



Counterflow flame experiments and chemical kinetic modeling of dimethyl ether/methane mixtures

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ABSTRACT

As advanced engines become more controlled by the fuel reactivity, it is important to have a complete understanding of combustion chemistry of fuel blends at both high and low temperatures. While the high-temperature chemistry coupling with transport and heat release can be examined through the use of flame experiments, low-temperature chemistry has been traditionally limited to homogeneous reactor experiments at fixed temperatures, which leaves the heat release rate unconstrained. In this study, the kinetic coupling between dimethyl ether and methane is examined by studying hot flames, cool flames, and ozone-assisted cool flames in a counterflow burner. At fixed fuel mass fraction, it is found that methane addition to dimethyl ether raises the hot flame extinction limit but lowers the cool flame extinction limit. Ozone addition to cool flames is seen to lead to a substantial increase in the extinction limit, but it also produces a decrease in sensitivity of the extinction limit to the fuel mass fraction.

The cool flame extinction measurements are then used to examine the uncertainties of reactions contributing significantly to the low-temperature heat release. The measurements indicate that the original kinetic model significantly overpredicts the cool flame extinction limits. However, by targeting the H-abstraction reaction of dimethyl ether by OH, among other reactions, an updated chemical kinetic model for dimethyl ether/methane mixtures is developed and validated. This study shows the value of the ozone-assisted counterflow cool flame platform in examining the key low-temperature reactions contributing to the heat release rate in cool flames.

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1. Introduction

Over the past decade, natural gas production has grown by more than 40%, most of which has been driven by newfound access to shale gas [1,2]. As a result, natural gas has become an increasingly inexpensive option for combustion applications. Power-generating gas turbines are already designed with natural gas in mind, but internal combustion (IC) engines are usually not. The use of natural gas in IC engines has produced mixed results. Methane (CH₄) is the main component of natural gas [3] and has characteristically poor ignition properties [4]. Moreover, since the amount of heavier hydrocarbons can vary dramatically [5], natural gas is an inconsistent fuel for ignition control in IC engines.

Dimethyl ether (DME) is produced from coal and biomass via syngas [6,7] and has been proposed as an alternative fuel for the

future [8,9]. Neat DME has been implemented successfully in IC engines [10,11], where it has been shown to produce lower soot emissions than diesel fuel [12]. Since methane displays significantly increased reactivity when blended with DME [13], mixtures of DME and CH₄ can also be used in IC engines [14]. Moreover, for advanced homogeneous charged compression ignition (HCCI) engines [14], it is primarily the chemical kinetics which controls the ignition timing and therefore the overall engine efficiency. Therefore, a detailed understanding of combustion chemistry is crucial for investigating whether DME/methane blends have potential for use in HCCI and other advanced engines.

Previous chemical kinetic studies of DME/CH₄ mixtures have focused on ignition [15,16] and high-temperature flames [13,17,18]. It was seen in [15] that the addition of a small amount of DME can sharply reduce the ignition delay times for methane at high temperatures. Burke et al. [16] performed DME/CH₄ ignition experiments in both shock tubes and rapid compression machines and constructed a detailed chemical kinetic model that included pressure-dependent low-temperature DME reactions.

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Chen et al. [13] measured ignition delay times and laminar flame speeds of DME/CH₄ blends. It was seen that DME addition to methane increases the laminar flame speed across all equivalence ratios. Measurements of laminar flame speed for DME/CH₄ mixtures have since been extended to elevated pressures [17] and considered the effects of preheating and dilution [18].

Real engines, however, are pushing more and more towards lower temperatures and near-limit conditions in order to decrease emissions while simultaneously increasing efficiency [19]. In near-limit flames, the extinction limit is governed by chemical kinetics coupled with transport and heat release [20]. However, to the authors' best knowledge, the extinction limits of DME/CH₄ blends have never been measured. Moreover, it was recently observed that an "experimental blind spot" [21] is present in the study of low-temperature oxidation in systems with strong coupling between chemistry, transport, and chemical heat release. Specifically, it was found that many chemical kinetic models are validated using highly diluted homogenous experiments such as flow reactors, jet-stirred reactors, and shock tubes. Cool flames, however, are inherently inhomogeneous and produce substantial amounts of heat release. Therefore, many low-temperature chemical kinetic models for DME (and DME/CH₄ blends) are capable of reproducing homogeneous reactor experiments but are unable to predict cool flame behavior accurately. However, the emergence of the counterflow cool flame platform [21–23] has enabled such experiments to be performed.

The present investigation studies the near-limit behavior of DME/CH₄ hot and cool diffusion flames in a counterflow burner. In particular, the impacts of DME/CH₄ blending and the reaction heat release rate on the extinction limits and flame structures of hot flames and cool flames are examined. Both ozone-less and ozone-assisted cool flames are studied. An updated chemical kinetic model is developed using the cool flame extinction measurements and kinetic data from the literature. The model especially targets the CH₃OCH₃ + OH = CH₃OCH₂ + H₂O reaction, which is one of the major reactions contributing to low-temperature heat release and is disproportionately important in cool flame extinction compared to homogeneous reactors. Due to the tendency for ozone to decompose into O radicals, the ozone-assisted cool flames possess additional sensitivity to the CH₃OCH₃ + O = CH₃OCH₂ + OH reaction. Validations of experimental data from the literature are presented next. The model is then used to understand how CH₄ addition can decrease the reactivity of DME at low temperatures.

2. Experimental and numerical setup

The experimental setup for this study is an atmospheric counterflow burner identical to the one in [22,24,25]. A schematic of the burner is shown in Fig. 1. A distance of 2.25 cm separates the upper and lower nozzles, both of which are 1.3 cm in diameter. The upper nozzle issues a mixture of dimethyl ether, methane, and nitrogen at 550 K. The temperature is held constant by PID control. The oxidizer stream begins as pure oxygen but then passes through an ozone generator (Ozone Solutions, TG-20) to form a mixture of O₂ and O₃. The molar percentage of ozone is dictated by the oxygen volumetric flow rate [22,23]. Although the cool flames produced are extremely dim, an ICCD camera (Princeton Instruments, PI-MAX 4) is able to capture them using the intensifier on the highest setting without any filters. The main chemiluminescence in the cool flame is excited formaldehyde (CH₂O*) [26].

In order to examine the detailed flame structure, temperature measurements are performed using a 254- μ m K-type thermocouple. The uncertainty in temperature is approximately ± 10 K. The thermocouple's position along the centerline of the burner is controlled by a stepper motor with an accuracy of 5 μ m per step. Centerline species profiles are also measured through micro-probe

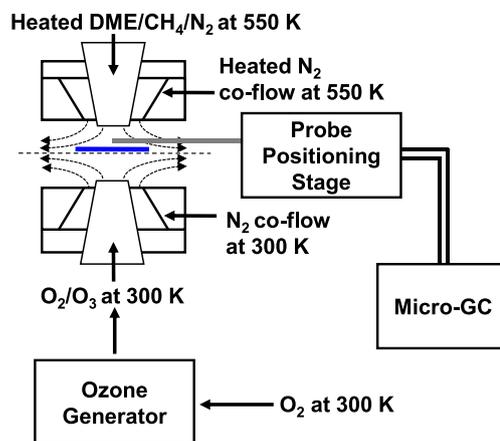


Fig. 1. Schematic of the counterflow burner setup, including the ozone generator and micro-GC.

sampling with a micro gas chromatography system (Inficon, 3000 micro-GC). The uncertainties in the species mole fractions are primarily due to the calibration of the GC and are estimated to be $\pm 5\%$ [22]. The micro-probe has an outer diameter of 630 μ m.

The numerical modeling in this study is centered upon the OPPDIF [27] module of the CHEMKIN package. To predict the extinction conditions numerically, the fuel-side N₂ dilution was increased at a constant strain rate. A slightly less diluted solution was used as a restart in OPPDIF. The value of the extinction strain rate using continuation methods with restarts (i.e., OPPDIF) is typically within less than 5 s⁻¹ of one determined using arc-length continuation methods [28], which is sufficient for the purposes of this study. Since the experiment showed some slight deviation from ideal plug flow conditions, radial velocity gradients of 20–40 s⁻¹ were imposed on the inlets [29]. Further details on the deviations from the plug flow assumption are presented in Section 3.3. For DME/CH₄ oxidation, a variety of DME chemical kinetic models (which naturally include a CH₄ sub-mechanism) are employed. These include the HP-Mech model [30] from Princeton University, the Burke model [16] from National University of Ireland Galway, the Dames model [31] from Massachusetts Institute of Technology, the UCSD model [32] from the University of California San Diego, the Wang model [33] from Bielefeld University, and the Zhao model [34] from Princeton University.

3. Results and discussion

3.1. Counterflow flame extinction experiments

The extinction strain rates (a_{Ext}) of DME/CH₄ mixtures have been measured experimentally for hot flames, ozone-assisted cool flames, and ozone-less cool flames (with the repeatability of the experiments typically being within ± 2 s⁻¹ for a_{Ext}). Figure 2 shows the results for hot flames. It is apparent that Fig. 2a and b shows opposing trends in that methane inhibits reactivity when blended with DME on a mole fraction basis but promotes reactivity on a mass fraction basis. The reason behind this is simple. DME is a larger molecule than CH₄ and therefore has a higher heat of combustion per mole (341 kcal/mol versus 213 kcal/mol). The difference in diffusivity between CH₄ and DME, moreover, is not large enough to make up this disparity (especially since the flame resides on the fuel side). However, CH₄ possesses a higher heat of combustion per gram (13.3 kcal/g versus 7.6 kcal/g) and therefore increases the extinction limit when substituted for DME on a mass basis. Figure 2c shows the fairly obvious scenario that replacing

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