

Experimental and Modeling Study on Ignition Characteristics of 2, 5-Dihydrofuran

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ABSTRACT

The ignition delay times of 2, 5-Dihydrofuran (25DHF) were measured behind reflected shock waves at the pressures of 4, 10atm, temperatures of 1110-1650 K, for the lean ($\phi=0.5$) and stoichiometric ($\phi=1.0$) mixtures with fixed fuel concentration of 0.5%. The correlations of ignition delay times to initial parameters were fitted in an Arrhenius-like form for the two fuels by multiregression analysis. Simulations based on Liu model, Somers model and Tran model were presented and compared to experiment data. Subsequently, reaction pathway and sensitivity analysis were performed in low and high temperature to obtain insight into the ignition kinetic by using Liu model. Reaction path analysis shows that there are two main ways in the consumption of 25DHF and the main intermediates are C_3H_5Y , sC_3H_5 and propylene etc. Some reactions which involved the main intermediate products presented important effect on the whole ignition of 25DHF. The comparisons to furan and MTHF on ignition delay time data were also conducted. The ignition delay times of 25DHF were shorter than that of furan and the slopes of ignition delay times of 25DHF were smaller than that of furan and MTHF, proving lower activation energy.

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INTRODUCTION

The energy crisis and environmental pollution have restricted the development of the society. Searching for sustainable alternative fuels is one of the most promising development tendencies of internal combustion engine industry. The application of ethanol and biodiesel proves the potential of biomass fuels on energy sustainability and emission reduction. Furans and tetrahydrofurans are the second generation biomass fuels produced from agricultural waste [1, 2], such as straw, bagasse. Unlike ethanol as the first generation of biomass fuel, furans and tetrahydrofurans consumed no agricultural resources in the production process and expressed further advantages.

Furans and tetrahydrofurans have been widely researched on internal combustion engines. The feasibility of the application of 2-methylfuran (MF) and 2, 5-dimethylfuran (DMF) on internal combustion engine was studied [3, 4, 5] and conclude that the aldehydes emission and combustion characteristic are better than that of gasoline. Favorable power output and emission characteristics were achieved by addition of 2-methyltetrahydrofuran into gasoline [6]. Matthias et al. [7] studied the spray and combustion of MF on a GDI engine, concluded that the full load thermal efficiency increased about 10% than that of 95# gasoline through improving compression ratio by 3.5. Combined with EGR, application of blended fuels of furans is a new way to improve the engine performance, emission and fuel economy.

The combustion characteristics of furans and tetrahydrofurans have also been comprehensively investigated. Detailed mechanism of furan combustion was developed by Tian et al. [8] and validated by three sets of low-pressure laminar premixed flame. Chemical kinetic of 2-methylfuran pyrolysis and oxidation was investigated by Somers et al. [9] and verified by ignition delay times and laminar flames. Xu et al. [10] optimized that mechanism at high temperature through shock tube experiment and carried out kinetic analysis work. Sirjean et al. [11] and Somers et al. [12] separately constructed and verified the kinetic of DMF oxidation. Researchers of Bielefeld University and Lorraine University [13, 14, 15] also optimized and validated the kinetic of furans combustion. The detail kinetic of THF oxidation was developed and verified by laminar flames, ignition delay times and combustion velocity by Tran et al. [16] Oxidation model of 2-methyltetrahydrofuran (MTHF) was developed and verified by Moshhammer et al. [17] in 2013. These models can reveal the internal processes of the furans and tetrahydrofurans combustion.

Dihydrofurans (DHF) are important intermediates in combustion action of furans and tetrahydrofurans and involved in detail mechanisms mentioned above. So, the investigation of DHFs oxidation is of significant for model optimization and understanding the combustion process of furans and tetrahydrofurans accurately. Lifshitz et al. [18] researched the thermal pyrolysis of 25DHF behind shock waves and discovered the main reactions in low temperature and concluded that 25DHF is less stable than furan and tetrahydrofuran (THF). Sudholt et al. [19] calculated the bond dissociation energies of carbon-hydrogen on the ring of 25DHF and

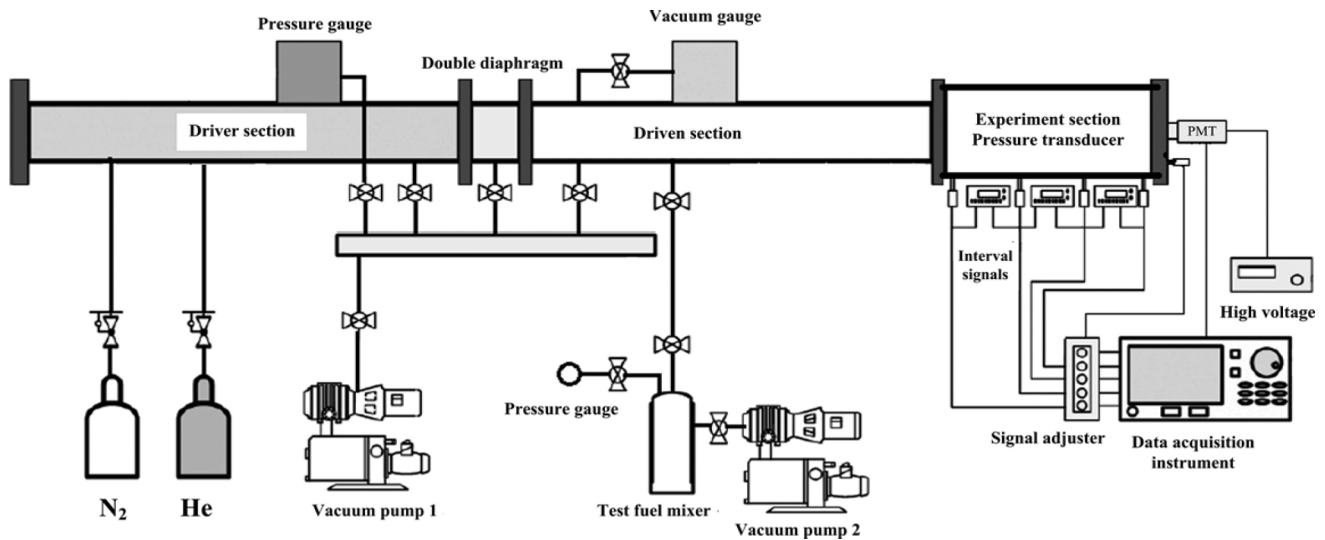


Figure 1. Schematic of the shock tube.[20]

investigated the derived cetane numbers of 25DHF in an Ignition Quality Tester. Ignition quality is not only a key factor in performance and emissions of internal combustion engines, but also a critical parameter in engine numerical simulation. Accurate ignition delay data measured in the shock tubes can be used in the development and verification of combustion models. In present study, the ignition delay times of 25DHF were measured behind reflected shock waves and the simulation of experiment based on Liu model was carried out. What's more, the comparisons to furan and MTHF were conducted to better perceive the combustion characteristics of 25DHF.

EXPERIMENTAL SETUP AND NUMERICAL APPROACH

The ignition delay data for the present study was collected behind the reflected shock waves. The present shock tube facility which has been described in details previously [20, 21] is consists of a 2000mm long driver section and a 7300mm long driven section, as shown in Figure 1. The driver section and the driven section are separated by a connecting flange (60mm long) with PET diaphragms on both sides.

Diaphragms of different thickness were selected according to the desired initial conditions. Before experiment, the tube is evacuated by vacuum system to the pressure below 1 Pa. High purity helium and nitrogen were mixed with precise quantities and ratios in the driver section to generate shock waves of desired velocities. 25DHF/O₂/Ar mixtures were mixed in a 128 L stainless steel tank and kept stationary for at least 12 h to ensure sufficient homogeneousness. Purities of 25DHF, oxygen and argon were 97%, 99.999% and 99.999%, respectively. The mole ratios of the reactant mixtures are shown in Table 1. The OH* chemiluminescence is detected by a 307±10 nm narrow band filter and a photomultiplier (Hamamatsu, CR131) at the endwall. The travel processes of the shock waves could be detected by four fast-response piezoelectric pressure transducers (PCB, 113B26) which located at the side wall of the driven section. Three time interval counters (Fluke PM6690) measured the times of the waves passing the pressure transducers. All signals were recorded

by a Yokogawa DL750 digital recorder. By extrapolation, the incident shock velocity at the end wall could be calculated, which is essential for the calculation of the temperatures behind the shock waves [22]. The ignition delay time is defined as the time interval between the arrival of incident shock wave at the end wall and the intersection of extrapolation of the maximum slope of the OH* radical curve to the zero baseline, as shown in Figure 2.

Table 1. Composition of fuel mixtures (in mole fraction)

$\phi(\%)$	2,5-DHF(%)	O ₂ (%)	Ar(%)	P(atm)
0.5	0.5	5	94.5	4
1	0.5	2.5	97	4 / 10

The ignition processes are simulated in an adiabatic and zero-dimensional homogeneous reactor based on the Senkin code [23, 24]. The calculated ignition delay time is defined as the time interval from the beginning of the reaction to the steepest rise of the temperature. The interaction between reflected shock wave and boundary layer could cause slight rise of pressure before the ignition. This phenomenon is simulated by setting 4%/ms in volume decrease, so the simulation of ignition could be more precise.

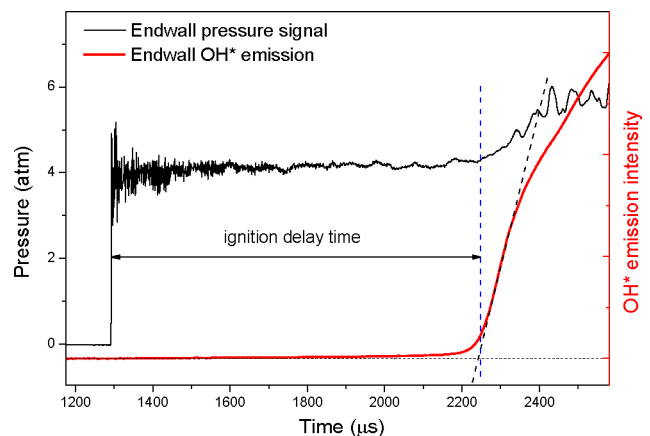


Figure 2. Definition of ignition delay times in experiments.

EXPERIMENTAL RESULTS AND DISCUSSIONS

Ignition Delay of 2, 5-Dihydrofuran

The experiments were carried out at the equivalence ratios of 0.5 and 1, pressures of 4atm and 10atm, with fixed fuel concentration of 0.5%. Correlation of ignition delay time with pressure, equivalence ratio and temperature was obtained by regression analysis.

$$\tau = 2.305 \times 10^{-2} \phi^{1.49} p^{-0.70} \exp(30.057 / RT) \quad (1)$$

Where τ is the ignition delay time in microsecond, and ϕ is the equivalence ratio and p represents the pressure in atm, and T is the temperature in kelvin, $R=1.987 \times 10^{-3}$ kcal/(mol·K). The correlation fitted the experiment well, as shown in Figure 3 ($R^2 > 98\%$). Note that the correlation is only suitable for the prediction at fuel concentration of 0.5%.

As can be seen from Figure 2, ignition delay times of 25DHF present obvious logarithmic relation with the reciprocal of temperature. The slopes of experiment data are almost the same at different pressures and equivalent ratios and the temperature from 1100 to 1650K, demonstrating the active energy is constant on a large range, as shown in Equation 1. The ignition delay times increase with the decrease of pressure and are lower at the equivalence ratio of 0.5 compared with that at stoichiometric condition. The elevation of the pressure could densify the mixture, so the possibility of molecular collision and the reactivity of reactions would increase and the ignition is accelerated in consequence. At high temperature, the ignition is mainly dominated by the reaction of $H + O_2 = O + OH$, which can strongly promote the ignition process. The increase of the oxygen concentration at fixed fuel concentration could boost the reactivity of this reaction and accelerate the ignition, thus the ignition delay time is lower at oxygen-rich mixture.

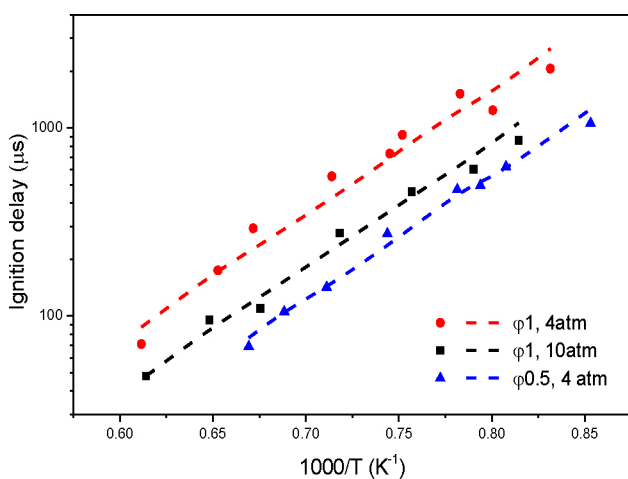


Figure 3. Ignition delay times of 25DHF/O₂/Ar mixtures. Symbols for measurements, dash lines for fitting curves.

Chemical Kinetic Analysis of 2, 5-Dihydrofuran

2, 5-dimethylfuran is an important intermediate in combustion of furans and tetrahydrofurans and involves in many chemical kinetic models. In present study, we chose Somers model [9], Liu model [13]

and Tran model [16] for the simulation and comparison with experiment. Both Somers model and Liu model are integrated with kinetics of furan, 2-methylfuran and 2, 5-dimethylfuran. The furan kinetic of Somers model is from Tian et al. [8] and Sendt et al. [25], which contains the sub-mechanism of 25DHF. Validations have been done for the C0-C4 kinetic in Somers model, which could ensure precise simulations. The 25DHF sub-mechanism of Liu model is also from Tian et al. [8] and was updated based on laminar flame experiments. The C0-C4 chemistry in this mechanism is from [26, 27, 28]. Two reaction pathways related to dihydrofuryl radicals have been added. Tran model was developed by using EXGAS taking into account the specific combustion characteristic of cyclic ethers.

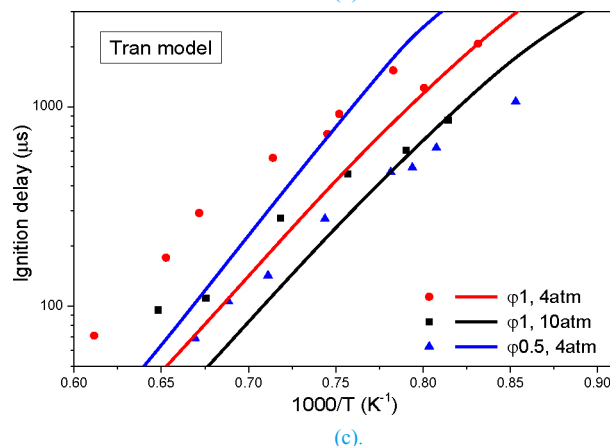
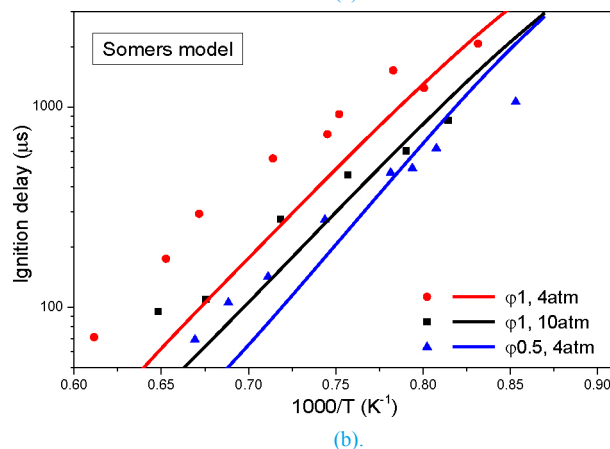
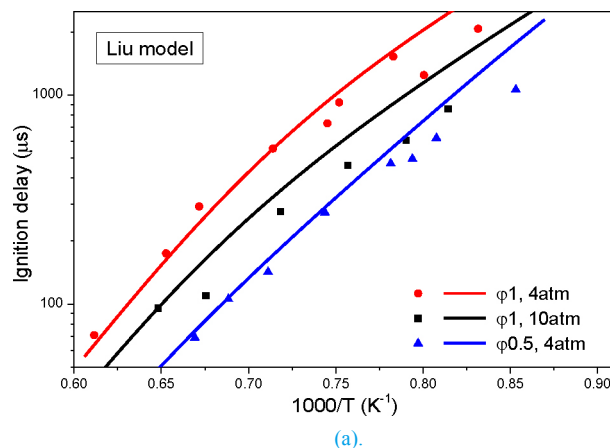


Figure 4. Measured and fitted, calculated ignition delay times of 25DHF/O₂/Ar mixtures. Symbols for Measurements, solid lines for simulation results of Liu model (a), Somers model (b) and Tran model (c).