



# An experimental chemical kinetic study of the oxidation of diethyl ether in a jet-stirred reactor and comprehensive modeling

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## ABSTRACT

The oxidation of diethyl ether was studied experimentally in a jet-stirred reactor. Fuel-lean, stoichiometric and fuel-rich mixtures were oxidized at a constant fuel mole fraction (1000 ppm), at temperatures ranging from 450 to 1250 K, pressures of 1 and 10 atm, and constant residence time (70 and 700 ms, respectively). In total, six mixtures were tested at both pressures. Mole fraction profiles were obtained using gas chromatography and Fourier transform infrared spectrometry. The fuel mole fraction profiles, as well as some reaction intermediate and product profiles indicated strong low-temperature chemistry at high pressure. On the other hand, at atmospheric pressure this behavior was observed to a very small extent and only with the lean and stoichiometric mixtures. These data were compared to modeling results using literature mechanisms for diethyl ether oxidation. None of these predicted low-temperature reactivity under present conditions. Therefore, a kinetic mechanism is proposed in this study, based on recently computed kinetic parameters from literature. It shows good performances for representing the present experimental data as well as experimental data found in literature consisting of ignition delay times, laminar flame speeds and flame structure.

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## 1. Introduction

Given the strict emission regulations for automotive sector and environmental concerns, there has recently been a growing need to find alternative feedstocks for the next generation biofuels. Diethyl ether (DEE) could represent an alternative fuel for compression ignition engines given its high cetane number ( $> 125$ ) and because it can be produced from bio-ethanol by dehydration.

Previous combustion related studies on diethyl ether include structure and burning velocity of laminar flames [1–3], ignition delay times [4] and pyrolysis/oxidation in a shock tube and jet-stirred reactor [5,6]. To the best of our knowledge, the earliest speciation study on DEE was reported in the 60s by Agnew and Agnew [7] in a stabilized flat flame for rich DEE/air mixtures at atmospheric pressure. They identified and quantified an important number of species among which the cyclic ether 2-methyl-1,3-dioxolane. Ya-

sunaga et al. [6] studied pyrolysis and oxidation of diethyl ether behind reflected shock waves, above 900 K. Tran and co-workers [2] reported species profiles in a rich premixed low-pressure flame as well as laminar burning velocities of DEE in a constant volume cylindrical chamber between 1 and 5 atm, and they have also studied the effect of blending DEE to n-butane flames and showed a decrease in soot precursor formation compared to a neat n-butane flame [3]. Vin et al. [5] studied pyrolysis of DEE in a jet-stirred reactor between 200–800 Torr and 600–1100 K. They observed complete destruction of the reactant at 1080 K for a residence time of 2 s and reported CO, methane, ethylene and acetaldehyde as major products. Werler and co-workers [4] measured ignition delay times of DEE in a shock tube (900–1300 K) and a rapid compression machine (500–1060 K) at high pressure. They observed two-stage ignition in RCM experiments. Laminar flame speed of DEE has also been studied by several groups [1,8,9]. There has been some recent theoretical investigations on the low-temperature chemistry of DEE by Sakai and co-workers [10,11], who computed thermochemistry and rate constants of the related species and reactions, and proposed a kinetic reaction mechanism.

This study investigates the oxidation of DEE in a jet-stirred reactor spanning an interval from low- to high-temperatures showing cool flame and negative temperature coefficient (NTC) be-

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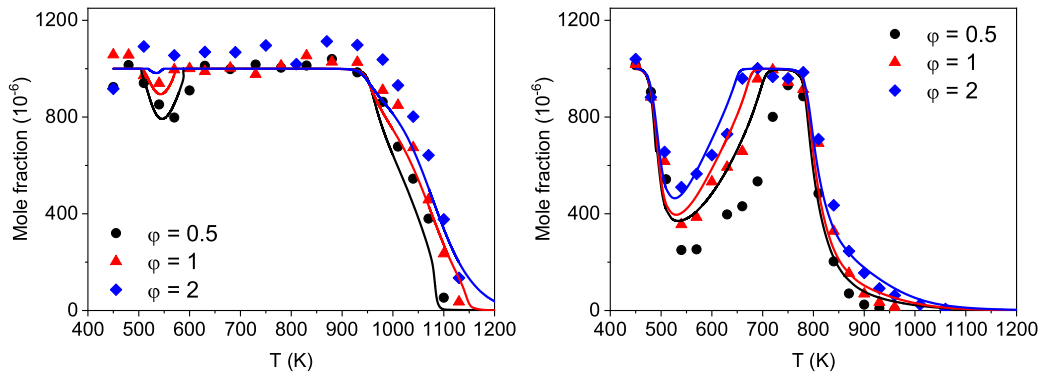


Fig. 1. DEE mole fraction evolution as a function of temperature, 1 atm (left), 10 atm (right), lines represent simulations.

behavior for all mixtures ( $\phi = 0.5, 1, 2$ ) at 10 atm. The experimental conditions chosen in this study are the same as in our dibutyl ether (DBE) experiments, previously reported [12]. Unlike the unconventional “double-NTC” behavior observed in DBE, DEE shows a conventional but very strong cool flame and NTC behavior, a comparison will be presented in coming sections.

## 2. Jet-stirred reactor experiments

Experiments were carried out in a fused silica jet-stirred reactor settled inside a stainless-steel pressure resistant jacket. An electrical oven enabled to perform experiments up to c.a. 1280 K. The temperature within the reactor was continuously monitored by a Pt/Pt-Rh thermocouple located inside a thin wall fused sil-

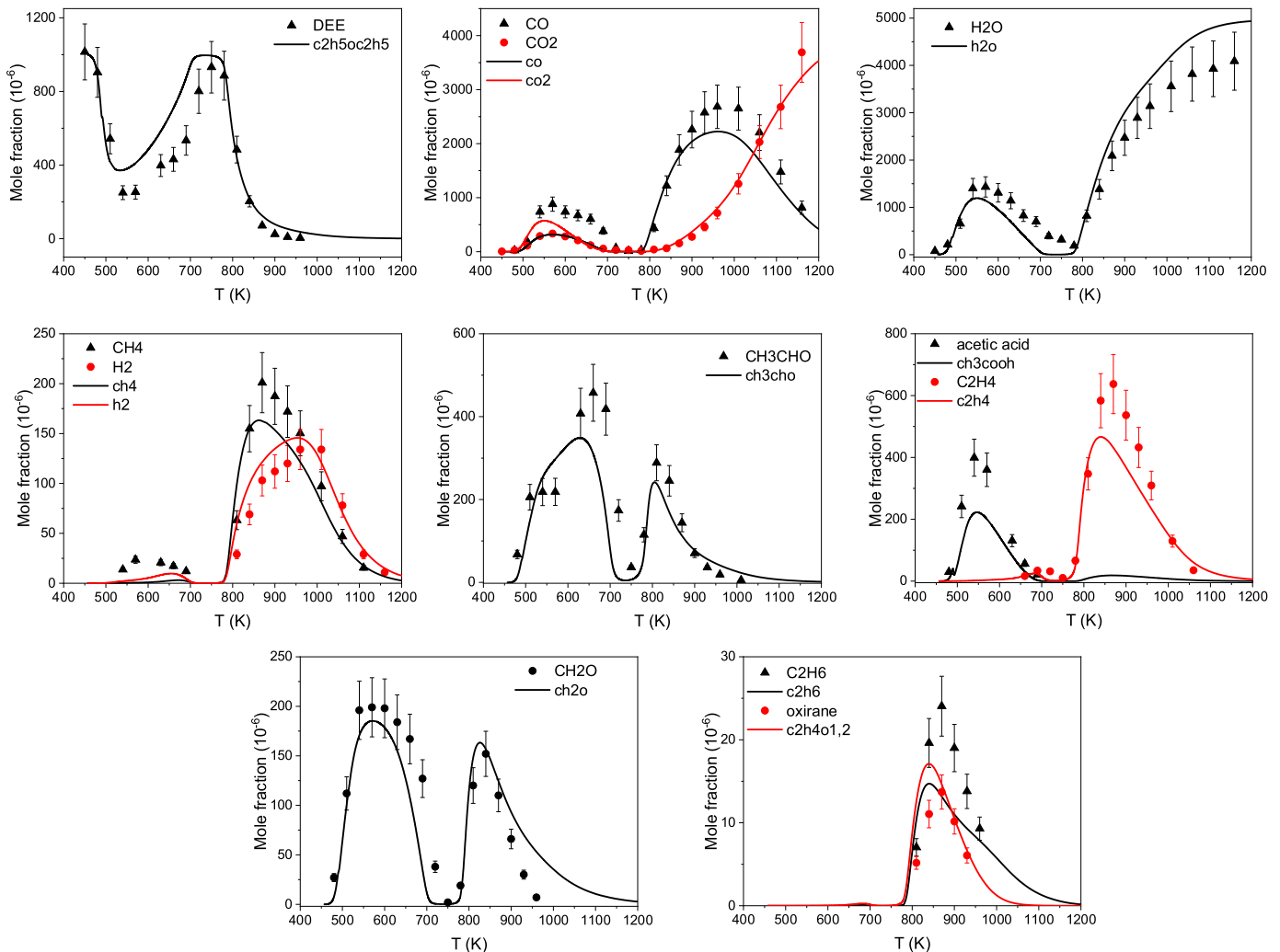


Fig. 2. Mole fraction profiles for the  $\phi = 0.5$  experiment at 10 atm, initial mole fraction of DEE: 1000 ppm,  $\tau = 0.7$  s.

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