

# An experimental and kinetic modeling study of methyl decanoate combustion

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## Abstract

Biodiesel is typically a mixture of long chain fatty acid methyl esters for use in compression ignition engines. Improving biofuel engine performance requires understanding its fundamental combustion properties and the pathways of combustion. This research study presents new combustion data for methyl decanoate in an opposed-flow diffusion flame. An improved detailed chemical kinetic model for methyl decanoate combustion is developed, which serves as the basis for deriving a skeletal mechanism via the direct relation graph method. The novel skeletal mechanism consists of 648 species and 2998 reactions. The skeletal mechanism reproduces the behavior of the fully detailed mechanism in plug flow and stirred reactors for temperatures of 900–1800 K, equivalence ratios of 0.25–2.0, and pressures of 101 and 1013 kPa. This mechanism well predicts the methyl decanoate opposed-flow diffusion flame data. The results from the flame simulations indicate that methyl decanoate is consumed via abstraction of hydrogen atoms to produce fuel radicals, which lead to the production of alkenes. The ester moiety in methyl decanoate leads to the formation of low molecular weight oxygenated compounds such as carbon monoxide, formaldehyde, and ketene.

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## 1. Introduction

Real biodiesel is a complex mixture of fatty acid methyl esters (FAME) with differing chain lengths and degrees of unsaturation, so it is much simpler to study the combustion chemistry of pure FAME. In order to simplify models and experiments, surrogate fuels with shorter chain lengths

are chosen for biodiesel combustion chemistry studies.

A number of studies have been conducted to study the combustion of methyl butanoate (MB), and some notable ones are Refs. [1–3]. Experimental and modeling studies have also been conducted on methyl *trans*-2-butenate (MC) [4,5] and ethyl propanoate [6,7]. The studies revealed that small esters are a good surrogate fuel for representing the thermochemistry of saturated long chain FAME, but they are not suitable surrogates for understanding the low temperature reactivity and autoignition properties of biodiesel. However,

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blends of *n*-heptane plus MB have been used to simulate combustion in engines [8,9].

Recently, the research focus has shifted to longer chain esters. Experimental and modeling studies of methyl hexanoate [10] and methyl heptanoate [11] in a jet stirred reactor (JSR) have been performed. Zhang et al. have presented motored engine experimental data of methyl heptanoate [12] and various C<sub>9</sub> FAME [13].

Dagaut et al. [14] studied the oxidation of rapeseed oil methyl ester (RME) in a JSR at various temperatures and pressures. A detailed chemical kinetic mechanism for *n*-hexadecane gave a good description of the RME experimental results, with a good agreement for RME reactivity and the relative importance of C<sub>2</sub>–C<sub>6</sub> alkenes.

Herbinet et al. [15] developed a detailed chemical kinetic mechanism for methyl decanoate (MD) consisting of 3012 species and 8820 reactions. The MD mechanism reproduces early CO<sub>2</sub> formation observed for RME in the JSR [14], a behavior that the *n*-hexadecane model by Dagaut et al. could not reproduce. The large size of this mechanism requires enormous computing resources when attempting to model combustion in some configurations (e.g., laminar flames).

Seshadri et al. used the direct relation graph (DRG) method to reduce the detailed mechanism to a skeletal mechanism consisting of 713 elementary reactions and 125 species [16]. The skeletal mechanism predicts experimental extinction and ignition of MD in an opposed-flow diffusion flame. Their results indicate that low temperature chemistry is of minor importance in an opposed-flow diffusion flame.

The existing detailed MD mechanism [15] and the skeletal mechanism [16] have not been validated against fundamental flame structure data for MD because such experiments have not been performed. This study presents new experimental temperature and species concentration profiles for an MD opposed-flow diffusion flame, and uses this data to validate an improved skeletal mechanism for MD combustion.

## 2. Experimental methods

A detailed explanation of the experimental opposed-flow diffusion flame and corresponding sampling setup has been described by Sarathy et al. [17]. A fuel mixture of 98.2% N<sub>2</sub> and 1.8% fuel (99% pure MD) is fed through the bottom port at a mass flux of 0.0142 g/cm<sup>2</sup> s, while an oxidizer mixture of 42.25% O<sub>2</sub> and 57.75% N<sub>2</sub> is fed through the top port at a mass flux of 0.0137 g/cm<sup>2</sup> s. At these plug flow conditions, the Reynolds Number is in the laminar flow regime (i.e.,  $Re < 400$ ), the flame is on the fuel side of the stagnation plane, and the fuel side strain rate is approximately 31 s<sup>-1</sup>. An ultrasonic atomizer

sprays the liquid fuel into a stream of N<sub>2</sub> gas. The temperatures of the gases exiting the top and bottom burner ports were 420 K and 400 K, respectively.

Analytical techniques used to measure the species in the sample included: non-dispersive infrared detection (NDIR) for CO and CO<sub>2</sub>; gas chromatography/flame ionization detection (GC/FID) with an HP-Alt/S PLOT column for C<sub>1</sub> to C<sub>5</sub> hydrocarbons; and GC/FID equipped with a methanizer (i.e., Ni catalyst) and Poraplot-U column for oxygenated hydrocarbons such as acetaldehyde/ethanol, formaldehyde, and acrolein. The Poraplot-U column separates the low molecular weight oxygenates and the methanizer converts the C–O bonds to C–H bonds for detection on the FID. The precision of species measurements is estimated to be ±15%. Temperature measurements were obtained using a 254 μm diameter wire R-type thermocouple (Pt–Pt/13% Rh) in an apparatus similar to that used by McEnally et al. [18]. The measured temperatures were corrected for radiation losses. This apparatus was unable to accurately measure temperatures on the oxidizer-rich side of the flame (i.e., 10.5 mm above the fuel port).

## 3. Computational methods

The kinetic modeling for MD oxidation in the opposed-flow diffusion flame was performed using the OPPDIF code within the CHEMKIN package [19]. The inputs to each simulation include a detailed chemical kinetic reaction mechanism, a dataset of thermochemical properties, and a dataset of transport properties.

The chemical kinetic mechanism developed here is an extension of the previously published detailed [15] and skeletal [16] mechanisms for MD. The large size of the detailed mechanism makes it impractical for use in the one-dimensional flame code (i.e., OPPDIF), and we found that the skeletal mechanism does not contain enough species and reactions to accurately predict many species concentration profiles in the opposed-flow diffusion flame to be studied in the following. Therefore, the present study develops an intermediate sized mechanism, which balances computational performance and chemical fidelity. First, several modifications were made to the detailed chemical kinetic mechanism to better predict MD combustion, and then this modified mechanism was reduced using the DRG method.

### 3.1. Detailed mechanism

Herbinet et al.'s detailed chemical kinetic mechanism [15] includes low temperature chemistry to simulate fuel ignition with NTC behavior, as well as intermediate and high temperature

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