two shock tubes. The experiments with undiluted THF/air mixtures were performed at 20 and 40 bar in a high pressure shock tube (HPST) at an equivalence ratio of $\Phi = 1$ covering an overall temperature range of 780–1100 K and 691–1006 K, respectively. Undiluted 2MF/air mixtures ($\Phi = 1$) were also investigated in the HPST at 40 bar in the temperature range of 820–1215 K. The experimental data of 2MF obtained at 40 bar were supported with kinetic simulations of existing models from literature. Additionally, sensitivity analyses of 2MF at several temperatures were performed for finding out the most sensitive reactions. Schlieren imaging was employed in a rectangular shock tube (RST) utilizing a high speed video camera through which the ignition process was captured for a stoichiometric 2MF/O_2/Ar mixture at pressures of about 10 bar and in the temperature range of 871–1098 K.

The pressure signals of THF and 2MF at 40 bar indicate two types of pre-ignition at low temperatures: a short two-stage ignition for THF and a relatively long and smooth increase in pressure before main ignition for 2MF. Furthermore, in case of 2MF at 40 bar, far-wall ignitions at low temperatures could be observed. The deviation between simulation and experiment as well as the presence of pre-ignitions in the low temperature regime were the main reasons for undertaking optical investigations of 2MF. The Schlieren images show that the ignition process at low temperatures ($T \leqslant 940$ K) begins as a deflagrative phase in the form of flame kernels and ends in a strong ignition (explosion in explosion).

The current study analyzes the auto-ignition of THF and 2MF at engine relevant pressures and temperatures. The optical investigations have been conducted to analyze the ignition behavior of 2MF.

1. Introduction

The necessity of surrogate fuels which should replace the conventional fuels in the near future led to the growing interest in the last years in finding new sustainable fuels from biomass.

THF is colorless and a water-miscible cyclic ether with a low viscosity at standard temperature and pressure. It can be used as a solvent for biodiesel production [1]. Moreover, it is a good biofuel candidate for HCCI engines. The knowledge of THF oxidation can be further applied for studies of alkylated tetrahydrofurans. On the other hand 2MF is getting more attention for spark ignition engines. It has favorable physicochemical properties like high energy density similar to RON 95, relatively fast evaporation (h_{vap} = 358 kJ/kg) and hence a good spray formation in direct-injection spark-ignition engines [2]. Further it exhibits less hydrocarbon emission compared to RON 95 and a higher octane number of 100.7. Although higher NOx emissions were measured in comparison to RON 95 and ethanol, the better leanability of 2MF and higher efficiency at lean mixtures makes this biofuel more attractive. Thewes et al. [2] concluded that 2MF is a promising potential biofuel candidate and further called for measuring laminar burning velocities and ignition delay times at higher pressures to better understand the observed autoignition and combustion delay behavior of 2MF. Autoignition is one of the crucial parameters to describe the properties of a fuel and provides useful information of its applicability for practical use e.g. in engines and turbines.

2MF has not been investigated at engine related temperature and pressure conditions so far. A detailed kinetic model of 2MF has recently been developed by Somers et al. [3]. They have validated their kinetic model with shock tube data in the temperature

* Corresponding author. Fax: +49 2418022175.
E-mail address: uygun@swl.rwth-aachen.de (Y. Uygun).
URL: http://www.swl.rwth-aachen.de/ (Y. Uygun).

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range of 1200 K to 1800 K at atmospheric pressures with different equivalence ratios (Φ) of 0.5, 1 and 2. Measurements of flat flame laminar burning velocities at atmospheric pressure over a temperature range of 298 K to 398 K for Φ ranging between 0.55 and 1.65 have also been taken. In addition, Wei et al. [4] have recently measured ignition delay times of 2MF/O_2/Ar mixtures in the temperature range of 1120–1700 K at average pressures of 1.25–10.65 bar with Φ ranging from 0.25 to 2. Several theoretical works confirm the similarities between 2MF and 2,5DMF oxidation kinetics. More recently Somers published a comprehensive study of 2,5DMF, where experiments were done with shock tubes, jet stirred reactor and a flat flame burner [5]. Simmie and Metcalfe [6] concluded that $\dot{H}$ atom addition reactions are dominant at temperatures up to 2000 K. $\dot{H}$ atom addition to C2 of the furan ring leads to a ring opening process competing with demethylation i.e. formation of 2MF and $\dot{C}H_3$ radical. Sirjean et al. [7] also highlighted the $\dot{H}$ addition to C2 where the ring opening process by building 1, 3-butadiene and acetyl radical ($CH_3\dot{C}O$) competes with the demethylation forming the intermediate products 2MF and $\dot{C}H_3$ radical.

Similarly, there have been previous ignition, oxidation and kinetic studies on THF [8–14]. Previous THF experiments have been conducted at 50–300 Torr in a heated bulb over a temperature range of 530–569 °C [10,11] and lately by Lifshitz et al. [12] in a single pulse shock tube under reflected shock conditions over a temperature range of 1070–1530 K. Molera et al. [8] have studied gas phase oxidation of THF under static conditions at 220 °C. Dagaut et al. [9] have studied the ignition delay times of THF in a single pulse shock tube under reflected shock conditions and oxidation in a high pressure jet-stirred reactor at pressures ranging from 2–10 atm, with Φ of 0.5, 1.0 and 2.0 and in the temperature range of 800–1800 K. Kasper et al. measured the mole fractions of major and intermediate species at 2000 Pa and 3333 Pa for Φ varying from 1 to 1.75 using a flat flame burner [13].

In the present work, the ignition of THF and 2MF has been studied at engine operating pressures and temperatures. The ignition delay time studies are accompanied by optical investigations which should also help in understanding the pre-ignition phenomena at low temperatures. This study deals, as far as our knowledge goes, for the first time with the ignition behavior of these biofuel candidates at high pressures and low to intermediate temperatures.

2. Experimental facilities

Both 2MF and THF were investigated in a high pressure shock tube (HPST) and optical investigations were performed for 2MF in a rectangular shock tube (RST) under reflected shock wave conditions. These facilities are briefly described in the following sections.

2.1. High pressure shock tube (HPST)

The experiments have been performed in a high pressure stainless steel (X2CrNiMoN22-5-3) shock tube described in detail in [15]. Having an inner diameter of 140 mm and a total length of about 15.5 m the HPST is optimally suited for ignition delay time measurements. The high pressure driver section is separated from the low pressure driven section by a double diaphragm chamber. Two aluminum diaphragms of 4 mm and 6 mm thicknesses are used for the current study at 20 bar and 40 bar, respectively. Having a large inner diameter reduces the facility influence on ignition delay and having longer sections increases the available test time. Ideally the conditions behind reflected shock waves should be constant with time, but in a real shock tube process the pressure and temperature behind reflected shock waves increase with time due to shock attenuation caused by boundary layer effects and also due to non-ideal bursting of diaphragms. Detailed information on effects of shock attenuation can be found in [16]. For investigations of fuels with low vapor pressures the whole facility can be resistively heated up to 200 °C. At this temperature the maximum working pressure of the shock tube amounts to 950 bar. Eight piezoelectric sensors (Kistler 603B), which are installed at 0 mm, 10 mm, 260 mm, 510 mm, 760 mm, 1010 mm, 1510 mm and 2510 mm from the end wall, have been used for pressure measurements and determination of the shock speed. A photomultiplier (Hamamatsu, RR212UH) with a narrow band pass filter (LOT 430FS10, FWHM 10 ± 2 nm) for the detection of CH^* emission is positioned 10 mm away from the endwall. The pressure transducers are shielded with a layer of high temperature silicone to protect them from heat loads of the shock heated gas which may otherwise lead to significant errors in the pressure signals. The gas temperature behind the reflected shock is calculated from the initial conditions and the shock velocity. For this purpose the in-house code KASIMIR [17] was utilized which considers equilibrium real gas effects like molecular vibration and electronic excitations. Ignition delay times can be accurately determined by means of acquired pressure time histories as well as a photo multiplier for CH^* emission detection. The ignition delay times presented in this paper are obtained from the pressure sensor located 10 mm away from the endwall. The uncertainties in the temperature behind the reflected shock wave (T_5) are estimated by taking into account the measurement uncertainties of the shock velocity and are close to ±10 K for both facilities. The available test time in shock tubes is limited due to arriving pressure or expansion waves at the endwall which are caused by the interaction between the reflected shock wave and the contact surface. As the available test time depends on several parameters which are different for each experiment, the available test time varies. Its maximum value for the current study amounts to 7 ms. Before each experiment, the shock tube was evacuated below 2×10^{-5} bar. Gas mixtures can be prepared in a separate mixing vessel of 260 l volume. For the current study, the fuel was injected directly into the shock tube and the pressure was monitored after complete vaporization of the fuel. In a subsequent step the tube was filled with synthetic air. A mixing time of one hour has been found to be sufficient as no differences in the ignition delay times could be observed for longer mixing times.

2.2. Rectangular shock tube (RST)

In the present work, experiments with 2MF at 10 bar have been performed in a rectangular stainless steel shock tube with a Z-type optical set up as shown in Fig. 1. The shock tube includes a double diaphragm chamber for accommodating two aluminum diaphragms separating the 5.4 m long driver section from the 6.9 m long driven section. The driver section has an inner diameter of 100 mm, while the rest of the tube has a 54 mm × 54 mm internal cross section. In order to capture the ignition process as well as incident and reflected shock wave parameters, four conventional pressure transducers (Kistler 603B) are mounted near the end wall. The distances from the end wall to each pressure transducers are 8 mm, 58 mm, 108 mm and 830 mm. Visualization of the flow field and the ignition process was conducted by time resolved Schlieren imaging using a high speed camera with a maximum frame rate of 1 MHz (Shimadzu, HPV 1). For this purpose a pair of fused silica windows is mounted near the end wall allowing the visualization of the whole region between lower and upper shock tube wall. The available visible area is approximately 121 mm × 54 mm. The temperatures behind the reflected shock wave were estimated with the same method described in Section 2.1. The preparation and homogenization of the mixture was also done in the same way as explained in Section 2.1.