



The temperature dependence of the laminar burning velocities of methyl formate + air flames



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HIGHLIGHTS

- The burning velocities of methyl formate + air flames at several temperatures were measured.
- Comparison of predictions of 3 mechanisms with the experimental data showed mixed agreement.
- The temperature dependence of the burning velocity was interpreted using empiric power law.
- For the first time, a sensitivity analysis of the power exponent, alpha, of the temperature dependence was performed.

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ABSTRACT

Laminar burning velocities, S_L , of methyl formate and air flames were determined at atmospheric pressure and initial gas temperatures, T , of 298, 318, 338 and 348 K. Measurements were performed in non-stretched flames, stabilized on a perforated plate burner at adiabatic conditions, generated using the heat flux method. These new experimental data shed light on discrepancies seen in previously published results, and the temperature dependence of the laminar burning velocity of methyl formate was analysed using expression $S_L = S_{L0}(T/T_0)^\alpha$. It was found that the power exponent, α , has a minimum close to equivalence ratio, ϕ , of 1.0. Both the laminar burning velocities and alpha coefficient were compared with predictions of the mechanisms of Glaude et al. (2005), Dooley et al. (2010) and Dievart et al. (2013). While the two latter mechanisms are in generally good agreement in lean mixtures, the Glaude mechanism over predicts the experimental burning velocities over the entire range of equivalence ratios. The temperature dependences predicted by the Glaude and Dievart mechanisms, however, are rather close and agree well with the measurements. To elucidate these differences and similarities in the performance of two mechanisms, the sensitivity analysis of the power exponent α was performed for the first time. It was demonstrated that examination of the temperature dependence of the burning velocity provides an independent approach for analysis of experimental data consistency.

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1. Introduction

Limited fossil fuel resources and the need to maintain an environmentally sustainable society have led to an increased use of biofuels. One promising renewable fuel is biodiesel, it is mostly produced from a variety of vegetable oils and primarily consists of methyl and ethyl esters with 16–18 carbons in the hydrocarbon chain [1,2]. The chemical complexity of biodiesel, as a result of the long carbon chains, makes development of chemical kinetic models for its combustion challenging. There is a lack of chemical

understanding and kinetic information as well as computer capacity necessary to run the mechanisms [1,2].

To gain insight into the combustion characteristics of biodiesel, information about the kinetics of smaller alkyl esters, for instance methyl butanoate, MB, can be used. MB is considered to be a good surrogate for biodiesel as it possesses the essential chemical structure of longer chained methyl esters [1]. When larger esters decompose and undergo reactions under combustion conditions the reactions commonly proceed via smaller intermediate esters. An example of this is the vital role played by the smallest methyl ester, methyl formate, MF ($C_2H_4O_2$), in the combustion of MB. As a result of this MB mechanisms contain a subset of MF reactions. The importance of MF as an intermediate holds true for larger esters as well, and by determining combustion characteristics of MF, pertinent reaction subset can be validated independently.

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This has led to several experimental studies over a wide range of conditions, and in a conjunction to this, kinetic models have been developed. The models have been validated against results of the laminar burning velocity, S_L , flame structure, as well as other data obtained using static and flow reactors, and shock tubes.

The first model for combustion of small esters was proposed by Fisher et al. [3]. Constructed for combustion of MF and MB, using bond additivity methods and extended rules for estimating kinetic parameters, the mechanism became the starting point for ester mechanisms development. The reaction subsets of MF and MB were added to a n-heptane mechanism [4]. Previously published results of MF combustion studies, obtained in a static reactor at low temperatures and sub atmospheric pressure [5], were used to validate the mechanism. While some qualitative agreement was seen, the experimental data indicated lower reactivity than that predicted by the model. This was ascribed to wall reactions in the experiments [3].

Further development of ester modelling was motivated by new experimental data for smaller alkyl esters [6]. Westbrook et al. [7] developed a mechanism for MF, methyl acetate, ethyl formate and ethyl acetate. Built on C₁–C₄ mechanism of Petersen et al. [8], the ester mechanism was constructed by relating reactivity in molecules of similar molecular structure to the esters investigated. The model was validated against intermediate species profiles measured in fuel-rich, low pressure premixed laminar flames [7] with good agreement.

Dooley et al. [9] developed a kinetic model with several rate constants pertinent to MF estimated by investigating the hydrogen bond and reactivity of similar compounds. The mechanism is built upon the works of Fisher et al. [3] and Westbrook et al. [7], and C₁ and C₂–C₃ subsets of Zhao et al. [10] and Healey et al. [11], respectively. Experimental data [9] from a shock tube and flow reactor as well as the laminar burning velocity, determined using the spherical bomb technique, were used for model validation. The mechanism could successfully reproduce experimentally determined ignition delays and species mole fractions measured during oxidation and pyrolysis. For the laminar burning velocity, determined at 1 atm and 295 K, the model over predicted the experimental results at equivalence ratios below 1.2 by 1–2 cm/s and under predicted the velocity at richer conditions by 1–2 cm/s. The mechanism was later used to model flame structures of low pressure MF flames [7,12] with an overall good agreement.

To investigate the chemical kinetic effects due to molecular structure of C₂–C₁₁ methyl esters, Dievart et al. [13] developed a mechanism based on a methyl decanoate model [14] and the MF reaction subset originating from Dooley et al. [9]. The mechanism was successfully validated against experimental data of extinction limits of C₂–C₁₁ methyl ester diffusion flames [13] from a counter flow setup. It was later used by Wang et al. [15] to model the laminar burning velocities of several small methyl esters, including MF. The study by Wang et al. [15] is a thorough investigation of the laminar burning velocity of several methyl and ethyl esters at standard conditions, including measurements performed using a counter flow setup and analysis of four kinetic mechanisms. The experimental MF laminar burning velocities of Wang et al. [15] are in agreement with the results of Dooley et al. [9] up to an equivalence ratio of 1.2, at richer conditions the results of Wang et al. are lower by up to about 6 cm/s. The mechanism of Dievart et al. [13] are within error bars of the experimental results of both Wang et al. [15] and Dooley et al. [9] at the lean side, while at equivalence ratios above 1.2 it over predicts the data of Wang et al. [15] and is in agreement with the data of Dooley et al. [9]. The experimental results were also compared to two new mechanisms, created by combining the reaction subset of smaller alkyl esters from Westbrook et al. [7] and the C₀–C₄ subsets originating from Bourque et al. [16] or Wang et al. [17]. The two latter

mechanisms both over predicted the laminar burning velocity of MF [15].

The combustion reactions of MF are important for non-ester fuels as well. A notable example is the combustion of dimethyl carbonate, DMC, where MF is itself an intermediate and in addition the two fuels share an important intermediate, the methoxycarbonyl radical, CH₃OCO [18]. Knowledge of MF oxidation can thus increase the understanding of DMC combustion. Glaude et al. [18] developed a DMC mechanism using rate constants estimations for similar oxygenated fuels and group additivity rules. The mechanism is based on a model of dimethoxy methane and dimethyl ether [19], from which the reaction subset of MF originates. Experimentally determined species profiles in opposed flow DMC diffusion flames [18] were used for model validation with reasonably good agreement.

Validating kinetic models against the laminar burning velocity is vital, but with only two prior studies of the laminar burning velocity of MF [9,15], and discrepancies seen between these results [15], more experimental data are needed. The present study was performed to provide new reliable laminar burning velocities measured in stretch free adiabatic flames using the heat flux method. A wider range of initial gas temperatures, 298–348 K, compared to previous studies, was covered. The experimental results shed further light on the deviation between the experimental data by Wang et al. [15] and Dooley et al. [9]. A detailed description and uncertainty analysis of all three methods can be found in [20].

In addition, the paper presents a comparison of the experimental results with the modelling by use of three mechanisms: of Glaude et al. [18], Dievart et al. [13] and Dooley et al. [9]. Included in this paper is a new approach for analysis of experimental data consistency, based on the behaviour of the power exponent, α , from the temperature dependence equation of the laminar burning velocity, $S_L = S_{L0}(T/T_0)^\alpha$. This analysis will be further described and discussed below.

2. Experimental details

The laminar burning velocities were measured using two heat flux setups; one of which is described in [21]. The central part of the setup is the perforated plate burner that generates a stretch-free flat flame [22,23]. The burner consists of a plenum chamber and a burner plate, separated by a ceramic ring for insulation and thus allow for temperature control using two different water baths. The temperature of the plenum chamber controls the temperature of the unburned gas, regulated between 298 and 348 K in the present study. To maintain the fuel in a gaseous state, a heating tube was connected between the Controlled Evaporator Mixer, (CEM), used to evaporate the fuel, and the burner inlet. The heating tube was set to the same temperature as the plenum chamber.

To measure the laminar burning velocity, the flame must be adiabatic; however flame stabilization occurs via heat loss of the flame to the burner creating a non-adiabatic situation. The heat flux method compensates for this heat loss by heating the burner plate to temperatures above that of the unburned gas, and creating a temperature increase of the unburned gas as it passes the burner plate. In the present study the burner plate temperature was set to 370 K.

At experimental conditions when the unburned gas velocity is lower than the laminar burning velocity, the flame will position itself closer to the burner and the burner plate will gain heat from the flame. During opposite conditions, when the unburned gas velocity is higher than the laminar burning velocity, the flame will position itself further away, and the burner plate lose more heat to the unburned gas than it gains from the flame.

The difference in the heat loss and heat gain of the burner plate results in a parabolic temperature distribution that can be

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