



Scaling relation for high-temperature biodiesel surrogate ignition delay times



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HIGHLIGHTS

- A scaling relationship for high-temperature biodiesel ignition times is presented.
- Negative pressure, carbon chain length, and oxygen mole fraction scaling are seen.
- The equivalence ratio scaling depends on the oxygen mole fraction.
- The activation energy depends on the oxygen mole fraction and pressure.

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ABSTRACT

High-temperature Arrhenius ignition delay time correlations are useful for revealing the underlying parameter dependencies of combustion models, for simplifying and optimizing combustion mechanisms for use in engine simulations, for scaling experimental data to new conditions for comparison purposes, and for guiding in experimental design. We have developed a scaling relationship for Fatty Acid Methyl Ester (FAME) ignition time data taken at high temperatures in 4%O₂/Ar mixtures behind reflected shocks using an aerosol shock tube:

$$\tau_{\text{ign}} [\text{ms}] = 2.24 \times 10^{-6} [\text{ms}] (P [\text{atm}])^{-0.41} (\phi)^{0.30} (C_n)^{-0.61} \exp\left(\frac{37.1 [\text{kcal/mol}]}{\bar{R}_u [\text{kcal/mol K}] T [\text{K}]}\right)$$

Additionally, we have combined our ignition delay time data for methyl decanoate, methyl palmitate, methyl oleate, and methyl linoleate with other experimental results in the literature in order to derive fuel-specific oxygen-mole-fraction scaling parameters for these surrogates. In this article, we discuss the significance of the parameter values, compare our correlation to others found in the literature for different classes of fuels, and contrast the above expression's performance with correlations obtained using leading FAME kinetic models in 4%O₂/Ar mixtures.

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1. Introduction

Increasingly stringent regulations for heavy-duty diesel engine exhaust have led manufacturers to search for methods of reducing nitrogen oxide (NO_x) and particulate matter (PM) emissions [1–3]. Such techniques include Exhaust Gas Recirculation (EGR), in which a portion of the exhaust gases are combined with the pre-combustion fuel/air blend in order to decrease the oxygen content

of the mixture and hence reduce NO_x [4,5], and blending fossil diesel fuel with small fractions of biodiesel fuel, which can reduce PM [6–10]. However, these prevention techniques are complicated by the fact that EGR sometimes results in increased exhaust PM [4,5], and in some engines biodiesel has been linked with increased levels of tailpipe NO_x [6–12]. Thus, care must be taken in using EGR and biodiesel in conjunction [13]. This motivates a thorough understanding of biodiesel combustion in lower-oxygen-content (<21%) mixtures.

Shock tube ignition delay times are a critical component for developing and validating combustion models [14–17]. These models are used to evaluate fuel blends and design diesel engines [18–26]. High-temperature shock tube ignition delay time data can

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be summarized by correlations that serve to reveal the underlying dependence of ignition times on important parameters such as pressure or equivalence ratio [27]. Such correlations are useful for simplifying/optimizing combustion models for use in diesel engine Computational Fluid Dynamics (CFD) simulations, for scaling experimental data to new conditions for comparison purposes, and for guiding in experimental design [28–32]. Several authors have suggested high-temperature Arrhenius-like correlations for various fuels (normal alkanes, oxygenates, etc.), including those listed in References [27,33–46] (see also Table 1). Other more complex ignition delay time correlations have also been suggested that cover both high and low temperatures [47–49]. However, we are unaware of any such correlation for large biodiesel surrogates at high temperatures and low oxygen concentrations; this provides motivation for the present work.

2. Previous biodiesel ignition studies

Recently, our research group published two articles containing high-temperature ignition delay times measured in 1%, 4%, and 21% oxygen/argon mixtures behind reflected shock waves in an aerosol shock tube for a series of biodiesel surrogate molecules in the Fatty Acid Methyl Ester (FAME) family [51,52]. These fuels included methyl decanoate (MD, $C_{11}H_{22}O_2$; see Fig. 1), which was measured at 1% and 21% oxygen mole fractions, and methyl laurate (MLA, $C_{13}H_{26}O_2$), methyl myristate (MM, $C_{15}H_{30}O_2$), methyl palmitate (MP, $C_{17}H_{34}O_2$), methyl oleate (MO, $C_{19}H_{36}O_2$), and methyl linoleate (ML, $C_{19}H_{34}O_2$), which were measured in 4% oxygen mixtures. Importantly, the fact that these shock tube studies were performed at oxygen concentrations at or below 21% allows these experiments to serve as a proxy for EGR behavior. Our first goal in this work was to use these two data sets to develop an ignition delay time correlation for large FAMES in 4% O_2 /Ar mixtures that captures the effects of temperature T , pressure P , equivalence ratio ϕ , molecular size (carbon chain length) C_n , and, if necessary, hydrogen unsaturation (number of C=C double bonds) U_d . Moreover, our second ambition was to synthesize other FAME ignition delay data available in the literature [45,46,53–61] in order to develop scaling parameters for the dependence of ignition time on the mixture oxygen mole fraction x_{O_2} .

Before proceeding, we wish to note that other shock tube studies have specifically simulated EGR conditions by adding

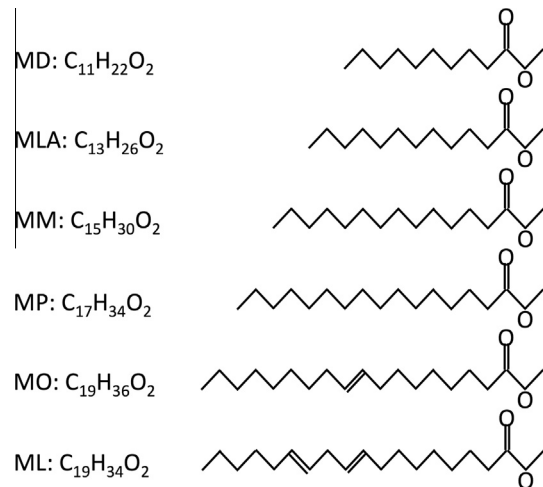


Fig. 1. Molecular diagrams for the FAMES examined in this work [51,52].

$CO_2/H_2O/O_2/N_2$ blends to the pre-shock mixture [48,56,62]. However, these works do not include experimentation at oxygen concentrations as low as used in our studies [51,52]. Also, it should be mentioned that many shock tube studies are performed with fuel/oxygen mixtures that are diluted in argon rather than in nitrogen [29]. The effects of the choice of diluent are well-understood and thus will not be considered here [63].

3. Experimental methods

Complete experimental details for our previous biodiesel studies can be found in References [51,52,64]; therefore, only a brief overview will be given here. All ignition delay shock-tests were conducted using the Stanford University Aerosol Shock Tube (AST). Experimental conditions are summarized in Table 2.

The AST uses a series of gate valves and pressure differentials to deliver a spatially uniform aerosol of micron-sized fuel droplets suspended in a carrier gas consisting of oxygen, argon, and fuel vapor into the last meter of the shock tube driven section. An incident shock wave, generated via strain-induced rupture of a diaphragm by high-pressure helium in the driver section, passes

Table 1
Select high-temperature ignition time correlations found in the literature. Controls: τ_{ign} : ignition delay time; [brackets]: concentration; \hat{R}_u : ideal gas constant; P : pressure; T : temperature, ρ : density; ϕ : equivalence ratio. The activation energy values (\hat{E}_A and B), the letter A , and the various lower-case letters (a, b, \dots, n, m) represent fitting parameters. Similar listings can be found in References [27,29,30].

Equation	Number	Fuel(s)	References
$\tau_{ign} = AP^a \phi^b C_n^c \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(1)	<i>n</i> -Pentane, <i>n</i> -Hexane, <i>n</i> -Octane, and <i>n</i> -Nonane	Davidson et al. [42]
$\tau_{ign} = AP^a \phi^b \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(2)	<i>i</i> -Octane	Burwell and Olson [33]
$\tau_{ign} = A[\text{fuel}]^f [O_2]^g [Ar]^h \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(3)	Methane, propane, and <i>n</i> -heptane	Burcat et al. [34,35,37]
$\tau_{ign} = \left(\frac{P}{R_u T}\right)^a \exp\left(A + \frac{B}{T}\right)$	(4)	<i>i</i> -Octane and <i>n</i> -heptane	Vermeer, Meyer and Oppenheim [36]
$\tau_{ign} = AT^m [\text{fuel}]^f [O_2]^g [Ar]^h \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(5)	Ring-structured hydrocarbons	Burcat et al. [50]
$\tau_{ign} = A[\text{fuel}]^f [O_2]^g \rho^k \exp\left(\frac{B}{T}\right)$	(6)	Blends of primary reference fuels	Ryan and Callahan [38]
$\tau_{ign} = AP^a C_n^c x_{O_2}^d \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(7)	Propane, <i>n</i> -butane, <i>n</i> -heptane, and <i>n</i> -decane	Horning et al. [27]
$\tau_{ign} = AP^a \phi^b \exp(n x_{fuel}) \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(8)	<i>i</i> -Octane	Davidson et al. [39]
$\tau_{ign} = AP^a \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(9)	Cyclopentane and cyclohexane	Daley et al. [40]
$\tau_{ign} = AP^a \phi^b T^m \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(10)	Number 2 diesel fuel (DF-2)	Haylett et al. [41]
$\tau_{ign} = A \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(11)	Hydrogen	Zhao et al. [43]
$\tau_{ign} = AP^a \phi^b \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(12)	<i>n</i> -Decane, <i>n</i> -hexadecane, and methyl decanoate	Haylett et al. [45]
$\tau_{ign} = A[\text{fuel}]^f [O_2]^g \exp\left(\frac{\hat{E}_A}{R_u T}\right)$	(13)	<i>n</i> -Nonane, methyl octanoate, and methylcyclohexane	Rotavera et al. [44,46]

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