



Ignition delay times of very-low-vapor-pressure biodiesel surrogates behind reflected shock waves



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HIGHLIGHTS

- The aerosol shock tube allows measurements of very-low-vapor-pressure fuels.
- Aerosol shock tube data compare favorably with that of a heated shock tube.
- Mechanisms generally predict ignition activation energy but not ignition delay time.
- Extra FAME components did not affect MO ignition delay times significantly.

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ABSTRACT

Ignition delay times for a variety of low-vapor-pressure biodiesel surrogates were measured behind reflected shock waves, using an aerosol shock tube. These fuels included methyl decanoate ($C_{11}H_{22}O_2$), methyl laurate ($C_{13}H_{26}O_2$), methyl myristate ($C_{15}H_{30}O_2$), methyl palmitate ($C_{17}H_{34}O_2$), and a methyl oleate ($C_{19}H_{36}O_2$)/Fatty Acid Methyl Ester (FAME) blend. Experiments were conducted in 4% oxygen/argon mixtures with the exception of methyl decanoate which was studied in 1% and 21% oxygen/argon blends. Reflected shock conditions covered initial temperatures from 1026 to 1388 K, pressures of 3.5 and 7.0 atm, and equivalence ratios from 0.3 to 1.4. Arrhenius expressions describing the experimental ignition delay time data are given and compared to those derived from applicable mechanisms available in the literature. Graphical comparisons between experimental data and mechanism predictions are also provided. Experiments of methyl laurate, methyl myristate, and methyl palmitate represent the first shock tube ignition delay time measurements for these fuels. Finally, experiments with methyl palmitate represent, to the authors' knowledge, the first neat fuel/oxidizer/diluent gas-phase shock tube experiments involving a fuel which is a waxy solid at room temperature.

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1. Introduction

In light of the finite supply of fossil fuels and recent concerns about the impact of combustion engine emissions, a search has begun for alternative energy resources. Such fuels would ideally have characteristics such as a high energy density, lower pollutant (hydrocarbon, soot, nitrogen oxide, etc.) emissions, the ability to be produced and refined geographically close to the location of consumption, and the ability to be consumed using currently existing infrastructure. With the possible exception of lower nitrogen oxide emissions, biodiesel fuel realizes all of these qualities and as such has become a leading candidate to blend with, supplement, or replace traditional fossil diesel fuel [1–4]. To facilitate such changes in fuel stock, a comprehensive understanding of biodiesel

oxidation chemistry is needed. One key component of such an understanding is a fuel's ignition delay time at elevated temperatures and pressures.

This study measured ignition delay times for several biodiesel surrogate molecules behind reflected shock waves using an aerosol shock tube. Biodiesel fuel is composed of Fatty Acid Methyl Esters (FAMES), and the actual fuel mixture has only five of such components: methyl palmitate (MP, $C_{17}H_{34}O_2$), methyl stearate (MS, $C_{19}H_{38}O_2$), methyl oleate (MO, $C_{19}H_{36}O_2$), methyl linoleate (ML, $C_{19}H_{34}O_2$), and methyl linolenate (MLN, $C_{19}H_{32}O_2$). Neat MO and ML were studied in another work [5]. MP and MS are fully saturated molecules, meaning they have no double bonds in their normal-alkane-like carbon chain; at room temperature they are waxy solids and normally they are found dissolved into the other three biodiesel components. Other saturated FAMES can be formed by varying the carbon chain length; three such molecules covered in this study are methyl decanoate (MD, $C_{11}H_{22}O_2$), methyl laurate

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(MLA, C₁₃H₂₆O₂), and methyl myristate (MM, C₁₅H₃₀O₂). Studying ignition delay times of smaller surrogate compounds can elucidate the chemistry of these molecules' larger counterparts.

2. Previous studies

2.1. Methyl decanoate

Of the surrogate fuels examined in this study, methyl decanoate (MD) has been the subject of the majority of research efforts to date. This is because its vapor pressure at 315 K (186 milliTorr) makes it experimentally accessible using traditional techniques [6]; its melting point is 260 K [7] (more fuel property information can be found in Table 1). Moreover, it is the largest component in cuphea biodiesel (65% by mass), hailed for its beneficial properties [8]. Previous studies of MD include microgravity experimentation [9–11], motored engine studies [12], pre- and non-pre-mixed flame examinations [13–18], pyrolysis studies [19], and jet-stirred reactor analyses [20,21]. Shock tube studies were performed by Wang and Oehlschlaeger, who worked at pressures of 15–16 atm in 21% O₂/N₂ mixtures with lean, stoichiometric, and rich equivalence ratios [22]; Haylett et al., who worked at a pressure of 8 atm in 21% O₂/Ar mixtures with very lean equivalence ratios [23]; and Li et al., who examined methyl decanoate autoignition at engine exhaust gas recirculation (EGR) conditions in air [24]. Other researchers have conducted modeling studies [25–32], and some of the experimental papers also include sections concerning mechanism development or reduction [10,13–15]. A summary of kinetic mechanisms designed for the fuels explored in this study is given in Table 2.

2.2. Methyl laurate

Methyl laurate (MLA) has been studied by far fewer researchers. Its vapor pressure at 315 K is 21 milliTorr [6] and its melting point is 278 K [7]. Vaughn et al. [9] and Marchese et al. [10] studied MLA droplets in microgravity environments, Schönborn et al. examined it in an engine study [4], and Herbinet et al. [29] developed a kinetic mechanism for this fuel using an automatic compilation program known as EXGAS.

2.3. Methyl myristate

Methyl myristate (MM) has also been relatively untouched in the literature. Its vapor pressure at 315 K is 3 milliTorr [6] and its melting point is 292 K [33]. One motored engine study [4] and one modeling study [29] have addressed this fuel.

2.4. Methyl palmitate

Despite being one of the five primary components of real biodiesel blends, to the authors' knowledge, methyl palmitate (MP) has been the subject of only two published experimental kinetic studies and two kinetic modeling studies. Its low vapor pressure (327 μTorr at 315 K) [6] and its high melting point (304 K) [33]

make it inaccessible to typical experimental techniques. Schönborn et al. studied MP in an engine using PID-controlled heaters to melt this waxy fuel [4], and Hakka et al. dissolved MP in *n*-decane (at a ratio of 26:74 mol:mol respectively) in order to examine it using a jet-stirred reactor [34]. The two modeling studies are Herbinet et al. [29] and Westbrook et al. [35]. (We also were made aware of another heated shock tube study by Wang et al. [36], currently under review, during the refereeing process for this manuscript.)

2.5. Methyl oleate

Methyl oleate (MO) has been the subject of multiple studies. Its vapor pressure at 315 K is 97 μTorr [6] and its melting point is 254 K [7]. Early work from the food industry is summarized by Porter et al. [37]. More recent work includes tubular reactor studies [38,39], cetane number determination work [40], microgravity experimentation [9,10], a motored engine study [4], a jet-stirred reactor analysis [41], an aerosol shock tube study [5], and kinetic modeling [35,42–44].

2.6. Summary of previous studies

The literature review above demonstrates that a solid base of research in the area of large biodiesel surrogates has been established. However, key pieces of information which are necessary to improve kinetic mechanism accuracy are still lacking. In the case of MD, shock tube studies at oxygen contents other than 21% are needed. For MLA, MM, and MP, no shock tube data is currently available. Finally, for MO, shock tube data demonstrating the effect of blending this methyl ester with other FAMES would be enlightening. The current study has sought to explore these research problems.

3. Experimental setup

3.1. Aerosol shock tube

Ignition delay times were measured behind reflected shocks in a second-generation aerosol shock tube. Details of this facility and the associated optical diagnostics are available elsewhere [5,23,45,46], so only a brief overview will be given here. The aerosol shock tube consists of a driver section filled with high-pressure helium separated by a polycarbonate diaphragm from a low-pressure bath gas mixture (1%, 4%, or 21% oxygen in argon; gas/fuel supplier and purity information can be found in Table 3). Nebulizers (Ocean Mist DK12NS) in a tank adjacent to the endwall with rotating fans produce a uniform mixture of fuel droplets and bath gas, and this mixture is introduced into the last 1.3 m of the shock tube via a sliding endwall gate valve. An incident shock wave, generated upon bursting of the diaphragm, propagates through the aerosol mixture and evaporates the droplets, producing a uniform gas-phase fuel–oxidizer–diluent mixture. The size of the droplets follows a log-normal distribution with an approximate 2.5 μm number median diameter as measured using a Malvern Spraytec Particle Sizer; this small size allows the droplets to evaporate

Table 1
Physical property information for the fuels investigated in this study [6,7].

Fuel	Molecular formula	Molecular weight (g/mol)	Vapor pressure (315 K) (Torr)	Melting point (1 atm) (K)
Methyl decanoate	C ₁₁ H ₂₂ O ₂	186.3	186 × 10 ⁻³	260
Methyl laurate	C ₁₃ H ₂₆ O ₂	214.3	21 × 10 ⁻³	278
Methyl myristate	C ₁₅ H ₃₀ O ₂	242.4	3 × 10 ⁻³	292
Methyl palmitate	C ₁₇ H ₃₄ O ₂	270.5	327 × 10 ⁻⁶	304
Methyl oleate	C ₁₉ H ₃₆ O ₂	296.5	97 × 10 ⁻⁶	254

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