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DME-Propane Blends Ignition Experiments and Modeling for Heavy-Duty Mixing Controlled Compression Engines

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A blend of dimethyl ether (DME) and propane (C_3H_8) is being studied in a shock tube at heavy-duty engine conditions at 110 bar. Due to its intrinsic combustion properties, DME/propane blend can potentially replace diesel in mixing controlled compression ignition engines. A blend of DME/propane can reduce emissions in mixing controlled compression ignition in heavy-duty engines through modifications, which require simulations using a high-fidelity chemical kinetics model that can accurately predict the chemistry of the blend. An essential aspect of testing the chemical kinetics model is doing baseline fundamental chemistry studies on neat DME and propane, which include ignition delay time measurements. In this work, using a high-pressure shock tube, ignition delay times were gathered for DME/Propane blends at 110 bar diluted with AR to test chemical kinetic models published in the literature. These models include Aramco 3.0, NUIG V1.1, C3mech V3.3, and Dames et al. Comparisons with the experimental IDTs and models were conducted, and general agreement was observed. A sensitivity analysis was conducted, and important reactions were outlined.

I. Nomenclature

CI	=	*Compression Ignition*
DME	=	*Dimethyl Ether*
IDT	=	*Ignition Delay Time*
K	=	*Kelvin*
MCCI	=	*Mixing Controlled Compression Ignition*
NTC	=	*Negative Temperature Coefficient*
LHV	=	*Lower Heating Value*
P_5	=	*Reflected shock wave pressure*

II. Introduction

In the U.S., the transportation sector is the most significant contributor to emissions based on CO_2 emissions, where over 94% of the fuels are primarily petroleum-based [1], and the transportation sector is the second largest energy consumer. It consumed around 28 quadrillion British thermal units (BTUs) in 2019 [2]. The rising global temperatures drive the industry to find alternative fuels significantly beneficial in combating global warming and adhering to stricter emission regulations locally in the U.S. by the U.S. Environmental Protection Agency (EPA) and worldwide. Alternative fuels being thoroughly researched are biofuels produced from renewable sources. These include biomatter, which popularly consists of organic waste, which helps mitigate the production of CO_2 emitted from many sources [3].

For a biofuel, DME is a second-generational biofuel with an LHV of 28.43 MJ/kg, [4] and is the simplest ether, which contains no carbon-to-carbon bonds in its chemical structure. DME is also non-toxic, non-carcinogenic, non-teratogenic, and non-mutagenic. This results in engines utilizing a higher exhaust gas recirculation (EGR) rate to reduce NOx further [5]. Also, its lower autoignition temperature (508 K) allows it to operate at lower temperatures to reduce NOx in systems further, enabling the extra utilization of EGR in some compression ignition (CI) engines.

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Other studies on ignition delay times of DME/propane at 60-80 bar pressures conducted at UCF showed that state-of-the-art chemical kinetic mechanisms for DME/propane chemical kinetics needs to be improved for accurate IDT predictions [6, 7]. Hence, in this work, we extend this pressure range to 110 bar to check the validity of these chemical kinetic models.

III. Experimental Procedure

The study occurred at the University of Central Florida's High-Pressure Extended Range Shock Tube for Advanced Research (HiPER-STAR) facility. [8, 9]. The shock tube is an excellent tool for creating high-pressure environments using shock waves, and it has been instrumental in combustion studies since the 1940s [10]. The HiPER-STAR shock tube can withstand pressures up to 1000 atm, allowing for safe experimentation at post-combustion pressures exceeding 900 bar for previous IDT experiments. The experiments involved achieving State 5 conditions by rupturing aluminum diaphragms and calculating the shock conditions using normal shock equations. Measurements were taken in the test section located 1 cm from the end wall. Piezoelectric dynamic pressure transducers were used to record pressure traces, and the shock velocity was determined using time interval counters triggered by the arrival of the incident shock at each pressure transducer. The shock tube is separated into two sections by an aluminum diaphragm, as seen in Figure 1. The inert gas flows into the high-pressure driven side, causing the diaphragm to burst and create a shock wave. State 1 consists of the low-pressure driven side with the test mixture (Mix 1). This study involves recording ignition delay times (IDT). The IDT is the time between the departure of the reflected shock until ignition, which was defined as the time of peak hydroxyl radicals (OH*) measured by a Newport 2032 photodetector with an Edmund Optics 306 nm narrow bandpass filter.

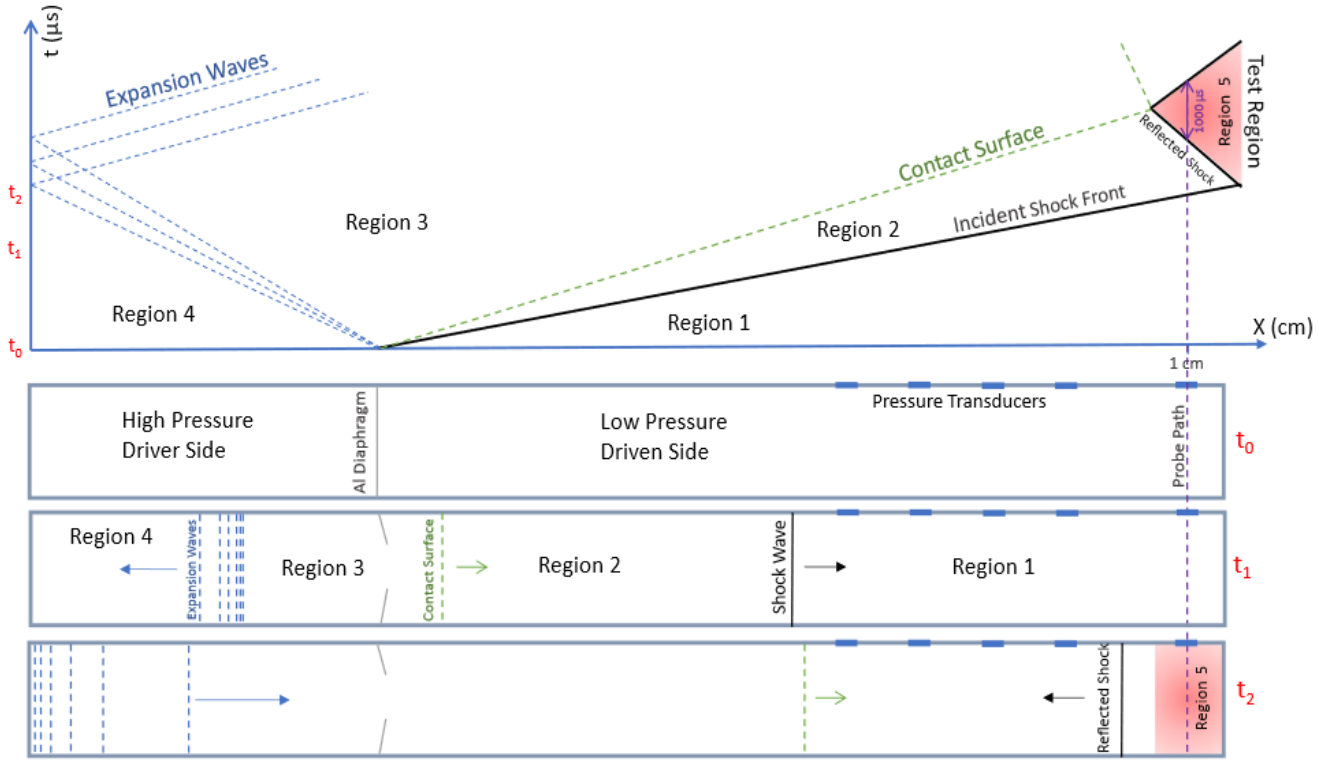

Figure 1: Shock tube x-t Diagram

Mixture details are available in Table 1 for the blend of DME/propane diluted in AR by 75%. Mixtures were combusted at stoichiometric conditions ($\varphi = 1$). Argon is an excellent inert gas that limits combustion pressures, as exceeding 1000 atm pressure peaks can damage equipment. The simulations were run using Chemkin–Pro [11] by using OH* as the IDT indicator. This mixture was prepared in a high-pressure tank using neodymium nickel-coated magnetic stirrers that mix the gas, ensuring gas homogeneity and separation from the shock tube. Initially, 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 ensured no impurities in the shock tube before the experimental mixture was introduced.

Table 1: Mixture information for neat DME/C_3H_8 and the blend of DME and C_3H_8.

Mixture #	Mixture	φ	C_3H_8	CH_3OCH_3	O_2	N_2	AR	P_5 (bar)
1	DME/Propane	1	0.002243	0.01271	0.04935	0.18568	0.75	110

From utilizing the software Ansys Chemkin-Pro [11], a sensitivity analysis was conducted. This allows a quantitative understanding of how the solution depends on various parameters. This allows for identifying important elementary reactions within DME/propane combustion. The sensitivity analysis conducted is an A-factor sensitivity analysis where the A-Factor from the modified Arrhenius Rate Equation is altered and how it influences the species for which the sensitivity analysis was conducted. For IDTs, OH* is used for sensitivity analysis because of its significant influence on IDTs. Equation 1 is the modified Arrhenius equation where the rate constants for all the single-step reactions are determined. The rate constant is k; A is the pre-exponential factor; E is the activation energy; β is the temperature coefficient; R is the gas constant, and T is the temperature. Equation 2 represents the sensitivity analysis equation dependent on the rate of mole fraction change as a function of time dependent on the rate fraction. This is done for each single-step reaction about the production or consumption of X. Afterwards, when the species is half consumed, the sensitivity coefficients are normalized, as shown in equation 3.

$$k = AT^{\beta} e^{-E/(RT)} \qquad \textit{Equation 1}$$

$$S = \left(\frac{dX(t)}{dk_i}\right)\left(\frac{k_i}{X(t)}\right) \qquad \textit{Equation 2}$$

$$S_N = \left(\frac{S_i}{S_{max}}\right) \qquad \textit{Equation 3}$$

IV. Results and Discussion

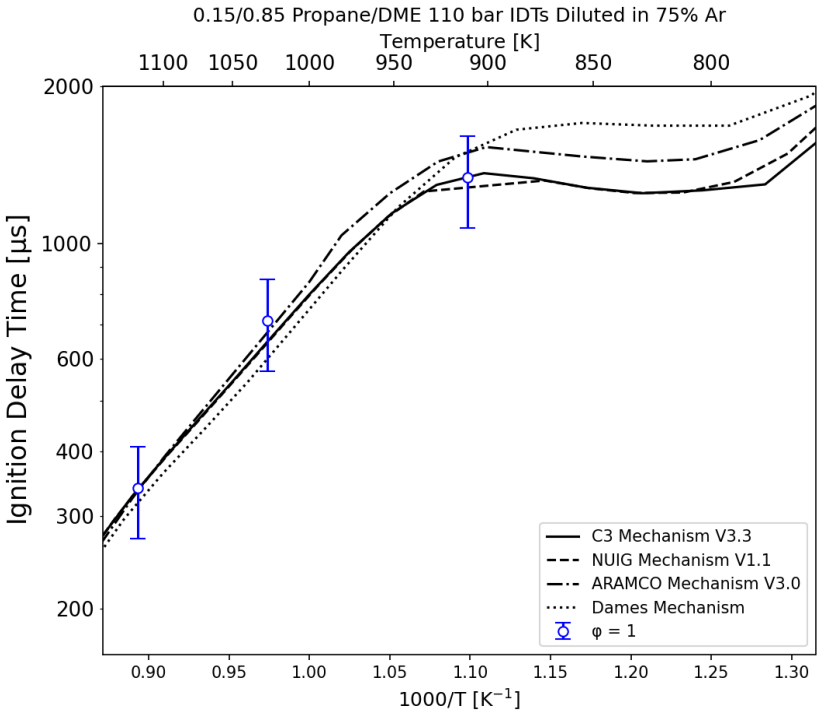

Figure 2: Comparison of models for Mix 1 at Φ = 1 for 110 bar

In Figure 2, simulations were conducted using the C3 Mechanism V3.3 [12], NUIG V1.1 [13], Aramco [14], and Dames et al. [15] for mixture one from Table 1 for a temperature range of 730 K to 1300 K. During the NTC region, discrepancies can be seen between the four chemistry model predictions of neat DME. NUIG V1.1 and C3 V3.3 align well with each other. Dames et al. predict the NTC region to occur faster, while according to ARAMCO V3.0, the NTC is between Dames et al. and NUIG V1.1. The temperature range of the NTC for the models is 730 K to 950 K for all models. Deviations can be seen at lower temperatures, and all the models converge as temperatures increase. Experimental IDTs were conducted from 900 to 1150 K. At these experimental IDTs. All models can predict IDTs within the uncertainty. The experimental data follows a linear trend, and the lowest temperature conducted, around 900 K, was at the end of the NTC region predicted by the four chemical kinetic models.

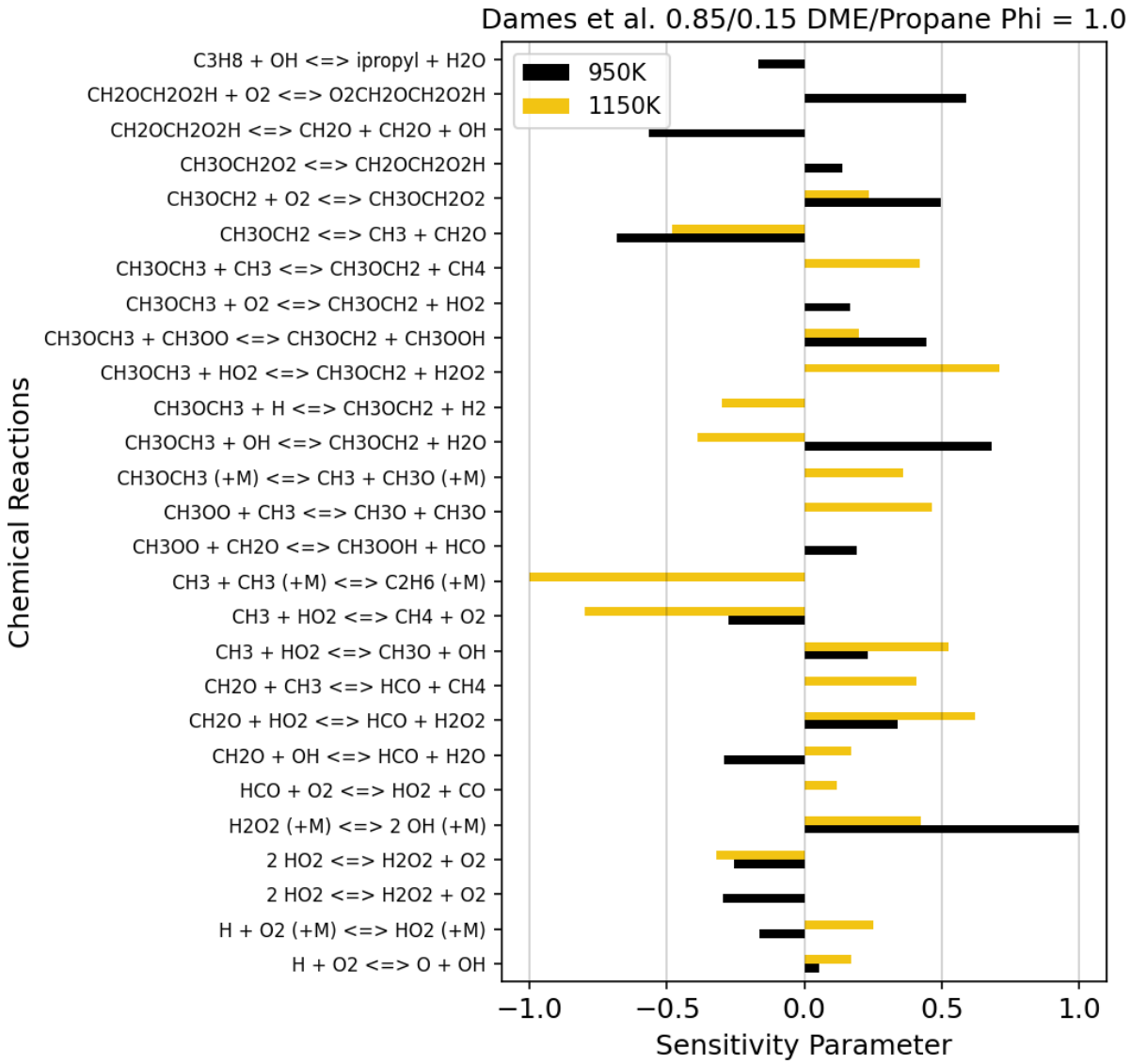

Figure 3: Sensitivity Analysis was conducted for Mix 1 at 950 and 1150 K temperatures.

Utilizing Chemkin-Pro [11], a sensitivity analysis was conducted at 110 bar via A-factor sensitivity as seen from Figure 3. The most sensitive terminating reaction for 1150 K is R65 in the Dames et al. mechanism, which is also a pressure-dependent reaction. Following R65 for 1150 K is R64, and for 950K, R363 is the most sensitive terminating reaction from the OH sensitivity analysis. The most prominent propagating reaction is R24, a pressure-dependent reaction of hydrogen peroxide decomposing into two radicals. For 1150 K, R356 has the highest sensitivity parameter and is an H abstraction reaction from DME to produce hydrogen peroxide and CH_3OCH_2. A summary of reactions can be found in Table 2.

Table 2: Reaction index and chemical reactions

Reaction Index	Chemical Reaction
R65	$CH_3 + CH_3 (+M) <=> C_2H_6 (+M)$
R64	$CH_3 + HO_2 <=> CH_4 + O_2$
R363	$CH_3OCH_3 + OH <=> CH_3OCH2 + H_2O$
R24	$H_2O_2 (+M) <=> 2\ OH (+M)$
R356	$CH_3OCH_3 + HO_2 <=> CH_3OCH_2 + H_2O_2$

V. Summary

As energy demand and global temperatures are rising, there is a need for alternate, more environmentally friendly fuels. DME is a more environmentally friendly biofuel that can be blended with a high energy content fuel (like C_3H_8). Due to the need for autoignition data for DME/C_3H_8 in the literature on engine-relevant conditions of heavy-duty MCCI engines, we gathered IDTs for DME/propane blends at 110 bar and compared them with literature models. All literature models can predict the experimental IDTs within uncertainty for the studied mixture (Mix 1). A sensitivity analysis was then conducted for two temperature points where significant elementary reactions were summarized for Mix 1.

Acknowledgments

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