

# Laminar flame speed measurement of multicomponent Jet A-1 and LUCHE kerosene surrogate fuels in elevated pressure and temperature conditions

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## Abstract

Understanding of combustion characteristics of real jet fuels is central to the development of affordable, efficient and friendly aero-combustors. Laminar flame speed at elevated pressure is a key parameter for refining the chemical kinetics that is relevant at engine conditions. Although the laminar flame speed has been investigated for decades by using various experimental methodologies, accurate measurements of laminar flame speeds in high-pressure and high-temperature conditions similar to aero-engines operating conditions is still required. In this present study, a high-pressure combustion chamber was specifically developed to measure the laminar flame speed of multicomponent liquid fuels such as kerosene (Jet A1) and surrogate kerosene (LUCHE) fuels using a preheated premixed Bunsen burner operated in elevated pressure and temperature conditions. The optical method used to determine the laminar flame speed is based on the flame contour detection by using OH\* chemiluminescence imaging. Experimental work was firstly performed by measuring the laminar flame speed of gaseous CH<sub>4</sub>/air and acetone/air premixed laminar flames for validating the experimental setup. Kerosene/air combustion was then investigated to deduce laminar flame speeds over a large range of operating conditions including equivalence ratio (0.5-1.3), inlet fresh gas temperature (300-550 K) and pressure (0.1-0.5 MPa). Experiments are complemented by numerical simulations conducted with the COSILAB software using various published detailed kinetic mechanism models for CH<sub>4</sub>, acetone and kerosene fuels. The observed results are compared with previous experimental data found in literature and discussed subsequently. Further experimental data analysis is finally investigated and empirical relationships of kerosene laminar flame speed with pressure, temperature and equivalence ratio effects are proposed.

## 1. Introduction

Due to the new European regulations on air pollution, it is foreseeable that the aircraft manufacturers will need to significantly reduce the emission of pollutants such as NO<sub>x</sub>, CO<sub>x</sub> and particles. To achieve this objective, improvement of performances of aeronautical propulsion systems therefore needs a better understanding of the chemical kinetic mechanisms of real multicomponent fuels such as conventional fuel Jet A-1 and kerosene surrogate fuel. Hence, there is a growing interest in complementing combustion database of liquid hydrocarbons that are relevant to the real transportation fuels. One particular interest to reduce the pollutant emission is to burn the fuel/air mixture in lean equivalence ratio to decrease flame temperature and consequently, decrease the level of NO<sub>x</sub>. Several tools and methodologies are previously conducted to study the effect of the fuel chemical composition on pollutant emissions. These methodologies are usually used to quantify fundamental properties such as ignition, laminar flame speed, flame stretch and extinction limit. Among these parameters, laminar flame speed is a key parameter for understanding reactivity, diffusivity and exothermicity of fuels and validating both the kinetic chemical mechanisms as well as turbulent models. Although laminar flame speed has been investigated over few decades using various combustion methodologies [1-4], accurate measurements of laminar flame speed of multicomponent liquid fuels in high-pressure and

high-temperature regimes are still required. For instance, kerosene fuel has been used for decades in aeronautical propulsion engines but the knowledge of fundamental properties such as ignition, combustion and oxidation is still limited. The use of experimental devices such as heated shock-tube operating over a wide range of temperature and pressure [5] recently contributed to complement the early ignition of kerosene database. For flame structure data, few data are available due to the rare experimental studies of laminar kerosene flame. For instance, laminar flame speed of kerosene was investigated with a large equivalence ratios range 1.0-1.4 and in an atmospheric pressure by using a Bunsen flame [6]. In the work of Xinhui et al., laminar flame speeds of jet fuels were investigated with a counter-flow burner in a preheated temperature 470 K and pressure up to 0.3 MPa [7]. Laminar flame speed of Jet A-1 was also measured by using the constant volume combustion-bomb approach [8]. The effect of equivalence ratio on laminar flame speed was studied for initial temperature up to 373 K and pressure up to 0.8 MPa. In Cheng et al.'s work, the PIV technique was used to measure laminar flame speed of liquid fuels including Jet A-1, Diesel, and fuel blends using a jet wall stagnation flame configuration. Pure components of Jet fuel such as n-Decane and Alkane were also investigated using the constant volume combustion-bomb approach [9-10].

The present study focuses on recent experiments and modeling of high-pressure laminar flame

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speeds of various fuels. The method employed here to measure flame speed consists to use an innovative laminar flame burner operating with gas and/or multicomponent liquid fuels specifically designed to measure laminar flame speed and flame structure in high-pressure and high-temperature conditions. This burner, detailed in section 2, enables an accurate monitoring and control of measurement conditions including temperature, pressure and equivalence ratio. Measurement of the burned flame area were performed using imaging of OH\* chemiluminescence emission combined with a specific image data processing which is described in section 3. A brief overview of the chemical kinetic mechanisms used to simulate the effect of pressure, temperature and equivalence ratio on laminar flame speed of the studied fuel/air mixtures is presented in section 4. Results from the experiments performed in the 0.1-0.5 MPa pressure, 373-550 K temperature and 0.5-1.3 equivalence ratio ranges are presented in section 5. Comparison between the experimental data with numerical prediction is then discussed.

## 2. Experimental details

### 2.1 High-pressure burner

A high-pressure Bunsen flame burner was designed and developed to generate a laminar conical flame stabilized on the outlet of a nozzle. The burner produces axisymmetric jet flames using contoured laminar nozzle (Fig. 1a). The shape of the converged nozzle is defined by a fifth order polynomial to provide a flat velocity profile at the exit plane. The exit diameter of the contoured nozzle is 10 mm. A sintered plate surrounding the nozzle exit ( $\varnothing=10.6$  mm) is used to produce a pilot flame to anchor the flame at high flow rates. The burner components are installed in a high-pressure vessel equipped with four large optical accesses. Preheating of the chamber was performed using

electrical wire heaters and controlled using thermocouples (Fig. 1a). The top of the vessel was designed as a convergent nozzle. A stainless steel pipe was connected to the exhaust chamber followed by sonic nozzles to control the pressure of the chamber measured with a piezoelectric transducer. Nitrogen flow used to increase the pressure inside the chamber was preheated by a heat exchanger and delivered to the chamber by a mass flow meter. The reactant temperature was monitored by a thermocouple placed at the exit of the nozzle before and after the experiments. With this experimental facility, the pressure chamber can withstand up to 3.0 MPa at a maximum wall temperature of 600 K.

### 2.2 Liquid fuel vaporization and gas feeding

The burner can operate with gaseous or liquid fuels. The reactant gases are stocked into pressurized tanks. The gas flow rates are measured and controlled individually using mass flow meters and allowed sufficient residence time to mix thoroughly before passing through the nozzle. Overall, the flow rate has an accuracy of better than 1 %. In case of liquid fuels, the liquid fuel was contained in a pressurized tank. The tank was connected to a Controlled Evaporator and Mixer (CEM, Bronkhorst) which heated and mixed fuel vapour with N<sub>2</sub> carrier gas at controlled mass flowrate. The exit of the CEM was connected to a stainless steel cell preheated at temperature between 445 and 600 K (controlled with a type K thermocouple) to prevent any vaporized fuel condensation. Additional nitrogen and oxygen was performed before the entrance of the burner in order to change the equivalence ratio of the fuel/air mixture composition. All the gases are finally premixed into a tank before to be introduced into the nozzle. In the present work, air is composed of a gaseous O<sub>2</sub>/N<sub>2</sub> mixture of 20 % and 80 % respectively.

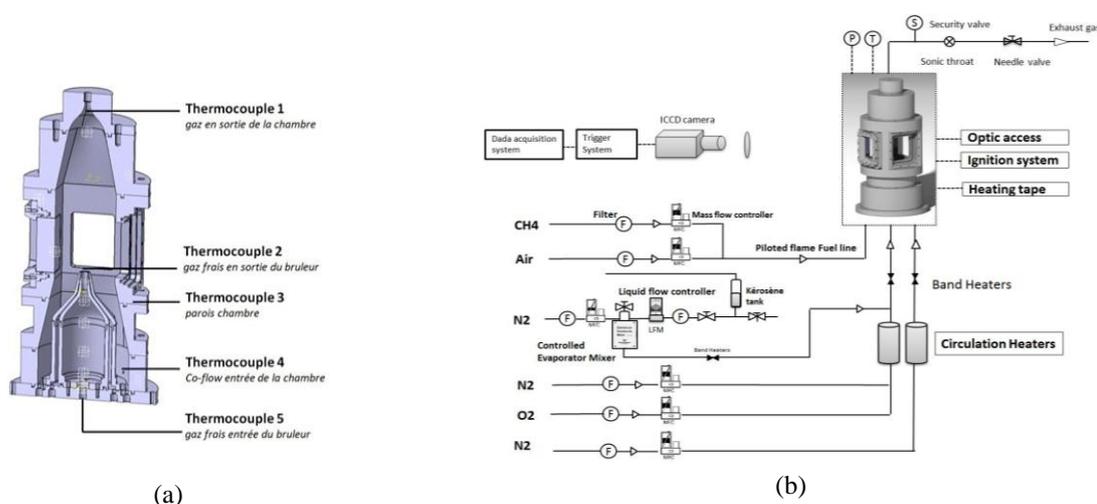


Fig.1 Schematic of the experimental facility: (a) high-pressure burner, (b) process Flow diagram

### 2.3 Optical diagnostics

The optical technique used in the present study is based on flame contour detection by using OH\* chemiluminescence imaging. The flame is imaged on 1024×1024 pixels<sup>2</sup> of a 16-bit, ICCD camera (Princeton instrument). The camera is combined with a UV 100F/2.8 lens with an optical filter centered at 310 nm allowing a 40×40 mm<sup>2</sup> field of view, which is a 0.45 μm/pixel magnification ratio. The acquisition frequency of the camera was kept in 50 Hz. For each operating condition, 30 instantaneous chemiluminescence images are typically recorded. The final flame speed was determined by processing the averaged image of these 30 instantaneous images. Examples of CH<sub>4</sub>/air flame images are shown in Fig.2 for equivalence ratio ranging between 0.7 and 1.4.

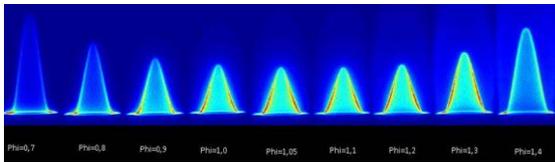


Fig.2 Laminar CH<sub>4</sub>/air flames for various equivalence ratios. T=300K, P=0.1MPa, fresh gas velocity =1.1m/s.

### 3. Laminar flame speed measurement

The principle of flame velocity measurements is based on the mass conservation between the outlet nozzle and the flame front. The average flame speed in the transverse plane can be expressed by

$$\rho_u S_u A = Q_m \rightarrow S_u = \frac{Q_m}{\rho_u A} \quad (1)$$

where  $Q_m$  is the total mass flow rate of the fuel/air mixture gas,  $\rho_u$  is the unburned gas density and  $A$  is the surface area. The flame front area  $A$  which allows to determine the laminar flame speed is deduced by flame imaging. The images are processed in Matlab software using an image processing algorithm based on the inverse Abel transformation to get first the location of the outside maximum intensity contour from OH\* chemiluminescence images. Since the laminar flame speed is defined relative to the unburned reactive mixture, the appropriated surface area  $A$  is the upstream boundary of the preheat zone. The upstream boundary of the preheat zone is then different from the maximum OH\* contours (See Fig. 3). In the present study, the best approximation of the location of the upstream boundary of the preheat zone is then obtained by adopting the following procedure.

The location of the surface  $A$  is determined by shifting the maximum OH\* contour by a ‘flame thickness’ defined as the  $\delta = X_{T=800K} - X_{[OH]_{max}}$  representing the difference between the location of the  $T = 800$  K isotherm, delimiting the position

between the fresh gases zone and the reaction zone, and the location of the maximum OH\* contour. Using 1D adiabatic premixed flame simulations for the studied mixtures, the  $T = 800$  K isotherm has been defined as the location where the radical OH appears. The resulting flame thickness was then ranging from 0.2 to 1.2 mm depending of the operating conditions of the experiments.

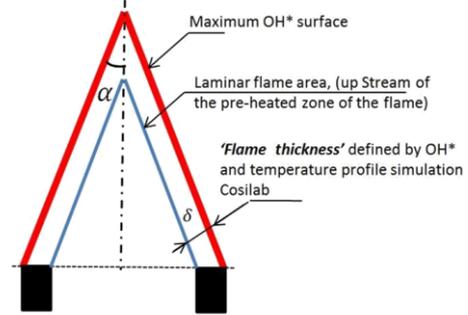


Fig.3. Illustration of the surface area methodology

### 4. Numerical analysis

Numerical simulations of laminar one-dimensional adiabatic unstretched flame are carried out with COSILAB code using detailed chemical kinetic mechanisms. The GRIMech 3.0 mechanism was used for CH<sub>4</sub>/air mixtures. A sub-mechanism including acetone oxidation and pyrolysis reactions are added to the GRIMech 3.0 mechanism to simulate acetone/air mixtures [13]. Combustion of kerosene/air mixtures cannot be easily modeled because of their complex and variable chemical composition. To overcome this problem, the calculation of kerosene laminar flame speed was carried out by using the Luche skeletal mechanism [11] derived from the El-Bakali-Ristori mechanism [12]. The Luche mechanism consists of a reduced mechanism with associated rates coefficient expressions and thermodynamical parameters for 91 species. This mechanism has been validated with perfectly-stirred reactor calculation in the range of initial temperature  $T = 300$ -1800 K, pressure 0.5-10 MPa, and equivalence ratios  $\phi = 0.5$ -2.0. It should be noted that the Luche kerosene chemical composition is a mixture of n-decane (C<sub>10</sub>H<sub>22</sub>), aromatic (C<sub>9</sub>H<sub>12</sub>) and naphthenic (C<sub>9</sub>H<sub>18</sub>) molecules (see the composition in table 2). CH<sub>4</sub>/air, Acetone/O<sub>2</sub>/N<sub>2</sub> and Luche kerosene/air laminar flame speeds were calculated in the 0.1-0.5 MPa pressure range and for equivalence ratios ranging from 0.6 to 1.4. The initial temperature was between 300 and 600 K. For each condition, the previous defined flame thickness was deduced from the numerical simulation profiles of  $T$  and OH.

	Composition	Mass fraction	Molar fraction
Linear	C <sub>10</sub> H <sub>20</sub>	0.767	0.7396
Aromatic	C <sub>9</sub> H <sub>12</sub>	0.132	0.1507
Naphthenic	C <sub>9</sub> H <sub>18</sub>	0.101	0.1097
Kerosene	C <sub>9.7396</sub> H <sub>20.0542</sub>	1.000	1.000

Table 1: Composition of Luche Kerosene.

## 5. Results and analysis

Four fuels were tested using this system, CH<sub>4</sub>/air, Acetone/air, Jet A-1/N<sub>2</sub>/O<sub>2</sub> and surrogate kerosene LUCHE/N<sub>2</sub>/O<sub>2</sub>. The experimental results of each fuel are presented and analyzed in the following sections comparing with the numerical simulated results.

### 5.1 CH<sub>4</sub>/air and acetone/air flame

The first measurement of laminar flame speed was performed using CH<sub>4</sub>/air to validate the system measurement accuracy in comparing with previous experimental measurements from literatures and numerical simulation results. As shown in Fig. 4, for an equivalence ratio range of  $\phi = 0.7-1.4$ ,  $T = 300$  K and ambient pressure  $P = 0.1$  MPa condition, a general good agreement is observed comparing with previous experimental works as well as numerical simulations which suggests the accuracy of our measurement system and image processing algorithm.

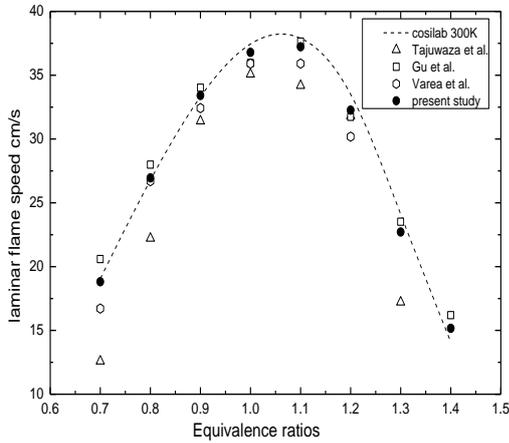


Fig.4. Laminar flame speed  $S_u$  comparison between experimental measurements and previous literature results and simulated results (CH<sub>4</sub>/air  $T = 300$  K,  $P = 0.1$  MPa).

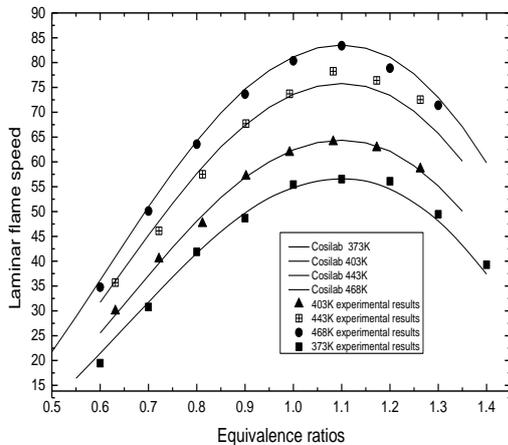


Fig.5. Laminar flame speed of acetone/N<sub>2</sub>/O<sub>2</sub> versus initial temperature variation. (Symbols represent experimental data, lines are modeling results)

There is a slight discrepancy for richer equivalence ratio side where the simulated CH<sub>4</sub>/air flame speed is greater than experimental measurement results. To study the piloted flame influence to flame speed accuracy, the flame speed comparison between a measurement with piloted flame and without piloted flame was performed. A small difference was observed (1~2 cm/s), moreover it was observed that the influence of piloted flame was less obvious in high temperature condition which enable us to neglect its influence in high temperature condition for liquid fuel flame speed measurements which is normally tested in a temperature minimum 373 K. The value presented here are averaged value considering the scatter and the number of data points in the raw dataset.

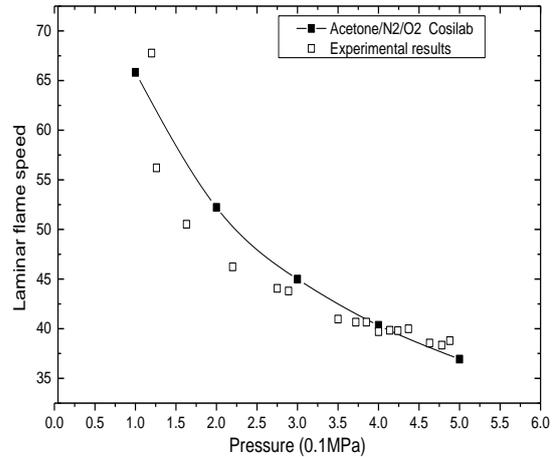


Fig.6. Acetone/N<sub>2</sub>/O<sub>2</sub> laminar flame speed versus pressure variation in  $T = 473$  K,  $\phi = 0.8$ ,  $P = 0.1-0.5$  MPa.

In order to valid the vaporization system and laminar flame speed measurement accuracy for liquid fuel, neat fuel/air mixtures was firstly tested. In considering acetone's low vaporization temperature property and its relatively well known chemical mechanism, which allows us to comparing with numerical simulation results, the acetone/N<sub>2</sub>/O<sub>2</sub> mixture was firstly tested in a working condition of  $T = 473$  K,  $P = 0.1-0.5$  MPa and equivalence ratio  $\phi = 0.6-1.3$ . Experimental results of laminar flame speed of acetone/air were shown in Fig.6 in variation of pressure; a higher pressure leads to a decrease of flame speed. The change in flame speed at lower pressure is more noticeable than at higher pressure levels. This is also in agreement with the literature where the influence of pressure on laminar flame speed was numerically investigated for higher pressure, whilst the flame speed becoming almost constant for pressure higher than 0.8 MPa. Comparing with the numerical simulation accomplished in this work, it is found that the numerical simulation gives a higher flame speed comparing with empirical results from 0.1 MPa to 0.3 MPa and a better accordance in 0.3 MPa to 0.5 MPa. The whole trend

shows a good agreement with literature and simulation results as well. Acetone/N<sub>2</sub>/O<sub>2</sub> laminar flame speed measurements were conducted prospectively in high temperature. Experimental and modeling results were shown in Fig. 5 at elevated initial gas mixture temperature: 373K, 403K, 443K and 468K. It can be found that experimental and modeling results are in good agreement on the lean side. On the equivalence ratio richer part, however it shows a discrepancy that experimental measurements are overestimated compared with simulation results.

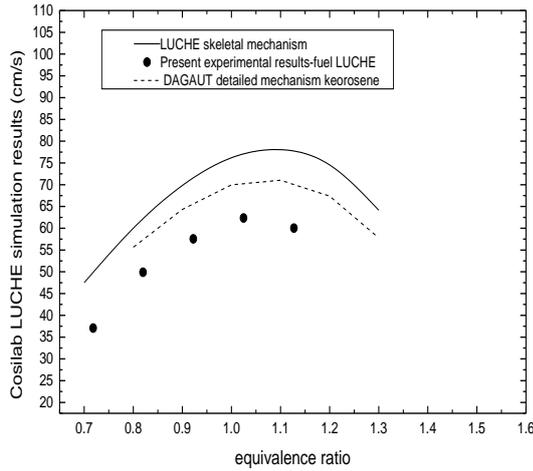


Fig.7. Laminar flame speed of fuel LUCHE/N<sub>2</sub>/O<sub>2</sub> versus equivalence ratio variation (T = 473 K, P = 0.1 MPa).

### 5.2 Kerosene (jet-fuel)/N<sub>2</sub>/O<sub>2</sub> flame

The experimental results of multi-component jet fuel laminar flame speed were discussed in this section. Two jet fuels were experimentally investigated, Jet A-1 fuel and surrogate jet fuel (LUCHE components). The components of LUCHE surrogate fuel were discussed in previous section. In order to avoid the condensation of the fuel, the working temperature was kept with minimum at 473 K. The LUCHE surrogate fuel was determined both experimentally and numerically in two temperatures T = 473 K and T = 523 K with equivalence ratio 0.75-1.35. As presented in Fig. 7 and Fig 8, the trends and the main features are well captured that the maximum flame speed was shown in equivalence ratio around 1.05 and the increase of initial temperature leads to an increase of flame speed. The measurements results of 473 K were compared with LUCHE mechanism simulation results accomplished in current work and compared with other chemical detailed mechanism simulation results found in literature (DAGAUT detailed mechanism scheme [5]). The shown data points in Fig.7 exhibits a discrepancy that the numerical results by LUCHE mechanism are overestimated the flame speed about 10 cm/s. The DAGAUT detailed mechanism simulation results are smaller and more approach to current experimental work.

This is also in agreement with shown results by Lu & Law [14] that a skeletal mechanism can predict a larger flame speed than its parent detailed mechanism.

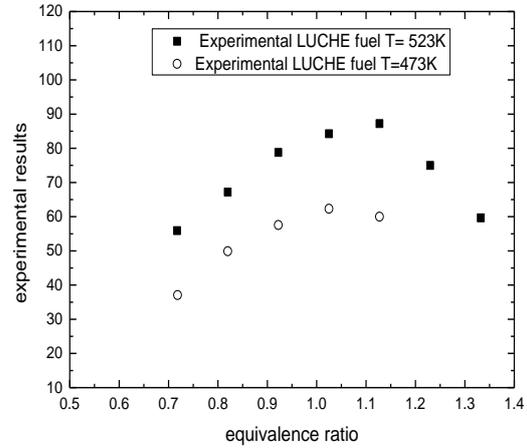


Fig.8. Experimental measurements of fuel LUCHE/N<sub>2</sub>/O<sub>2</sub> with T = 473 K and T = 523 K,  $\phi = 0.7-1.35$ , P = 0.1 MPa.

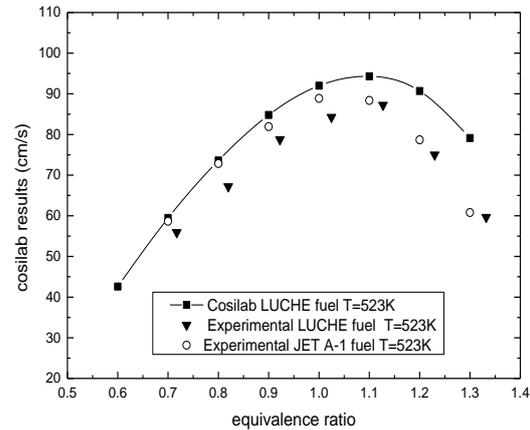


Fig.9. Experimental results of laminar flame speed comparison between fuel Jet A-1, surrogate kerosene LUCHE fuel and numerical simulation results at T = 523 K, P = 0.1 MPa and  $\phi = 0.6-1.3$ .

In order to learn the chemical difference between surrogate LUCHE fuel and Jet A-1 fuel which could yields to flame speed difference, experimental measurements were performed at the same temperature T = 523 K and pressure P = 0.1MPa condition for both surrogate LUCHE fuel and Jet A-1 fuel. As Jet A-1 fuel is a multi-component mixture of thousands of hydrocarbons, the average molecular formulation of kerosene Jet A-1 used in the present study was considered as C<sub>11.16</sub>H<sub>20.82</sub> with a molar mass 154g/mol [8]. In Fig. 9 the laminar flame speed of LUCHE surrogate fuel and Jet A-1 is represented with initial mixture temperature 523 K. The laminar flame speed of Jet A-1 exhibits greater value compared with LUCHE fuel on the fuel lean side, while still slightly under the simulated values. On the fuel rich side, flame tip opening phenomenon was observed when  $\phi >$

1.2. Flame area calculation can't proceed precisely that suggests the reason of the more obvious discrepancy on fuel rich side  $\phi = 1.3$ . The maximum flame speed was shifted to equivalence ratio 1.0 for Jet A-1 fuel results; this could be caused by the uncertainty of Jet A-1 fuel components. Due to the fact that the crude oil originates from a variety of locations on the earth, the chemical composition even for the same type of kerosene according to the ASTM standards can be different. From the view of similar flame speed of LUCHE fuel, it indicates that LUCHE surrogate fuel could be a possible alternative for jet fuel in aeronautic applications.

## 6. Conclusion

A laminar flame speed measurement system for liquid fuel was proposed using Bunsen flame with average surface method. Four different fuel/air mixtures flame speed were determined in a wide range of equivalence ratio, temperature and pressure conditions both experimentally and numerically. The measured laminar flame speed of acetone/N<sub>2</sub>/O<sub>2</sub> and CH<sub>4</sub>/air shows a good agreement with numerical simulation results in ambient pressure conditions. Laminar flame speed comparison between surrogate kerosene fuel and fuel Jet A-1 was accomplished, a similar flame speed was observed at temperature 523 K for both surrogate LUCHE kerosene and Jet A-1 fuel. However, the kerosene/air simulated results for laminar flame speed using LUCHE detail chemical mechanism exhibits an overestimation of laminar flame speed.

For high pressure laminar flame speed measurements, acetone/O<sub>2</sub>/N<sub>2</sub> flame shows good flame stability and the experimental results exhibits a satisfying agreement with numerical determined results. For high pressure kerosene fuel laminar flame speed measurements, as the flame stability in high pressure is difficult to maintain, the flow control system should be carefully regulated. In current research project, investigations of high pressure laminar flame speed measurement of kerosene/N<sub>2</sub>/O<sub>2</sub> using Bunsen flame is a work in progress.

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