



# Probing the low-temperature chemistry of ethanol via the addition of dimethyl ether

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## ARTICLE INFO

### Article history:

Received 24 August 2017

Revised 15 October 2017

Accepted 10 November 2017

### Keywords:

Ignition delay times

Ethanol

DME

Low-temperature chemistry

## ABSTRACT

Considering the importance of ethanol (EtOH) as an engine fuel and a key component of surrogate fuels, the further understanding of its auto-ignition and oxidation characteristics at engine-relevant conditions (high pressures and low temperatures) is still necessary. However, it remains difficult to measure ignition delay times for ethanol at temperatures below 850 K with currently available facilities including shock tube and rapid compression machine due to its low reactivity. Considering the success of our recent study of toluene oxidation under similar conditions [38], dimethyl ether (DME) has been selected as a radical initiator to explore the low-temperature reactivity of ethanol. In this study, ignition delay times of ethanol/DME/air mixtures with blending ratios of 100% EtOH, 70%/30% EtOH/DME and 50%/50% EtOH/DME mixtures were measured in a rapid compression machine and in two high-pressure shock tubes at conditions relevant to internal combustion engines (20–40 atm, 650–1250 K and equivalence ratios of 0.5–2.0). The influence of these conditions on the auto-ignition behavior of the mixture blends was systematically investigated. Our results indicate that, in the low temperature range (650–950 K), increasing the amount of DME in the fuel mixture significantly increases the reactivity of ethanol. At higher temperatures, however, there is almost no visible impact of the fuel mixture composition, whereas DME shows a lower reactivity. Furthermore, with the addition of DME, different kinetic regimes were observed experimentally: the reactivity is controlled by ethanol when the addition of DME is less than 30% while it is dominated by DME when the proportion of DME is over 50%. Literature mechanisms show reasonable agreement with the new experimental data for the 100% EtOH and the 70%/30% EtOH/DME mixtures but under-predict the reactivity of the 50%/50% EtOH/DME mixtures at temperatures below 850 K, suggesting that further refinement of the low-temperature chemistry of ethanol/DME is warranted. An updated binary fuel mechanism is therefore proposed by incorporating the latest experimental and/or theoretical work in the literature, as well as adding new reaction pathways. Results indicate that the proposed model is in satisfactory agreement with all of the mixtures investigated.

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## 1. Introduction

Ethanol and DME are considered to be promising transportation biofuels due to their sustainability [1–5] and low soot emissions [6–8] in internal combustion engines (ICEs). In order to determine its potential use in real internal combustion engines, it is important to investigate a priori how it will behave under practical engine relevant conditions. Ethanol also has an impact on the reactivity of surrogate fuels. Compared to mixtures made of pri-

mary reference fuels (PRF), *n*-heptane and iso-octane, ternary mixtures including ethanol present a reduced negative temperature coefficient (NTC) behavior at low temperature at a constant octane number. The reactivity is reduced at low temperatures (below 750 K) but increases at intermediate and high temperatures [9]. Thus, ethanol has previously been extensively studied under various range of conditions and facilities including flame speed measurements [10–16], ignition delay times measurements in shock tube [17–21] and rapid compression machines [21–23], species measurements in rapid compression facility [23], flow reactors [9,24–26] and jet-stirred reactors [27]. There is, however, limited experimental data with which to evaluate the auto-ignition behavior of ethanol under engine relevant conditions, namely at high

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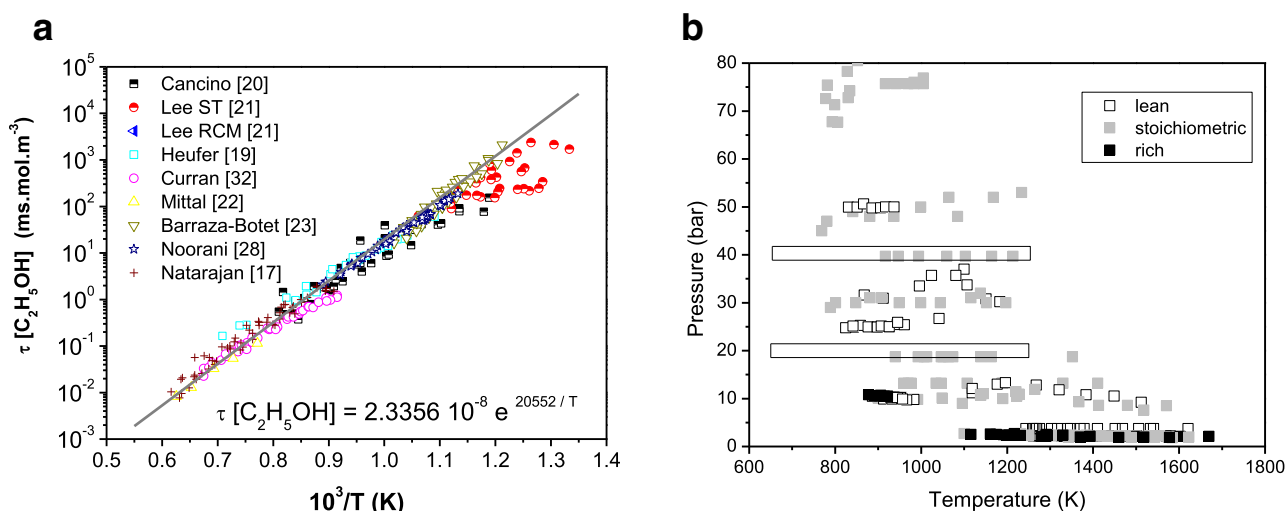


Fig. 1. Comparison of the available ignition delay time data (symbols) [17,19–23,28,32] with the experimental conditions presented in this study (boxes).

pressures and at intermediate to low temperatures (especially below 850 K) [22], since most of the experimental investigation has been performed at low pressure (below 5 bar) and at high temperatures (above 1000 K). Considering measurements performed at high pressures, Heufer and Olivier [19] measured the ignition delay times of the stoichiometric ethanol–air mixture at 13, 19 and 40 bar in the temperature range of 910–1410 K using a shock tube. Cancino et al. [20] investigated the ignition for lean ethanol–air mixture ( $\phi = 0.3$ ) at 30 bar between 860 K and 1180 K and for stoichiometric mixture over a pressure range of 10–50 bar with a temperature range of 800–1250 K in a shock tube. Lee et al. [21] performed a shock tube and RCM study of stoichiometric ethanol–air mixture under high pressure conditions (67–93 bar) in the intermediate temperature range (775–1000 K). Mittal et al. [22] investigated the auto-ignition behavior of lean ethanol–air mixture ( $\phi = 0.3$  and 0.5) in the intermediate temperature range (830–980 K) for a pressure range of 10–50 bar and of stoichiometric mixture at 10 bar and over limited temperature range (870–920 K). More recently, Barraza-Botet et al. [23] measured ignition delay times and species concentration for a diluted stoichiometric ethanol/ $O_2$  mixture in a rapid compression facility at temperature between 880 and 1120 K over a pressure range of 3–10 bar. Extended experimental work on ethanol ignition, including lean to rich mixtures, has been mainly performed at intermediate and high temperatures ( $>850$  K), low pressures ( $\leq 10$  atm) and at diluted conditions in shock tubes [17,28,29]. The available data are summarized in Fig. 1b. It appears that there is a lack of data at low temperatures ( $<850$  K) and at high pressures ( $>10$  atm). This lack of data limits the construction, validation and interpretation of chemical kinetic mechanism for the real combustor design. Such data are particularly important in assessing the influence of blending ethanol with practical fuels, in which the low reactivity of ethanol will inhibit the reactivity of a fuel at these low temperature conditions [30,31]. Moreover, Mittal et al. [22] revealed some discrepancies in the data available at low temperature ( $<910$  K) whereas there is a very good agreement at high temperature ( $>910$  K). However, some scatter appears at lower temperatures. The ignition delay times measured by Lee et al. [21] are shorter than expected. In their paper, Lee et al. scrutinized the ignition phenomenon using Schlieren imaging. They notice inhomogeneous ignition events with the occurrence of ignition kernels, leading to a pre-ignition pressure rise and associated pressure rise prior to ignition. Thus, the experiments cannot be considered as being at constant volume conditions. In order to use these pecu-

liar data for kinetic model validation, Lee et al. indicated that these non-ideal facility effects should be taken into account. Moreover, in RCMs, in the low temperature range, ignition delay times are slightly longer than expected as these are affected by heat transfer to the walls which lowers the temperature inside the combustion chamber and reduces the reactivity of the system.

Therefore, it is crucial to scrutinize the auto-ignition of ethanol at this low to intermediate temperature regime and provide reliable data in order to accurately predict the reactivity of ethanol which are of interest for internal combustion engine operation. The goal of the present study is to answer to this need and provide a comprehensive set of ignition delay times over a broad temperature range for fuel-lean to fuel-rich conditions and at high pressure.

The recent study from Barraza-Botet et al. [23] suggests that the accuracy of rate constants for ethanol +  $HO_2$  needs to be improved. This was confirmed by Olm et al. [33] who performed an optimization of an ethanol mechanism previously published by Saxena and Williams [15]. This also calls into question our understanding of the low temperature chemistry of ethanol.

Detailed chemical kinetics mechanisms have been proposed by several authors [11,15,20,21,25,27,34–36]. Dunphy et al. [34] validated a kinetic mechanism against ignition delay time measurements performed at low pressures (2–4.5 bar) and at high temperatures (1100–1500 K). Egolfopoulos et al. [11] proposed a mechanism tested under low pressure conditions (1 bar) including ignition delay times, species profiles measured in a flow reactor and laminar flame speeds. Marinov [35] validated his mechanism against a wide range of experimental conditions including laminar flame speeds, species profiles measured in a jet-stirred reactor and flow reactor and ignition delay times. Li et al. [25] studied the decomposition of ethanol in a flow reactor and proposed a rate constant for the decomposition reaction  $C_2H_5OH = C_2H_4 + H_2O$  in order to improve the mechanism previously developed by Marinov. Saxena and Williams [15] proposed a new mechanism validated at low pressures (1–4 bar) against flame speeds, ignition delay times and species profiles. Cancino et al. [20] built their mechanism based on that of Marinov and validated it against ignition delay times at high pressure conditions (10–50 bar) for fuel-lean and stoichiometric mixtures. Leplat et al. [27] derived their mechanism by combining the mechanism developed by Marinov [35] and GRI Mech [36]. They increased the pressure range to 10 bar by testing the mechanisms against species data measured in a jet-stirred reactor and flame speeds and reproduced these data with good agree-

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