



# Autoignition Delay Time for Heavy-Duty Mixing Controlled Compression Ignition Conditions Using Dimethyl Ether and Propane

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Dimethyl ether (DME) is a biofuel that has the potential to replace diesel in heavy-duty engines. A blend of propane ( $C_3H_8$ ) and DME could reduce emissions when compared to diesel at heavy-duty compression engine-relevant conditions. Testing a potential new mixture in a compression engine requires a high-fidelity chemical kinetics model that accurately predicts autoignition delay times, which is especially necessary for a compression engine. In this work, autoignition data has been gathered at an equivalence ratio of 2.0 for pressures of 60 and 80 bar. DME and propane were combusted in synthetic air while excited hydroxyl ( $OH^*$ ) chemiluminescence was used to gather ignition delay times. Data was compared to recent chemical kinetic mechanisms for the two different pressures. Using the mechanism with the best fit of autoignition data, a sensitivity analysis was conducted to analyze the chemical kinetics of the DME/ $C_3H_8$  combustion at elevated pressures.

## I. Nomenclature

<i>CI</i>	=	<i>compression ignition</i>
<i>DME</i>	=	<i>dimethyl ether</i>
<i>IDT</i>	=	<i>ignition delay time</i>
<i>K</i>	=	<i>kelvin</i>
<i>MCCI</i>	=	<i>mixing controlled compression ignition</i>
<i>NTC</i>	=	<i>negative temperature coefficient</i>
<i>LHV</i>	=	<i>lower heating value</i>
<i>P<sub>5</sub></i>	=	<i>reflected shock wave pressure</i>

## II. Introduction

In the U.S., the transportation sector is the second largest energy consumer, which consumed around 28 quadrillion BTUs in 2019 [1]. Rising global temperatures from greenhouse gases are driving transportation companies to find alternatives to petrol and diesel fuels that are less significant in contributing to global warming and which adhere to more emission regulations worldwide. An alternative to these fuels is liquified petroleum gas (LPG) [2], which consists of propane ( $C_3H_8$ ) (80-100%). A positive for LPG is the large, existing infrastructure [3], which can support propane. Compared to petrol (LHV of 43.2 MJ/kg) [4] and diesel (LHV of 42.5 MJ/kg) [5], propane (LHV of 46.4 MJ/kg) [5] has a higher energy content. Despite the high energy content, propane's autoignition characteristics are insufficient and thus need to be blended with a fuel that enhances its autoignition [6].

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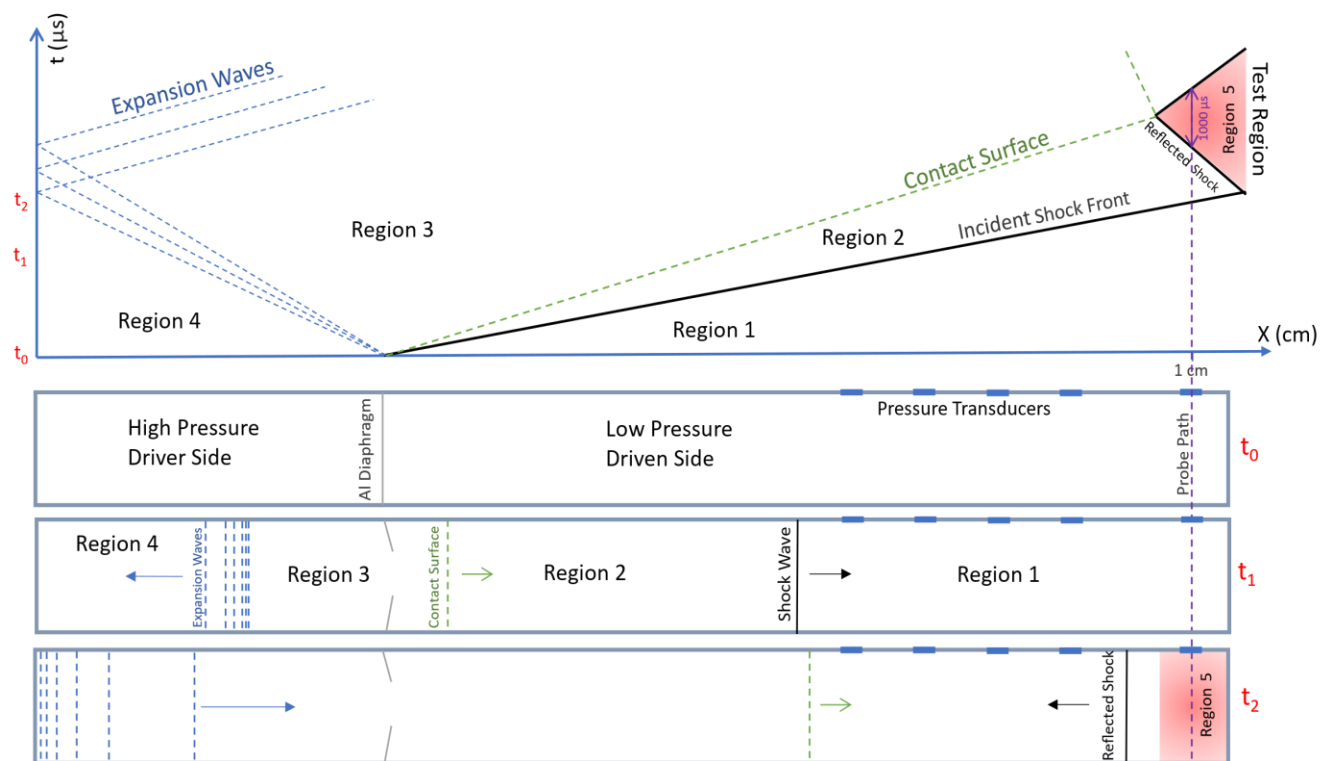
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A biofuel that accomplishes this is dimethyl ether (DME) (LHV of 28.43 MJ/kg) [5]. Dimethyl ether is the simplest ether with no carbon-carbon bonds in its chemical structure, which leads to soot-free combustion. Dimethyl ether is also a non-toxic, non-carcinogenic, non-teratogenic, and non-mutagenic fuel. This results in engines utilizing a higher rate of exhaust gas recirculation (EGR) to reduce nitrogen oxide emissions ( $\text{NO}_x$ ) [7]. Dimethyl ether's lower autoignition temperature (508K) also allows it to be operated at lower temperatures to further reduce  $\text{NO}_x$  in the Mixing Controlled Compression Ignition (MCCI) engine, which is the conventional mode for compression ignition (CI) engines. In literature, most DME studies are focused on ignition delay time (IDT) measurements, and for DME-propane blends specifically, IDT measurements up to 50 atm have been reported until recently [6]. Mohammed et al. reported stoichiometric IDTs for 60 and 80 bar [8]. In the same study, autoignition data was gathered at 90 and 120 atm at  $\phi=0.38$  [8].

Compression ignition engines have operating ranges from 30-70 bar [9] and heavy-duty compression engines operate at elevated pressures. Specifically, for an MCCI engine the fuel and oxidizer are not premixed and will encounter a wide range of equivalence ratios ranging from lean ( $<0.2$ ) to rich ( $>2.0$ ) [10]. Heavy-duty MCCI engines depend on autoignition data, and a chemical kinetic model needs to be developed for CFD simulations to accurately predict chemistry at engine-relevant conditions of an MCCI. In order to create and validate a chemical kinetic mechanism for DME-propane chemistry, high-pressure autoignition measurements are needed at varying equivalence ratios and temperatures at engine-relevant conditions. For this work, IDT measurements of DME-propane are shown for blends at 90-120 bar, 700-1100 K, for an equivalence ratio of  $\Phi=0.38$  using a shock tube.

### III. Experimental Procedure

This study was conducted at the University of Central Florida (UCF)'s High-Pressure Extended Range Shock Tube for Advanced Research (HiPER-STAR) facility [11, 12]. In general, a shock tube is ideal for creating a high-pressure environment by using the pressure and temperature behind a generated shock wave and has been used for numerous studies studying combustion since the 1940s [13]. The shock tube at HiPER-STAR is capable of withstanding high pressures reaching up to 1000 atm, allowing the experiments here within to be safely conducted as post-combustion pressures were recorded over 700 bar. State 5 conditions were achieved by rupturing aluminum diaphragms ( $T_5$  temperature,  $P_5$  pressure in Fig. 1), and measurements were taken in the test section, located 1 cm from the end wall. Piezoelectric dynamic pressure transducers (PCB 113B26) were used to record the pressure traces during the experiments. A total of five pressure transducers were used while they were connected to Agilent 53220A time interval counters on the driven side. The arrival of the incident shock at each pressure transducer triggered the time interval counters, which were used to find the shock velocity. Fig. 1 depicts shock tube methodology, which starts with the two sides of the shock tube separated by the aluminum diaphragm. The left side is the high-pressure driver side, while the right side is the low-pressure driven side. As the inert gas flowing into the high-pressure driven side reaches a critical pressure, the diaphragm will burst, creating a shock wave. State 1 is the low-pressure driven side and is composed of the test mixture (Mix 1). When the shock wave is reflected off of the end wall, the desired  $P_5$  is reached, and test time begins. Once ignition occurs, the IDT is recorded based on the maximum  $\text{OH}^*$  emission location.



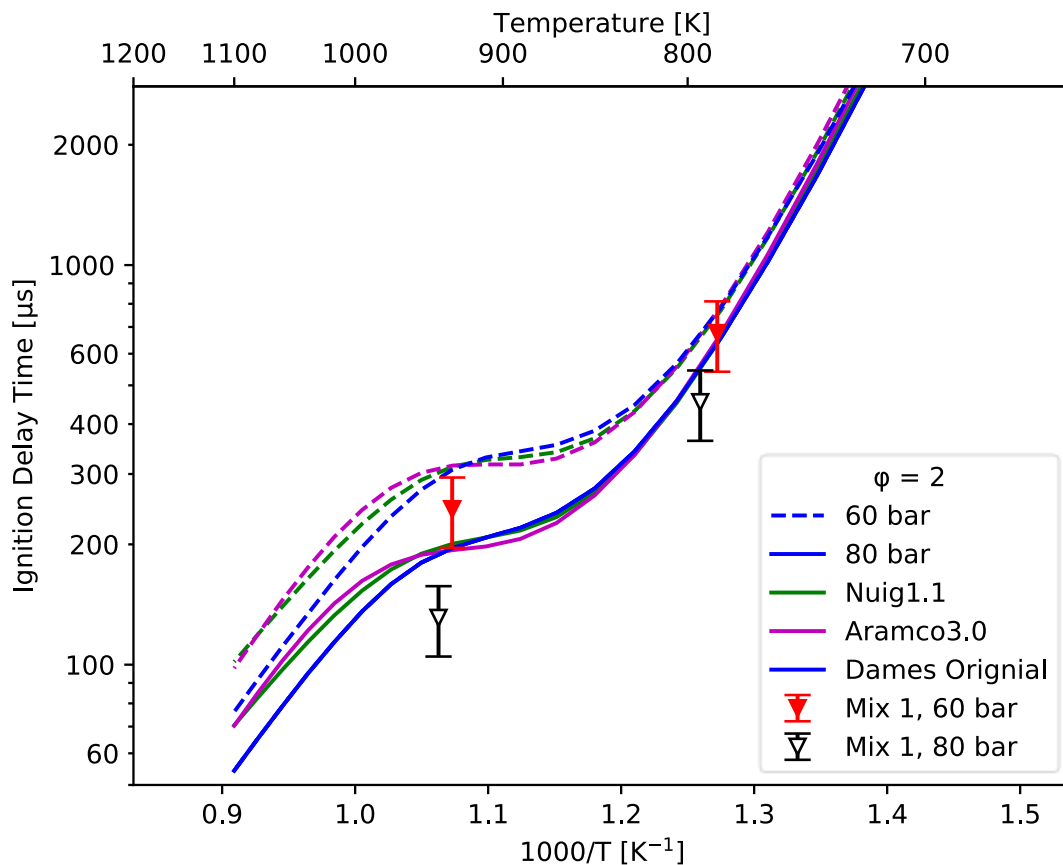
**Fig. 1: Shock tube x-t Diagram**

The mixture was prepared in a high-pressure mixing tank, separated from the shock tube. Gas homogeneity is achieved by using neodymium nickel-coated magnetic stirrers that continually mix the gas. Before the start of experiments, the driver section of the shock tube was vacuumed using the combination of an Agilent dual-stage rotary vane pump (DS 102), a Kurt J. Lesker TRIVAC B two-stage rotary vane pump (D&B), and an Agilent turbomolecular pump (TwisTorr 305 FS). These pumps were used to ensure that there were no impurities present in the shock tube before the experimental mixture entered. The IDT was defined as the time between the departure of the reflected shock up until ignition, which was defined as the time of peak hydroxyl radicals ( $\text{OH}^*$ ) measured by a Newport 2032 photodetector with an Edmund Optics 306 nm narrow bandpass filter. The mixture concentrations are presented in Table 1. Neat DME and propane were used as a baseline for model comparison while the blend was made on recommendation by literature [9].

**Table 1: Mixture information from temperatures of 700-1100 K for neat DME/ $\text{C}_3\text{H}_8$  and the blend of DME and  $\text{C}_3\text{H}_8$ .**

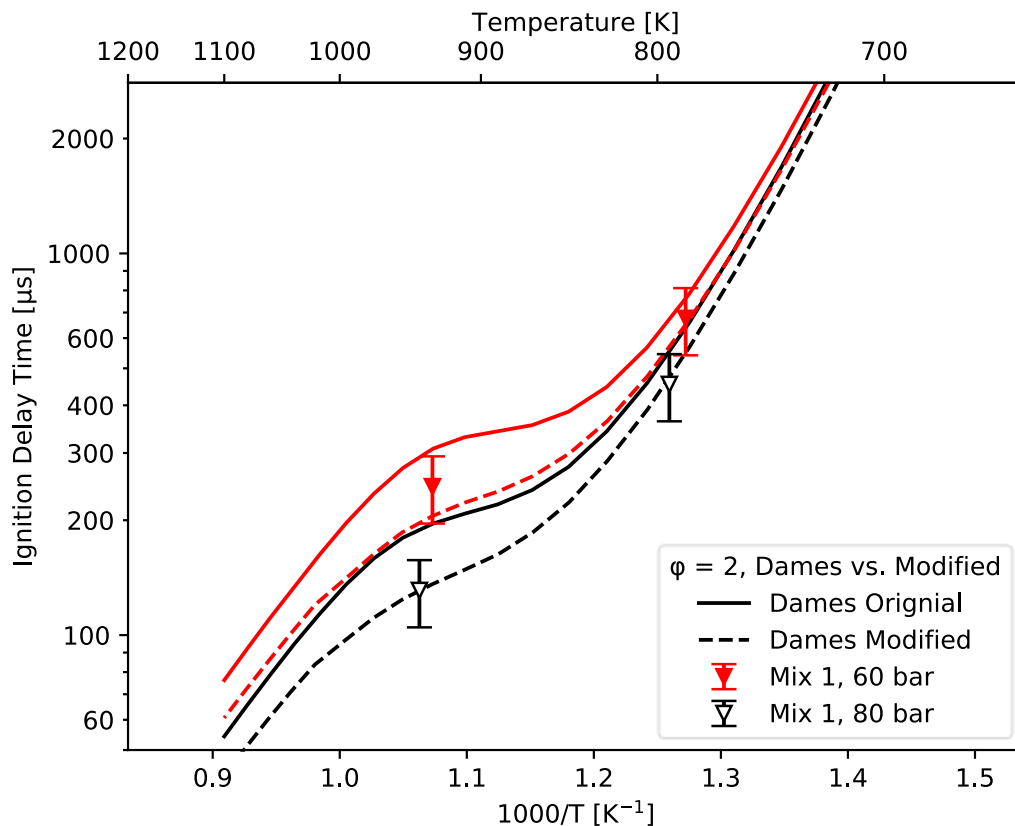
Mixture #	Mixture	$\phi$	$\text{C}_3\text{H}_8$	$\text{CH}_3\text{OCH}_3$	$\text{O}_2$	$\text{N}_2$	$P_5$ (bar)
1	DME-Propane	2	0.060	0.040	0.189	0.711	60, 80

#### IV. Results and Discussion



**Fig. 2: Comparison of IDT for Mix 1 in air at  $\Phi = 2$  for 60 and 80 bar with the Dames et al. [6], NUIG1.1[14] and Aramco3.0 [15].**

From Fig. 2, four experiments were conducted at high pressures of 60 and 80 bar for Mix 1 and for an equivalence ratio of 2.0. The pressure dependency of the DME/propane seen from the IDTs for 60 bar experiments was higher than the 80-bar experiment also shown by the simulations from the mechanisms. All three mechanisms are shown to follow the NTC trend as seen previously for stoichiometric 60–80 bar shock tube experiments with Dames et al. [6, 8]. Looking at the temperature, accurate assumptions about the NTC temperature range can be estimated to be around 850–1000K, where DME and propane’s low-temperature heat release interact with its high-temperature chemistry. The NTC region from Fig. 2 also shows a strong sense of pressure dependency from the 80-bar simulation for all mechanisms and shows less prominence for the NTC region.



**Fig. 3: Experiments from Mix 1 at  $\Phi=2.0$  for 60 and 80 bar compared to Dames et al. [6] and Dames modified.**

Fig. 3 shows the modified Dames mechanism where Reaction 356's A factor was altered. This reaction was chosen by conducting a sensitivity analysis using Chemkin Pro. Reaction 356 is  $\text{CH}_3\text{OCH}_3 + \text{HO}_2 = \text{CH}_3\text{OCH}_2 + \text{H}_2\text{O}_2$  where an H-abstraction occurs for DME by the hydroperoxyl radical. This results in  $\text{CH}_3\text{OCH}_2$  and hydrogen peroxide. The reaction rates are from works done by Mendes et al. [16], where they had estimated an uncertainty of 2.5. The reaction was modified by a factor of 2.5 and the results are represented as the dashed lines in Fig. 3. The model has increased its predictability of IDTs by a large margin. The model accurately predicts IDTs for all 60 and 80 experiments present in Fig. 2.

## V. Summary

As energy demand rises and so do global temperatures, there is a need for alternative, more environmentally friendly fuels. DME is one such biofuel that is more environmentally friendly and can be blended with a high energy content fuel (like  $\text{C}_3\text{H}_8$ ). Due to the lack of autoignition data for DME/ $\text{C}_3\text{H}_8$  at engine-relevant conditions of heavy-duty MCCI engines in literature, autoignition data was gathered at 60 and 80 bar for a blend of DME-propane at  $\phi$  of 2. The results were compared to numerous mechanisms which overpredicted the IDTs by a large margin. Reaction 356 was modified within uncertainty for the Dames et al. mechanism [6], and the modified mechanism is now able to better predict the chemistry of a DME/propane blend.

## Acknowledgments

This material is based upon work supported by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE) under Award Number DE-EE0009879. Partial support from the University of Central Florida is also acknowledged.

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