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Autoignition Delay Time Measurements of Dimethyl Ether at 110 bar inside a Shock Tube

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Fuel mixtures of propane and dimethyl ether have been proposed as potential diesel substitutes for use in compression-ignition engines. There is an interest in phasing out diesel fuel because its combustion byproducts are harmful to the environment. Propane and dimethyl ether burn cleaner and produce significantly less carbon dioxide than diesel. The combustion of these fuels at engine-relevant conditions must be characterized to create an engine capable of running on propane and dimethyl ether. In this work, IDT measurements of stoichiometric neat DME diluted in 75% argon were completed for temperatures spanning 800-1200K at 110 bar. A shock tube will be used for all experiments in this work. Experimental IDTs were then compared to simulated values using several well-established mechanisms in the literature.

I. Nomenclature

DME = Dimethyl Ether
IDT = Ignition Delay Time
Φ = Equivalence Ratio
NTC = Negative Temperature Coefficient
T_5 = Shock tube test temperature
P_5 = Shock tube test pressure
LPG = Liquified Petroleum Gas

II. Introduction

Higher global temperatures due to the increased concentration of carbon dioxide in the atmosphere have been a concern of politicians and scientists for decades. There are several culprits for the increase atmospheric carbon dioxide concentration, but one of the primary focuses is the transportation industry. In 2019, the United States transportation sector was the second largest energy consumer in the country. The transportation sector expended roughly 28 quadrillion British thermal units (BTUs) of energy in that year [1]. In 2021, 90 percent of all the energy used by the United States transportation sector was from petroleum products [2]. Petroleum combustion is one of the largest sources of carbon dioxide emissions. The carbon dioxide coefficient for a fuel defines the amount of carbon dioxide produced per unit mass of fuel burned. The carbon dioxide coefficient for diesel fuel is 22.45 pounds per gallon and 19.37 pounds per gallon for gasoline [3]. The combination of these statistics is concerning. There are arguments in the scientific community about how much of the observed carbon dioxide increase in the atmosphere is caused by human activity. However, it is alarming that the current rate of global heating is at a 10,000-year high while carbon dioxide concentration in the atmosphere is simultaneously the highest it has been in millennia [4]. The most plausible explanation for this is the rapid industrialization of societies worldwide in the last two centuries. Thankfully, alternative fuels have been studied in recent years to curb some of the damage caused by petroleum fuels.

A popular alternative fuel is liquified petroleum gas (LPG), which consists of almost entirely propane. This fuel has many desirable properties, such as a higher energy content than petroleum, no soot particulates, abundance, and ease of transportation. However, an issue with LPG combustion is its high autoignition temperature. For LPG to

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be used in compression ignition engines, its autoignition temperature must be reduced. Dimethyl ether (DME) is a biofuel that solves this problem. Propane has an autoignition temperature of 743 K at atmospheric pressure, while DME has an autoignition temperature of 523 K [5]. Until recently, propane and DME combustion studies have not exceeded 50 bar [6]. An ongoing effort to gather combustion data for these fuels at higher pressures to capture compression ignition engine-relevant conditions A study by Mohammed et al. collected data for various propane-DME blends at pressures of 55-84 bar [7].

To build an engine capable of running on propane and DME, the combustion of both fuels blended and on their own must be thoroughly studied. Chemical kinetic mechanisms simulate the outcome of combustion experiments under user-specified conditions. Chemical kinetic mechanisms rely on experimental data to increase their accuracy. To develop an accurate chemical kinetic model for propane and DME, measurements of these fuels must be conducted at various temperatures, pressures, equivalence ratios, and fuel mixtures. For this work, IDT measurements of stoichiometric neat DME diluted in 75% argon were completed for temperatures spanning 800-1200K at 110 bar. A shock tube was used for all experiments in this study.

III. Experimental Procedure

This study was conducted at the University of Central Florida High-Pressure Extended Range Shock Tube for Advanced Research (HiPER-STAR) facility [8, 9]. A shock tube is an ideal device for replicating engine conditions while decoupling walls and transport effects. In Fig. 1, t_0 represents the stagnant condition in the shock tube. The tube is filled with the desired test mixture on the driven side of the shock tube, while the driver gas is filled to high pressure before the diaphragm ruptures. After the diaphragm ruptures (t_1), a shock wave propagates down the tube and compresses the test mixture as the driver gas behind the contact surface expands. The shock wave then reflects off the end wall and compresses the test mixture a second time, which creates engine-relevant conditions (T_5 and P_5) and eventually causes it to combust (t_2). The time between the reflected shock's passage and the ignition's onset is ignition delay time (IDT).

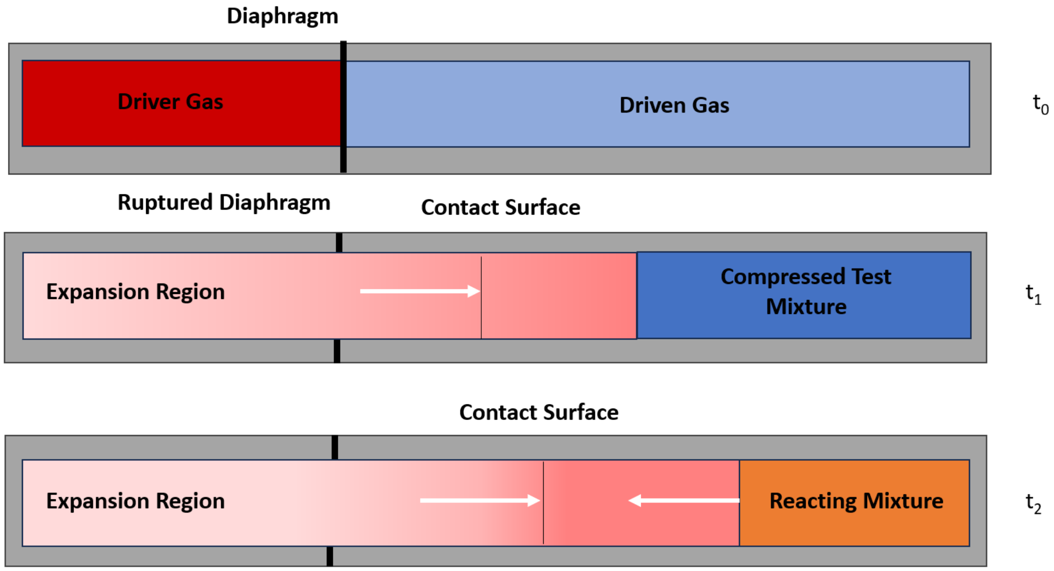

Fig. 1. Snapshots of the cross-section of a shock tube experiment.

The fuel mixture was prepared in the facility's mixing tank using the partial pressure method. After the gases were fed into the tank, they were stirred using an impeller coupled with neodymium magnets to ensure the mixture was homogenous. Before the mixture was fed into the driven side of the shock tube, it was vacuumed to cleanse impurities from previous experiments. The shock tube was also routinely cleaned with isopropyl alcohol to prevent soot buildup on the walls. The vacuuming process involved a series of pumps: Agilent dual-stage rotary vane pumps (DS 102), a Kurt J. Lesker TRIVAC B two-stage rotary vane pump (D8B), and finally an Agilent turbomolecular pump (TwisTorr 305 FS). A mixture of Neat DME and air diluted in argon was used for all experiments in this work. Experimental conditions and mixture information can be found in Table 1. All experiments were conducted at stoichiometric conditions ($\Phi = 1$).

Mixture	DME	Argon	O_2	N_2	P_5 [bar]	T_5 [K]
Neat DME	0.01614	0.75	0.049065	0.184579	105.8 – 118.8	828 – 1157

Table 1: Mixtures and Experimental Conditions

Nonintrusive optical diagnostic tests were used to measure the experimental IDTs. The IDT was defined as the time between when the reflected shock passed the test section (measured by pressure transducers) and the point of maximum OH* emissions measured by a detector.

Simulated IDTs were generated using the Ansys Chemkin Pro 2022 software. First, a closed, homogenous batch reactor with a constrained volume approach was selected. The fuel and planned experimental conditions were then imported, and the simulations were run. Several temperature points were plotted between 800 - 1200K to accurately capture the behavior IDTs as temperatures vary for the mixture.

IV. Results and Discussion

In Fig. 3, simulated IDTs for DME at 110 bar are shown for several mechanisms commonly used in the literature, demonstrating varying predicted behavior between each of the mechanisms [6, 10-12]. The negative temperature coefficient (NTC) region is where IDTs rise as temperatures increase due to internal chemistry. Dimethyl ether exhibits this behavior, which can be seen in the plot from roughly 850-930K. The Dames mechanism predicts the IDTs in the NTC region very accurately. Simulations deviated from the experimental values at higher temperatures for all mechanisms.

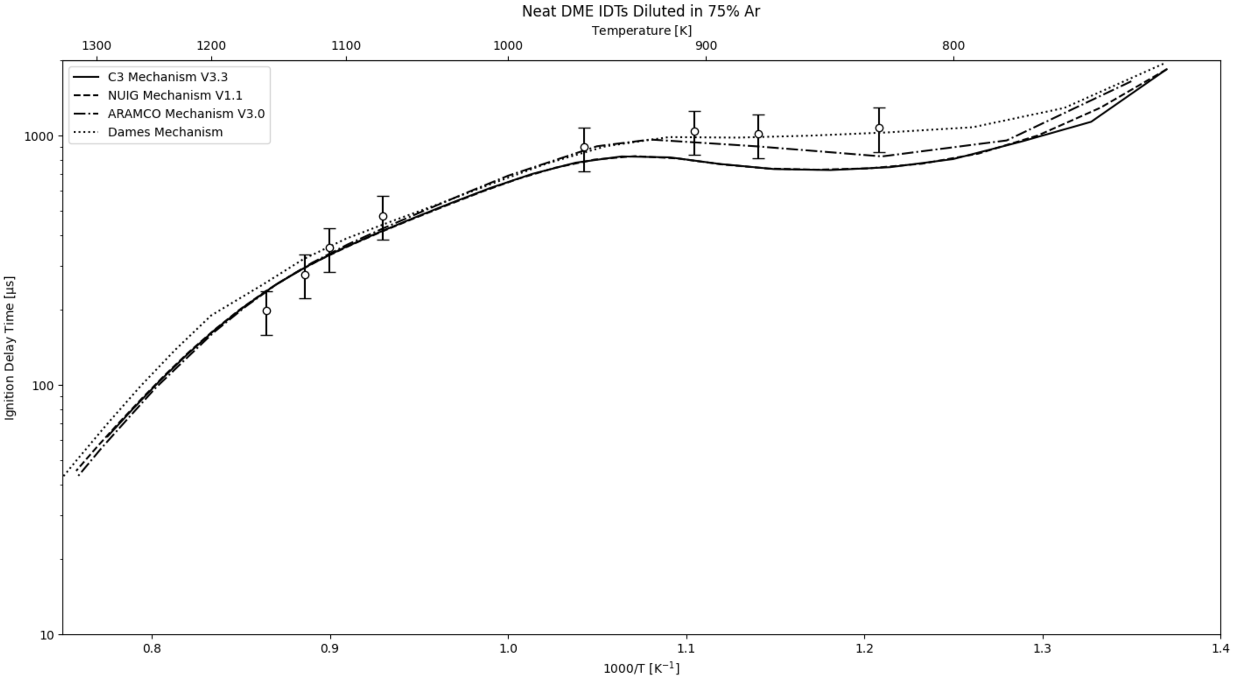

Fig. 2. Simulated IDTs for neat DME at 110 bar.

V. Conclusion

The fuels currently used by the transportation sector in the United States have been shown to have detrimental environmental effects. Cleaner alternatives to petroleum, such as batteries, natural gas, and hydrogen, have been explored in the industry in recent years. Propane and dimethyl ether fuel blends have been proposed as a cleaner substitute for diesel for use in compression-ignition engines. Currently, little information is available on propane-DME combustion at compression ignition engine-relevant conditions. This data is essential to building an engine capable of running on propane and DME. Autoignition data for stoichiometric neat DME diluted in 75% argon at 110 bar was gathered using the shock tube at the University of Central Florida HiPER-STAR facility due to its ability to replicate engine-relevant conditions. This experimental data was plotted against several chemical kinetic mechanisms in the literature. The Dames et al. model performed best at these conditions but deviated at higher temperatures.

Accurate chemical kinetic mechanisms are an essential tool for engine designers. Because of this, future work may include temperature sensitivity analyses to correct deviations, compiling IDT data for several propane/DME mixtures for model modifications and reduction, and doing direct laser absorption spectroscopy (LAS) using quantum cascade lasers (QCLs) for time history measurements of critical intermediate species.

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VI. References

[1] E.-E. I. Administration, "Annual Energy Outlook 2020," 2020. [Online]. Available: https://www.eia.gov/outlooks/aeo/pdf/aeo2020.pdf.

[2] "Use of energy for transportation - U.S. Energy Information Administration (EIA)." https://www.eia.gov/energyexplained/use-of-energy/transportation.php (accessed June 11th, 2023).

[3] E. I. Administration. "Carbon Dioxide Emissions Coefficients." https://www.eia.gov/environment/emissions/co2_vol_mass.php (accessed.

[4] NASA. "Climate Change Evidence." https://science.nasa.gov/climate-change/evidence/ (accessed.

[5] S. H. Park and C. S. Lee, "Applicability of dimethyl ether (DME) in a compression ignition engine as an alternative fuel," *Energy Conversion and Management,* vol. 86, pp. 848-863, 2014.

[6] E. E. Dames, A. S. Rosen, B. W. Weber, C. W. Gao, C.-J. Sung, and W. H. Green, "A detailed combined experimental and theoretical study on dimethyl ether/propane blended oxidation," *Combustion and Flame,* vol. 168, pp. 310-330, 2016.

[7] Z. P. Mohammed, R. K. Rahman, M. Pierro, J. Urso, and S. Vasu, "DME-Propane Ignition Delay Time Measurements at Mixing Controlled Compression Ignition Engine-Relevant Conditions," SAE Technical Paper, 0148-7191, 2023.

[8] M. Pierro *et al.*, "High-Fuel Loading Ignition Delay Time Characterization of Hydrogen/Natural Gas/Ammonia at Gas Turbine-Relevant Conditions Inside a High-Pressure Shock Tube," in *Turbo Expo: Power for Land, Sea, and Air*, 2022, vol. 86007: American Society of Mechanical Engineers, p. V03BT04A002.

[9] J. J. Urso *et al.*, "Characterization of a new ultra-high pressure shock tube facility for combustion and propulsion studies," *Review of Scientific Instruments,* vol. 93, no. 6, p. 063905, 2022.

[10] S. Dong *et al.*, "A new detailed kinetic model for surrogate fuels: C3MechV3. 3," *Applications in Energy and Combustion Science,* vol. 9, p. 100043, 2022.

[11] C.-W. Zhou *et al.*, "An experimental and chemical kinetic modeling study of 1, 3-butadiene combustion: Ignition delay time and laminar flame speed measurements," *Combustion and Flame,* vol. 197, pp. 423-438, 2018.

[12] Y. Wu *et al.*, "Understanding the antagonistic effect of methanol as a component in surrogate fuel models: A case study of methanol/n-heptane mixtures," *Combustion and Flame,* vol. 226, pp. 229-242, 2021.