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A detailed combined experimental and theoretical study on dimethyl ether/propane blended oxidation

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ABSTRACT

In this paper, a binary fuel model for dimethyl ether (DME) and propane is developed, with a focus on engine-relevant conditions (10–50 atm and 550–2000 K). New rapid compression machine (RCM) data are obtained for the purpose of further validating the binary fuel model, identifying reactions important to low-temperature propane and DME oxidation, and understanding the ignition-promoting effect of DME on propane. It is found that the simulated RCM data for DME/propane mixtures is very sensitive to the rates of $C_3H_8 + OH$, which acts as a radical sink relative to DME oxidation, especially at high relative DME concentrations. New rate evaluations are conducted for the reactions of $C_3H_8 + OH = products$ as well as the self-reaction of methoxymethyl peroxy (in competition with $RO_2 = QOOH$ isomerization) of $2CH_3OCH_2O_2 = products$. Accurate phenomenological rate constants, $k(T, P)$, are computed by RRKM/ME methods (with energies obtained at the CCSD(T)-F12a/cc-pVTZ-F12 level of theory) for several radical intermediates relevant to DME. The model developed in this paper (120 species and 711 reactions) performs well against the experimental targets tested here and is suitable for use over a wide range of conditions. In addition, the reaction mechanism generator software RMG is used to explore cross-reactions between propane and DME radical intermediates. These cross-reactions did not have a significant effect on simulations of the conditions modeled in this paper, suggesting that kinetic models for high- and low-reactivity binary fuel mixtures may be assembled from addition of their corresponding submodels and a small molecule foundation model.

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1. Introduction

Dimethyl ether (DME, CH_3OCH_3) is widely known to be a good transportation fuel, in part because it can act as a drop-in replacement for diesel while reducing soot, carbon monoxide (CO), and unburned hydrocarbon emissions [1]. As a fuel additive to conventional fossil fuel in internal combustion engines, DME has the potential to greatly reduce particulate (soot) formation [2]. Fuel additives have been studied for their potential to control ignition timing of homogeneous-charge compression-ignition (HCCI) engines, stratified-charge compression-ignition (SCCI) engines, and reactivity-controlled compression-ignition (RCCI) engines. In combination with intelligent fuel mixture and composition design, these advanced engines offer the prospect of cleaner burning and higher thermal efficiencies [3–6]. Many of these future engines may rely on dual fuel systems or those with adjustable

concentrations of fuel additives that advance combustion [7]. However, these same engines will also rely more heavily on fundamental knowledge of the underlying combustion chemistry that drives the low-temperature autoignition of fuel mixtures with both high- and low-reactivity components.

The promoting effect of DME on fuels such as methane (CH_4) under conditions of both low- and high-temperature combustion has been studied in some detail [8,9]. Under high-temperature regimes, the rapid build-up of radicals formed from DME promotes methane ignition, as noted by Chen et al. [8]. Although there is a nonlinear ignition enhancement, the laminar flame speeds of DME/methane mixtures are linearly proportional to the DME fraction [8]. The ignition promoting effect of DME on high-octane fuels is of particular importance for controlling ignition timing in internal combustion engines. Fundamental kinetic studies of fuel blends and quantification of ignition enhancement may therefore be useful in modeling, optimizing, and ultimately developing more advanced and cleaner combustion engines.

Dual fuel combustion embodies a conceptually novel approach to internal combustion engine technology, relying on mixtures of

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Table 1

Recent experimental studies of DME combustion with their corresponding experimental conditions, including temperature, pressure, equivalence ratio (ϕ), diluent, and residence time (t_{res}). Adapted from Rodriguez et al. [19].

Type of experiment	Experimental conditions	Reference
Jet-stirred reactor	$T = 800\text{--}1300\text{ K}$; $P = 101\text{--}1013\text{ kPa}$; $\phi = 0.2\text{--}2$ in N_2 ; $t_{res} = 0.1\text{--}1\text{ s}$	Dagaut et al. 1996 [32]*
	$T = 550\text{--}1100\text{ K}$; $P = 1013\text{ kPa}$; $\phi = 0.2\text{--}1.0$ in N_2 ; $t_{res} = 1\text{ s}$	Dagaut et al. 1998 [21]*
	$T = 540\text{--}850\text{ K}$; $P = 101\text{ kPa}$; $\phi = 0.5\text{--}2$ in N_2 ; $t_{res} = 1.5\text{ s}$	Le Tan et al. 2015 [33]
	$T = 550\text{--}1100\text{ K}$; $P = 107\text{ kPa}$; $\phi = 0.25\text{--}2$ in He, $t_{res} = 2\text{ s}$	Rodriguez et al. 2015 [19]†
Plug flow reactor	$T = 600\text{--}1500\text{ K}$; $P = 101\text{ kPa}$; $\phi = 0.01\text{--}\infty$ in air	Alzueta et al. 1999 [34]
	$T = 1080\text{--}1086\text{ K}$; $P = 101\text{ kPa}$; $\phi = 0.5$ in N_2 ; $t_{res} = 0.1\text{ s}$	Fischer et al. 2000 [17]
	$T = 550\text{--}855\text{ K}$; $P = 1216\text{--}1825\text{ kPa}$; $\phi = 0.7\text{--}4.2$ in N_2 ; $t_{res} = 1.8\text{ s}$	Curran et al. 2000 [18]
	$T = 513\text{--}973\text{ K}$; $P = 101\text{ kPa}$; 340 ppm in 10% O_2 ; $t_{res} = 2\text{--}4\text{ s}$	Liu et al. 2001 [35]
	$T = 490\text{--}750\text{ K}$; $P = 101\text{ kPa}$; $\phi = 0.6$ in He; $t_{res} = 107\text{ s}$	Guo et al. 2013 [36]
	$T = 500\text{--}1200\text{ K}$; $P = 101\text{ kPa}$; $\phi = 0.8\text{--}1.2$ in Ar	Herrmann et al. 2013, 2014 [37][38]
	$T = 739\text{--}902\text{ K}$; $P = 200\text{--}400\text{ kPa}$; $\phi = 0.225\text{--}0.675$ in N_2	Schönborn et al. 2014 [39]
	$T = 555\text{--}585\text{ K}$; $P = 101\text{ kPa}$; $\phi = 0.835$ in air	Wada et al. 2013 [40]
	$T = 500\text{--}1150\text{ K}$; $P = 101\text{ kPa}$; $\phi = 0.2\text{--}1.6$ in He/Ar; $t_{res} = 0.19\text{--}2\text{ s}$	Kurimoto et al. 2015 [41]
	$T = 500\text{--}1150\text{ K}$; $P = 101\text{ kPa}$; $\phi = 1$ in Ar; $t_{res} = 1.5\text{ s}$	Wang et al. 2015 [42]
Shock tube	$T = 650\text{--}1300\text{ K}$; $P = 1317\text{--}4053\text{ kPa}$; $\phi = 1$ in air	Pfahl et al. 1996 [22]*
	$T = 1200\text{--}1600\text{ K}$; $P = 350\text{ kPa}$; $\phi = 0.5\text{--}2$ in Ar	Dagaut et al. 1998 [21]*
	$T = 1175\text{--}1900\text{ K}$; $P = 161\text{--}666\text{ kPa}$; $\phi = 0.5\text{--}3$ in Ar	Cook et al. 2009 [43]*
	$T = 1134\text{--}2015\text{ K}$; $P = 101\text{--}1010\text{ kPa}$; $\phi = 1$ in Ar	Tang et al. 2012 [44]*
	$T = 1100\text{--}1500\text{ K}$; $P = 2000\text{ kPa}$; $\phi = 0.5\text{--}2$ in Ar	Hu et al. 2013 [29]†
	$T = 1200\text{--}1600\text{ K}$; $P = 120\text{--}530\text{ kPa}$; $\phi = 1$ in Ar	Hu et al. 2013 [29]
	$T = 697\text{--}1239\text{ K}$; $P = 2200\text{--}2300\text{ kPa}$; $\phi = 0.5\text{--}1.5$ in air/ N_2	Li et al. 2013 [23]†
	$T = 1300\text{--}1600\text{ K}$; $P = 152\text{ kPa}$; 0.5–2% DME in Ar	Pyun et al. 2013 [45]*
	$T = 900\text{--}1700\text{ K}$; $P = 122\text{--}1013\text{ kPa}$; $\phi = 0.5\text{--}2$ in H_2 /Ar	Pan et al. 2014 [46]*
	$T = 400\text{--}1160\text{ K}$; $P = 1111\text{--}3030\text{ kPa}$; $\phi = 0.3\text{--}2$ in air	Burke et al. 2015 [9]*
RCM	$T = 1000\text{--}1600\text{ K}$; $P = 122\text{--}2030\text{ kPa}$; $\phi = 0.5\text{--}2$ in Ar	Pan et al. 2015 [47]
	$T = 615\text{--}735\text{ K}$; $P = 1010\text{--}2010\text{ kPa}$; $\phi = 0.43\text{--}1.5$ in N_2	Mittal et al. 2008 [15]†
Burner	$T = 630\text{--}1250\text{ K}$; $P = 1111\text{--}3030\text{ kPa}$; $\phi = 0.3\text{--}2$ in air	Burke et al. 2015 [9]*
	premixed flame; $P = 4\text{ kPa}$; $\phi = 0.98\text{--}1.2$ in Ar	McIlroy et al. 2000 [48]
	premixed flame; $P = 101\text{ kPa}$; $\phi = 0.67\text{--}1.49$ in air	Kaiser et al. 2000 [49]
	premixed flame; $P = 2.67\text{--}4\text{ kPa}$; $\phi = 1.2\text{--}1.68$ in Ar	Cool et al. 2007 [50]
	premixed flame; $P = 4\text{ kPa}$; $\phi = 0.5\text{--}2$ in Ar	Wang et al. 2008 [51]
	premixed flame; $P = 4\text{ kPa}$; $\phi = 1$ in Ar	Xu et al. 2011 [52]
	premixed flame; $P = 5\text{ kPa}$; $\phi = 1.63$ in Ar/ CO_2	Liu et al. 2013 [12]*
Spherical bomb	Single jet-wall stagnation flame; $T = 298\text{ K}$; $P = 101\text{ kPa}$; $\phi = 0.7\text{--}1.7$ in air	Zhao et al. 2008 [20]
	Counterflow flame; $T = 298\text{ K}$; $P = 101\text{ kPa}$; $\phi = 0.7\text{--}1.7$ in air	Wang et al. 2009 [53]
	$T = 295\text{ K}$; $P = 100\text{ kPa}$; $\phi = 0.7\text{--}1.7$ in air	Daly et al. 2001 [54]
$T = 298\text{ K}$; $P = 200\text{--}1000\text{ kPa}$; $\phi = 0.6\text{--}1.7$ in air	Qin and Ju 2005 [55]	
$T = 298\text{ K}$; $P = 80\text{--}150\text{ kPa}$; $\phi = 0.7\text{--}1.8$ in air	Huang et al. 2007 [56]	
$T = 293\text{ K}$; $P = 97\text{ kPa}$; $\phi = 0.7\text{--}1.8$ in air	Chen et al. 2009 [57]	
$T = 298\text{ K}$; $P = 100\text{--}1000\text{ kPa}$; $\phi = 0.7\text{--}1.6$ in air	De Vries et al. 2011 [58]	

* See the Supplementary material for comparisons with the model of the present work.

† See main text for comparisons with the model of the present work.

high-octane fuels and high-cetane fuels as well as their synergistic combustion characteristics in order to achieve high thermal efficiencies. These engines can be made from retrofitted diesel engines with modified intake manifolds to allow for fuel vapor mixing into the engine piston. For example, recent work [4] has identified a mixture of 20% DME with 30% propane (by mass) in concert with diesel fuel combustion, resulting in over 50% brake thermal efficiency (BTE) in a modified rail diesel engine, compared to a baseline BTE of 37%. The authors found that propane substitution delayed DME's early autoignition and shifted the combustion process closer to top dead center [4]. In addition, DME has been investigated as an additive for ignition control in HCCI engines [1,7]. The combustion kinetics of fuel blends has also received wide attention in efforts to understand the oxidation and pyrolysis of primary reference fuels [10]. As a result, studies of DME combustion abound in the literature. Recent work (see Table 1) includes studies of premixed and non-premixed flames, homogeneous ignition experiments, and studies in homogeneous flow reactors.

The uncertainties in low-temperature (400–900 K) DME oxidation kinetics primarily involve the first and second O_2 additions (typically denoted $R + O_2 = RO_2$ and $QOOH + O_2 = O_2QOOH$, respectively) to radical derivatives of DME as well as the fate of

ketohydroperoxide, HO_2CH_2OCHO (hydroperoxymethylformate), all of which can serve to generate OH radicals, thereby promoting heat release and ignition. Tomlin et al. [11] have clearly illustrated the need for further work in this area by pointing out that several literature models such as [12–14] fail to accurately reproduce earlier rapid compression machine (RCM) ignition delay time measurements of DME [15]. In particular, Tomlin et al. [11] highlighted the need for accurate pressure-dependent descriptions for both first and second O_2 additions to DME radical derivatives and subsequent OH forming pathways. Thus, a number of more recent studies have been published that include detailed rate theory calculations for these reactions. Notably, Eskola et al. [16] performed a combined theoretical and experimental study for both first and second O_2 additions. The subsequent corresponding $CH_3OCH_2O_2$ (RO_2) = CH_2OCH_2OOH ($QOOH$) isomerization step is determined to be faster than those used in previous models [17,18], suggesting that the O_2 addition to $QOOH$ may play a more important role than previously thought [16]. The rate theory calculations performed by Eskola et al. [16] resulted in a total of nine phenomenological rates, including four well-skipping reactions. The rate of the $RO_2 = QOOH$ isomerization is near its high-pressure limit at 1 bar, while the rate of the important $QOOH$ decomposition to $2CH_2O + OH$ is at its high-pressure limit at 10 bar. Rodriguez et al. [19] also

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