

Experimental investigation of laminar burning velocity for n-dodecane/air mixture at elevated temperatures

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1 Introduction

Commercially available liquid fuel (gasoline, diesel, and jet aviation), which is extracted from crude oil contains a complex mixture of various hydrocarbons in terms of carbon number and chemical structure. A basic understanding of the combustion kinetics of these fuels is critical in the design and optimization of an existing and next-generation combustor. These fuels contain a large number of hydrocarbons and a direct chemical kinetic simulation of their oxidation is not possible [1]. Modelling of combustion characteristics of such fuel becomes very difficult at a fundamental level. Therefore, to analyze the effect of these fuels on combustion efficiency, fuel surrogates, which are typically a mixture of a limited number of hydrocarbons, are used to mimic the physical and chemical properties of a real fuel [2].

In general, the formulation of the surrogate fuels and the accuracy of the simulated results obtained from a chemical kinetic model depends on the mechanisms of individual components of the surrogate considered in the model. Therefore, it is necessary to provide experimental data for important kinetic properties such as laminar flame speed for the development, validation, and optimization of a chemical kinetic mechanism of the individual components of the surrogate fuel [3]. Laminar burning velocity (LBV) is the physiochemical property of a fuel/oxidizer mixture for the combustion process depending on the mixture's reactivity, exothermicity, and transport properties. LBV measurements of liquid fuels are crucial because of the need to understand the reactivity of the inhomogeneous system. n-dodecane is the major n-alkane group found in diesel and jet fuel, it is considered the main component in the formulation of several surrogate mixtures for diesel and jet fuels [4].

An experimental study of laminar flame speed and extinction limits of premixed n-decane and n-dodecane with synthetic air by Kumar and Sung [5] using the counter-flow twin-flame technique has been carried out for the equivalence ratio of 0.7-1.4 at a mixture temperature of 400 and 470 K and 1 bar pressure condition. They compared the experimental data with the modified Utah surrogate mechanism and observed an over-prediction of the mechanism over the investigated range of equivalence ratios. Kumar and Sung [5] suggested the improvement of the kinetic study of the mechanism for better prediction of the laminar flame speed. Similar to this study, Ji et al. [6] experimentally investigated the flame propagation and extinction of the premixed C₅-C₁₂ alkane group using counter-flow flame configuration at elevated unburnt mixture temperature (403 K) and atmospheric pressure conditions for the equivalence ratio of 0.7-1.5. Nearly a 5% difference in

maximum flame speed is observed between linear and non-linear extrapolation of the result. Experimental results of laminar flame speed were compared with the detailed kinetic model of JetSurF version 0.2 [7] and good behaviour was observed between them. You et al. [1] proposed a detailed kinetic model for the oxidation of straight-chain alkane up to n-dodecane for high temperature conditions and the proposed model is validated with ignition delay times of n-decane and n-dodecane. A detailed model proposed by You et al [1] was able to predict the laminar flame speed of n-dodecane over the entire range of equivalence ratio with the experimental data of Ji et al [8] whereas good agreement was observed for fuel lean conditions with Kumar and Sung [5]. Hui and Sung [6] extended the work of Kumar and Sung [5] for the equivalence ratio of 0.7-1.4 at 400 K and elevated pressure conditions. The researcher compared his experimental data with computed laminar flame speeds of n-dodecane using the mechanism of Naik et al. [9] and JetSurF 2.0 [10] and reported a good match between the computational and experimental results. The modelling of laminar flame speed is mostly dominated by low hydrocarbon chemistry. Richter et al [11] and Liu et al [12] experimentally measured the laminar flame speed of jet fuel components at high pressure using the cone angle method for the equivalence ratio of 0.7-1.8 at 473 K and elevated pressure conditions. Dortz et al [13] used the spherical flame method to measure the unstretched laminar burning velocity of commercial kerosene and its components for the equivalence ratio of 0.7-1.4 at 400 K and atmospheric pressure condition. An excellent match of the laminar burning velocity of n-dodecane was observed with JetSurF 2.0 model at atmospheric pressure. Recently, Rajesh and Prathap [14] experimentally investigated the propagation and flame stability of n-dodecane/air premixed flame at an elevated pressure of up to 4 bar and temperature of up to 450 K using the spherical flame method. LBV is reported to reduce with increasing pressure because of third-body reactions and higher mixture density.

Various researchers have carried out experiments to study the laminar burning velocity of n-dodecane as a primary fuel and a surrogate. However, a limited number of experimental data is available at high temperatures for the measurement of the laminar burning velocity of n-dodecane and its surrogate mixture. The experimental data of laminar burning velocity at elevated temperatures is important for the validation, optimization and development of the chemical kinetic models for better predictions of the combustion characteristics.

In the present study, the externally heated diverging channel method is used for the measurement of laminar burning velocities of premixed n-dodecane/air mixture at atmospheric pressure and elevated temperatures (396-560 K) for various ranges of equivalence ratios ($\Phi = 0.7-1.3$). Chemical kinetic simulations using three kinetic mechanisms have been compared with the experiments.

2 Experimental Details

Figure 1(Left) shows the schematic diagram of the experimental setup used for the measurement of laminar burning velocity. A diverging channel consists of an initial rectangular cross-section of size 25 x 2 mm with a diverging section of 15° angle and 50 mm in length. This diverging channel is heated by an external infrared heater with a variable heating rate. The external heating rate of the infrared heater is controlled by a voltage controller. The external heating creates a positive temperature gradient in the channel along the mixture flow. The temperature profile along the channel can be varied by varying the heat flux of the heater. Liquid fuel (n-dodecane) is vaporized by preheated air which is heated by an air preheater before entering the diverging channel. An infusion syringe pump is used to supply the fuel to mix with air. Fuel is supplied in the heated air using a micro syringe as the fuel enters the heated air line, it instantly gets vaporized and mixes with the air. A homogeneous mixture of fuel and air is supplied to the diverging channel. The entire flow path is heated by a strip heater and insulation is provided to avoid fuel condensation. The fuel-air mixture is ignited at the exit of the diverging channel with the help of an igniter. The flame is established at the exit and propagates upstream in the diverging channel. The flame stabilizes at a location where the mixture velocity matches the burning velocity. Figure 2(Right) shows a stabilized planar flame for premixed n-dodecane/air for mixture velocity of $U_{inlet} = 1.17$ m/s at an equivalence ratio of 0.7. The fuel flow rate

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is controlled by the infusion syringe pump whereas the flow rate of air is controlled and monitored by using a mass flow controller connected to a command module and a computer. A thermocouple is used to measure the temperature of the mixture at the flame location using a traverse mechanism. The laminar burning velocity (S_u in m/s) is calculated using a modified mass conservation equation at the channel inlet and stabilized flame location and is given as:

$$S_u = U_{inlet} \times \left(\frac{A_{inlet}}{A_f} \right) \times \left(\frac{T_f}{T_{inlet}} \right)$$

Where U_{inlet} (m/s) is the mixture velocity at the diverging inlet, A_{inlet} (m^2) and T_{inlet} (K) is the cross-section area and mixture temperature at the inlet section and A_f (m^2) and T_f (K) is the cross-section area at the flame location. Laminar flame speed is obtained from the chemical kinetic mechanism (CRECK modelling [15], LLNL [16], and JetSurF 2.0 [10] mechanism) using Chemkin-pro software. Mixture-averaged transport properties are used in the current study. The adaptive grid parameters were set with CURV = 0.04 and GRAD = 0.01 with a maximum of 2000 grid points.

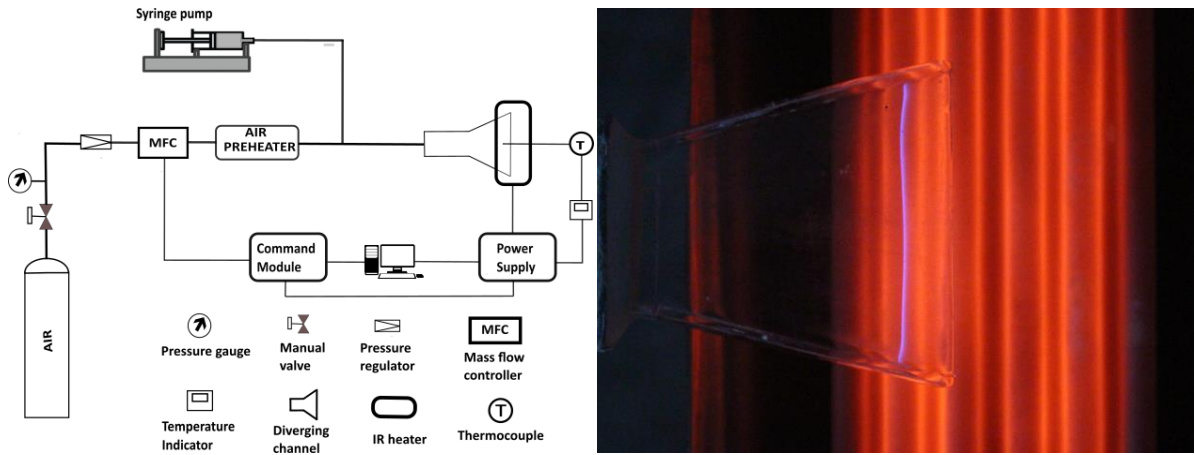


Figure 1: Left: Schematic diagram of an experimental setup. Right: Stabilized planar flame in the diverging channel for the mixture velocity of 1.17 m/s at an equivalence ratio of 0.7.

3 Results and Discussion

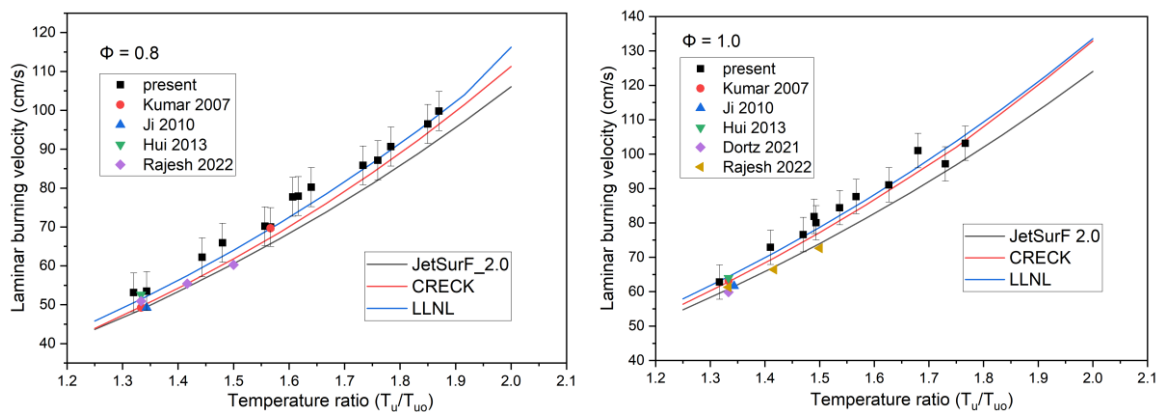


Figure 2: Variation of laminar burning velocity with mixture temperature at Left: lean condition. Right: stoichiometric condition.

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The effect of temperature on the laminar burning velocity of the n-dodecane/air mixture is shown in Figure 2 (Left) for fuel lean ($\Phi = 0.8$) and Figure 2 (Right) stoichiometric conditions ($\Phi = 1.0$). Normalized temperature is considered to show the variation of laminar burning velocity with mixture temperature (T_u) and reference temperature, taken as $T_{u0} = 300$ K. The experimental values are reported with an uncertainty band of $\pm 5\%$. The laminar burning velocity increases with an increase in mixture temperature due to an increase in the enthalpy of the mixture. Out of all the mechanisms, an excellent match is observed for LLNL [16] mechanism. Each data set reports the maximum LBV for $\Phi = 1.1$ similar to the literature and computations.

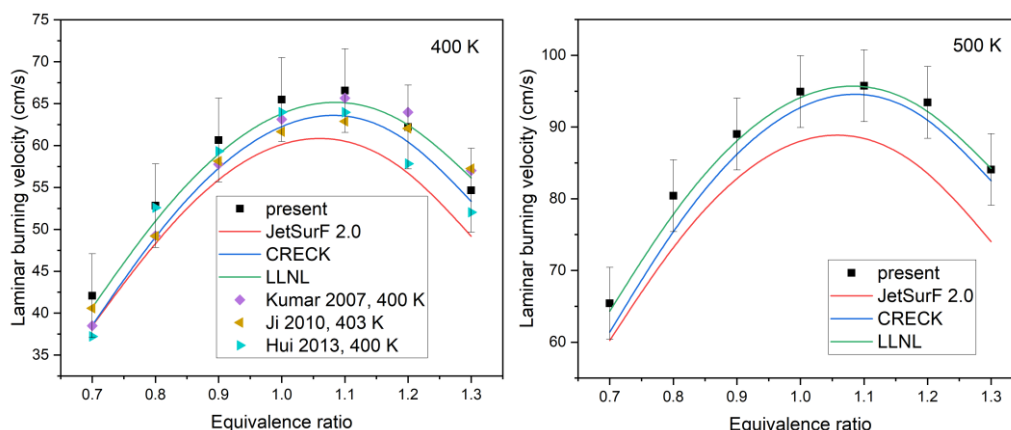


Figure 3: Comparison of the laminar burning velocity of n-dodecane-air mixture with literature and chemical kinetic mechanisms at Left: 400 K Right: 500 K.

Figure 3 shows the variation of laminar burning velocity at different equivalence ratios at 400 K and 500 K. The laminar burning velocity increases with an increase in mixture temperature at all the equivalence ratios. LLNL [16] mechanism better predicts the laminar burning velocity as compared to CRECK modelling [15] and JetSurF 2.0 [10] mechanism at both temperatures. JetSurF 2.0 [10] mechanism shows poor predictions with experimental data as the mixture becomes rich.

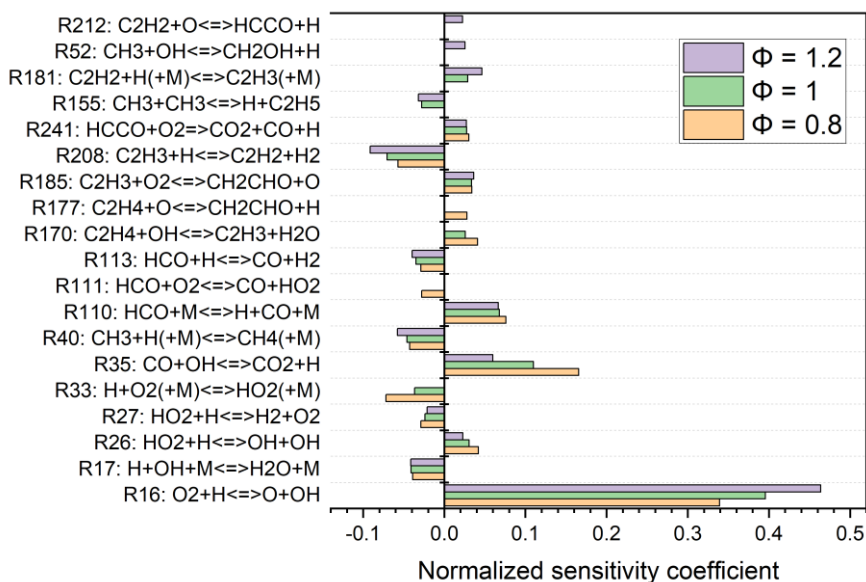


Figure 4: Normalized sensitivity coefficients for the laminar burning velocity of n-dodecane-air mixtures at 500 K.

Normalized sensitivity coefficient is used to assess the variation of laminar burning velocity from a kinetics perspective with mixture equivalence ratios. The normalized sensitivity coefficients of the laminar burning velocity using the LLNL [16] mechanism are shown in Figure 4. The major laminar burning velocity enhancement reactions are R16, R35, and R110 producing H, O, and OH radicals. The increasing rate of progress of these reactions increases the concentration of the radical pool, which then increases the energy extracted from the system. Therefore, the LBV increases with the rise in the concentration of these radicals. The chain branching reaction R16 shows the highest positive sensitivity among other reactions. The CO oxidation reaction R35: $\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$ and HCO decomposition reaction R110: $\text{HCO} + \text{M} \rightleftharpoons \text{H} + \text{CO} + \text{M}$ shows a reversal relationship in their sensitivity to the equivalence ratio as compared to R16.

The reactions: R17, R27, R40, R113, and R208 contributes negatively to flame speed at all the equivalence ratios ($\Phi = 0.8, 1.0, \text{ and } 1.2$) majorly due to the consumption of the H radicals. They compete with R16 which enhances the LBV of the system. The positive sensitivity value of a reaction corresponds to its participation in the enhancement of laminar burning velocity, whereas, the negative sensitivity value of a reaction reduces the laminar burning velocity.

4 Conclusions

The laminar burning velocity measurements is carried out for the n-dodecane/air mixture using an externally heated diverging channel method over the range of equivalence ratios (0.7-1.3) at elevated temperatures (396-560). The increase in laminar burning velocity is observed with an increase in mixture temperature due to a rise in the enthalpy of the mixture. For all equivalence ratios, a rise in mixture temperature causes an increase in the laminar burning velocity. For the mixture temperature from 400 to 500 K, peak laminar burning velocity is observed at $\phi = 1.1$. LLNL mechanism better predicts and the second best match is observed for CRECK modelling whereas, JetSurF 2.0 mechanism gives poor predictions of laminar burning velocity. The key reactions which influences the laminar burning velocity are analyzed using the sensitivity analysis for the unburnt mixture of 500 K at fuel-lean, stoichiometric and fuel-rich conditions.

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