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Laminar burning velocities of primary reference fuels and simple alcohols

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HIGHLIGHTS

- The laminar burning velocity has been measured for (m)ethanol-hydrocarbon blends.
- The temperature dependence for pure methanol and ethanol is shown.
- The temperature dependence has a minimum around peak burning velocity.
- Mixing rules to predict the laminar burning velocity of fuel blends are tested.
- These mixing rules are able to predict the laminar burning velocity of fuel blends.

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ABSTRACT

Laminar burning velocities for methanol, ethanol, and binary and quaternary mixtures of these with iso-octane and n-heptane, have been determined using the heat flux method on a flat flame adiabatic burner. Measurements were done for an equivalence ratio range between 0.7 and 1.5 and for a range of temperatures between 298 K and 358 K at atmospheric pressure. The present study expands the available data on laminar burning velocities of alcohol–hydrocarbon blends and validates simple mixing rules for predicting the laminar burning velocity for a wider range of fuel blends of hydrocarbons with methanol and/or ethanol. It is shown that simple mixing rules that consider the energy fraction of the blend's components are accurate enough to predict the experimentally determined laminar burning velocity of the mixtures.

1. Introduction

The use of fossil fuels on a massive scale has led to an intolerable stress on the local (air quality) and global (greenhouse effect) environment. An important and increasing share in the energy consumption goes to the transportation sector. Alcohols, methanol and ethanol in particular, are promising alternatives for fossil fuel replacement. These liquid fuels are largely compatible with the current fuel and distribution infrastructure and are easily stored in a vehicle. They can be used in the current vehicle internal combustion engines with little or no changes. Methanol and ethanol are also miscible with gasoline which enables a soft start to an alternative transport energy economy and in contrast to other alternatives, they have the well-known potential to increase the engine performance and efficiency over what is achievable with gasoline [1,2]. Much of the recent research efforts evaluating the potential of alcohols have focused on ethanol [3]. However, methanol is more versatile from a production point of view, its properties are even more beneficial for the power output and efficiency of internal combustion engines compared to ethanol and the addition of methanol to ethanol–gasoline blends can also have an economic advantage [4,5].

To fully exploit the characteristics of alcohols for increased efficiency and performance, engine cycle simulation models, which have become indispensable tools in the design of advanced engines, should be adapted to the combustion characteristics of these alcohol fuels. A fundamental property of a fuel and a key parameter in simulation tools for the characterization of the combustion behavior is the laminar burning velocity (u_l). Accurate and fast calculation of the laminar burning velocity is needed in simulation tools. Sileghem et al. [6] investigated if mixing rules could be used to determine the laminar burning velocity of fuel blends from the burning velocity of the fuel components with sufficient accuracy and without being computationally too demanding. In that work, different mixing rules for the prediction of the laminar

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burning velocity of ethanol–hydrocarbon mixtures were tested and compared. Three different mixing rules gave results in good agreement with the experimental determinations of the laminar burning velocities for mixtures. The mixing rules have been explained by Sileghem et al. [6], but are repeated here for the clarity of the present paper:

Mixing rule based on energy fraction of the fuels' components [7].

$$u_{l,blend}(\Phi) = \sum_{i=1}^{n} \alpha_1 \cdot u_{l,i}(\Phi) \tag{1}$$

In this expression α_i is the energy fraction of fuel component *i*. The energy fraction can be calculated as follows:

$$\alpha_i = \frac{\Delta c H_i^\circ \cdot x_i}{\sum_{i=1}^{n} \Delta c H_i^\circ \cdot x_i} \tag{2}$$

cH_i° is the heat of combustion and x_i is the mole fraction of the fuel component *i*.

Mixing rule based on Le Chatelier's rule [6].

$$u_{l,blend}(\Phi) = \frac{1}{\sum_{i=1}^{n} \frac{\alpha_i}{u_{l,i}(\Phi)}} \tag{3}$$

where α_i is the energy fraction of the fuel component (Eq. (2)).

Le Chatelier [8] first proposed a similar empirical mixing rule for predicting the flammability limit of lean fuel–air mixtures:

$$\mathrm{LFL}_{blend} = \frac{1}{\sum_{i=1}^{n} \frac{x_i}{\mathrm{LFL}_i}} \tag{4}$$

where x_i is the mole fraction of the *i*th component and LFL_i is the lower or lean flammable limit of the *i*th component in volume percent. Di Sarli and Di Benedetto [9] used Le Chatelier's rule to predict the laminar burning velocity of hydrogen–methane blends. They used the mole fraction instead of the energy fraction. These two approaches have been compared by Sileghem et al. [6] and it was found that the energy fraction gave better results for the laminar burning velocity of ethanol–hydrocarbon mixtures.

Mixing rule developed by Hirasawa et al. [10].

Hirasawa et al. [10] developed an empirical mixing rule, which depends on a mole fraction weighted average of the burning velocities and flame temperatures.

The expression for laminar burning velocity becomes:

$$u_{l,blend} = \prod_{i=1}^{n} u_{l,i}^{\beta_i} \tag{5}$$

with

$$\beta_i = \frac{x_i n_i T_{f,i}}{n_{blend} T_{f,blend}} \tag{6}$$

x_i is the mole fraction and *n* is the total amount of moles of the combustion products and diluents, and T_f represents the adiabatic flame temperature. '*i*' refers always to the *i*th fuel component and 'blend' refers to the fully blended fuel. More detailed information can be found in [6,10,11].

These three mixing rules gave similar predictions for ethanol–hydrocarbon blends [6] indicating that the flame temperature is the dominant factor for the laminar burning velocity, as was found by Hirasawa et al. [10]. Sileghem et al. [6] concluded that the mixing rule by Le Chatelier, based on energy fraction, was the most useful to represent the data of their study since it is relatively simple and give a prediction with satisfying accuracy. The data consisted of experimental laminar burning velocities of ethanol/n-heptane and ethanol/n-heptane/iso-octane mixtures at 1 atmosphere and 298 K and 338 K and modeling data of an ethanol/n-heptane blend and blends of ethanol and a toluene reference fuel at higher pressure and temperature. However, due to uncertainty limits and the limited data set used in the study of Sileghem et al. [6], further validation is needed. In this study, the laminar burning velocities of blends of methanol, ethanol, iso-octane and n-heptane at atmospheric pressure have been investigated. The laminar burning velocities for the pure fuels have been determined previously [12,13], but the data for methanol and ethanol were extended within the present work. For further discussion on the comparability of the laminar burning velocities of the pure fuels with previous determinations we refer to Sileghem et al. [14] in the case of ethanol, iso-octane and n-heptane.

2. Experimental setup

The measurements were performed using the heat flux method on a perforated plate burner. The experimental setup for the adiabatic flame stabilization is shown in Fig. 1. This method has been proposed by de Goey et al. [15] and was further developed by van Maaren and de Goey [16]. The present experimental rig is also used in the study of Sileghem et al. [14] to measure the laminar burning velocity of iso-octane, n-heptane, toluene and gasoline. Important features of the method are, therefore, only shortly outlined in the following.

The heat flux burner has two major parts: a burner head with a heating jacket supplied with thermostatic water to keep the temperature of the burner plate constant at 368 K and a plenum chamber with a separate temperature control system. This control system enables to set a temperature of the fresh gas mixture from 298 to 358 K. A burner plate of 2 mm thickness perforated with small holes (0.5 mm in diameter) is attached to the burner outlet. A theoretical analysis of the heat flux method has been given by de Goey and van Maaren [15,16]. A mixing panel shown in Fig. 1 was used to provide a controlled flow of the vaporized fuel and air at the required equivalence ratio. The key part of this mixing panel is the Bronkhorst High-Tech CORI-FLOW MassFlow Controller (MFC) connected to the Controlled Evaporator and Mixer (CEM, Bronkhorst High-Tech). The liquid fuel flow from the fuel reservoir, pressurized by nitrogen, is metered by the CORI-FLOW MFC and fed to the CEM. Part of the air flow, controlled by the gas MFC-1, is used as a carrier gas to facilitate vaporization in the CEM at temperatures up to 473 K. Another part of the air flow controlled by the gas MFC-2 is varied to provide the required mixture composition and is added downstream. For the measurements reported in this study, the tube connecting the CEM with the burner was a heated tube to avoid condensation of the fuel on its way to the plenum chamber.

3. Error assessment

Detailed analysis of these uncertainties was performed earlier [14,17,18]. The overall accuracy of the measurements presented in this work is commonly better than ±1 cm/s. Only for rich mixtures above the equivalence ratio of 1.3, the error could be slightly larger (maximum 1.3 cm/s). The laminar burning velocities measured by van Lipzig et al. [12] and Vancoillie et al. [13] using the same heat flux setup as in the present work are systematically higher than the present measurements by a few cm/s. The difference compared to the present work is larger than the stated experimental error. One of the reasons for the difference could be that in the present work the gas mixture was transported from the evaporator to the burner through a heated tube while in the previous experiments an insulated but unheated tube was used. A comparison of the measurements with and without a heated tube strongly indicated that some condensation did occur without it. Because