



An ignition delay and kinetic modeling study of methane, dimethyl ether, and their mixtures at high pressures



Ultan Burke^a, Kieran P. Somers^a, Peter O'Toole^a, Chis M. Zinner^c, Nicolas Marquet^c, Gilles Bourque^b, Eric L. Petersen^c, Wayne K. Metcalfe^a, Zeynep Serinyel^a, Henry J. Curran^{a,*}

^a Combustion Chemistry Centre, NUI Galway, Ireland

^b Rolls-Royce Canada, Montreal, QC H8T 1A2, Canada

^c Department of Mechanical Engineering, Texas A&M University, College Station, TX, USA

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ABSTRACT

The development of accurate chemical kinetic models capable of predicting the combustion of methane and dimethyl ether in common combustion environments such as compression ignition engines and gas turbines is important as it provides valuable data and understanding of these fuels under conditions that are difficult and expensive to study in the real combustors. In *this work*, both experimental and chemical kinetic model-predicted ignition delay time data are provided covering a range of conditions relevant to gas turbine environments ($T = 600\text{--}1600\text{ K}$, $p = 7\text{--}41\text{ atm}$, $\phi = 0.3, 0.5, 1.0, \text{ and } 2.0$ in 'air' mixtures). The detailed chemical kinetic model (Mech_56.54) is capable of accurately predicting this wide range of data, and it is the first mechanism to incorporate high-level rate constant measurements and calculations where available for the reactions of DME. This mechanism is also the first to apply a pressure-dependent treatment to the low-temperature reactions of DME. It has been validated using available literature data including flow reactor, jet-stirred reactor, shock-tube ignition delay times, shock-tube speciation, flame speed, and flame speciation data. New ignition delay time measurements are presented for methane, dimethyl ether, and their mixtures; these data were obtained using three different shock tubes and a rapid compression machine. In addition to the DME/CH₄ blends, high-pressure data for pure DME and pure methane were also obtained. Where possible, the new data were compared with existing data from the literature, with good agreement.

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1. Introduction

The depletion of crude oil resources has motivated the search for alternative energy sources. Currently, the combustion of hydrocarbons remains the biggest producer of energy throughout the world, and in the short- to medium-term will remain so. However, the combustion of fossil fuels has contributed to global warming and increased levels of pollution. Biofuels can be produced from renewable sources and can reduce undesirable emissions associated with conventional fossil fuels. Methane (CH₄), which is the predominant component of natural gas, is a relatively clean-burning fossil fuel and can be considered a renewable energy source when produced as biomethane via anaerobic digestion of biomass [1]. Dimethyl ether (DME) is also considered a second generation

biofuel as it can be produced from biomass. It is more commonly produced in a two-step process, where syngas is converted to methanol which can then be used to generate DME through a dehydration reaction [2]. Semelsburger et al. [3] found that DME ranks highly as an alternative fuel for the future.

It is for these reasons that a large number of studies have been performed on the combustion of these fuels. Due to its high cetane number (55), DME is considered a good alternative to diesel. DME has been studied experimentally in diesel engines [4–7] showing its advantages in terms of emissions and engine efficiency. Particulate matter (PM) emissions were found to be greatly reduced, as were NO_x and SO_x, while there was a slight increase in carbon monoxide (CO) and hydrocarbon (HC) emissions.

Methane is the main component of natural gas and is commonly burned in gas turbines. Due to DME's excellent auto-ignition characteristics, it has been used as an additive or alternative to natural gas in gas turbines [8,9], leading to interest in the combustion kinetics of mixtures of these two fuels. Mixtures of methane and DME have also been studied within homogeneous

* Corresponding author. Address: Combustion Chemistry Centre, School of Chemistry, NUI Galway, Ireland.

E-mail address: henry.curran@nuigalway.ie (H.J. Curran).

URL: <http://c3.nuigalway.ie/> (H.J. Curran).

charge compression ignition (HCCI) engines [10,11], where DME was found to be an excellent ignition improver. Several flame speed studies have been conducted on DME [12–17] using a variety of different methods such as constant-volume bomb using optical observation of the flame and counterflow flames; in some devices, particle image velocimetry has been utilized to determine the laminar flame speed from the observed gas velocities.

Species profiles were first measured by Dagaut et al. [18] in a jet-stirred reactor (JSR) using fuel mixtures highly diluted in argon, for equivalence ratios from 0.2 to 1.0, at a pressure of 10 atm, and in the temperature range 550–1100 K. Subsequently, flow-reactor data were taken by Fischer et al. [19] (1118 K, 3.5 atm, and 1085 K, 1 atm, $\phi = 0.32$ –3.40) and Curran et al. [20] (550–850 K, 12–18 atm, $\phi = 0.7$ –4.2). These studies [19,20] also developed a detailed chemical kinetic mechanism to simulate their experimental data, using it to identify the important reaction pathways controlling DME fuel oxidation. This mechanism was also used to simulate JSR data [18] and shock-tube ignition delay times.

Zhao et al. [21] used Rice–Ramsperger–Kassel–Marcus (RRKM)/master equation calculations to calculate rate constants for the unimolecular decomposition of DME as a function of temperature and pressure. Their study also reported flow reactor data at 980 K and 10 atm as a function of residence time. A chemical kinetic model was validated using experimental data which included flow reactor, JSR, shock tube ignition delays, laminar flame speciation and flame speed measurements. Wang et al. [22] and Cool et al. [23] used electron–ionization molecular-beam mass spectrometry and photoionization molecular-beam mass spectrometry performed using synchrotron radiation for the analysis of a stabilized flat flame to provide species profiles within DME flames.

Cook et al. [24] used laser absorption of OH radicals behind reflected shock waves to isolate and measure the rate constants of the decomposition of DME and the rate constant for H-atom abstraction from DME by OH radicals at high temperatures. These measurements were coupled with RRKM/master equation calculations which agreed well with the measurements. Recently, Pyun et al. [25] measured species profiles for CO, CH₄, and C₂H₄, during the pyrolysis of DME within a shock tube using tunable laser absorption with a quantum cascade laser. This laser absorption study was done at a range of reflected-shock temperatures (1300–1600 K) and at a reflected-shock pressure of 1.5 atm.

Previous ignition delay time studies of these fuels and their mixtures are summarized in Tables 1 and 2. These studies cover a wide range of conditions including low-to-high temperatures and pressures. Of these previous ignition delay time studies [26–37], only the work of Tang et al. [37] included mixtures of CH₄ and DME. It covered dilute mixtures within a pressure range of 1–10 atm. The current study covers a wider range of temperatures and pressures and includes fuel in ‘air’ mixtures.

Recent experimental studies of DME combustion also include a flame speed and flame speciation study by Liu et al. [38]. The effect of diluting DME flames with 20% CO₂ was studied, and flame speeds over a range of pressures were reported. Flame speciation

Table 1
CH₄ ignition delay time studies from the literature.

Instrument	Mixture	<i>p</i> (atm)	<i>T</i> (K)	Year	Reference
Review				1994	[26]
Shock tube	Dilute in Ar	3–300	1800	1974	[27]
Shock tube	Dilute in Ar	9–480	1410–2040	1996	[28]
Shock tube	Fuel-rich	35–260	1040–1600	1999	[29,30]
RCM	‘Air’	13–16	980–1060	2001	[31]
Shock tube	Fuel-lean	3–450	1200–1700	2003	[32]
Shock tube	‘Air’	16–40	1000–1350	2004	[33]

Table 2
Summary of DME ignition delay time studies from the literature.

Instrument	Mixture	<i>p</i> (atm)	<i>T</i> (K)	Year	Reference
RCM	‘Air’	9.87–19.74	615–735	2008	[34]
Shock tube	‘Air’	12.83–39.48	662–1266	1996	[35]
Shock tube	Dilute in Ar	1.58–6.51	1175–1900	2009	[36]
Shock tube	Dilute in Ar	1.00–9.87	1134–2105	2012	[37]

using electron–ionization molecular-beam mass spectrometry was measured. Guo et al. [39] measured low temperature species profiles in an atmospheric flow reactor with electron–ionization molecular-beam mass spectrometry used as the detection system. Herrmann et al. [40] used an atmospheric flow reactor to measure mole fractions of species related to DME oxidation at low temperatures (400–1200 K) by time-of-flight mass spectrometry. Both of these studies compared their measured data to models available in the literature.

In *this study*, we provide new ignition delay time data for these two important fuels over wide regimes of temperature and pressure at engine- and turbine-relevant conditions. We have developed a detailed chemical kinetic mechanism (Mech_56.54) based on the widely validated mechanism AramcoMech1.3 [41], which is capable of predicting these new ignition delay data and available literature data. Presented first is an overview of the experiments, including details on the mixtures studied, the facilities, the measurement techniques, and modeling approaches. The experimental section is followed by a summary of the chemical kinetic mechanism and the reaction rates that were modified for the present study. A results and discussion section comprises the bulk of this paper and presents all of the ignition delay time data as well as comparisons to the kinetic mechanism. Sensitivity analyses and relevant discussions on the observed trends are also provided.

2. Experimental

A common set of mixtures was selected for study in both the rapid compression machine (RCM) and in the shock tubes, Table 3.

For the experiments at NUIG, methane and DME gases were obtained from Sigma–Aldrich at $\geq 99.0\%$ and $\geq 99.9\%$ purity respectively, while all other gases were supplied by BOC Ireland; nitrogen (CP Grade) $\geq 99.95\%$, argon (Research Grade) $\geq 99.9995\%$, oxygen (Medical Grade) $\geq 99.5\%$ and all were used without further purification. At TAMU, the DME was Grade 2.6 purity (99.6%), the methane was Grade 3.7 (99.97%), and both the O₂

Table 3
CH₄/DME mixture compositions (%molar volume) tested in the present study.

	Mix No.	% CH ₄	% CH ₃ OCH ₃	% O ₂	% Diluent	ϕ
100% CH ₄	1	3.055	0.000	20.367	76.578	0.3
	2	4.990	0.000	19.960	75.050	0.5
	3	9.506	0.000	19.011	71.483	1.0
	4	17.361	0.000	17.361	65.278	2.0
CH ₄ /DME 80%/20%	5	2.228	0.557	20.423	76.792	0.3
	6	3.646	0.911	20.051	75.392	0.5
	7	6.974	1.743	19.177	72.106	1.0
	8	12.829	3.207	17.640	66.324	2.0
CH ₄ /DME 60%/40%	9	1.535	1.024	20.471	76.970	0.3
	10	2.516	1.677	20.127	75.680	0.5
	11	4.829	3.220	19.317	72.634	1.0
	12	8.939	5.959	17.878	67.224	2.0
100% DME	13	0.000	2.058	20.576	77.366	0.3
	14	0.000	3.383	20.298	76.319	0.5
	15	0.000	6.545	19.634	73.821	1.0
	16	0.000	12.285	18.428	69.287	2.0

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