

# Effects of Pressure and Temperature on Laminar Burning Velocity of a Kerosene Surrogate

Romain LE DORTZ<sup>1,2</sup>, Marc BELLENOUE<sup>2</sup>, Julien SOTTON<sup>2</sup>, Camille STROZZI<sup>3</sup>

<sup>1</sup> Safran Tech, Safran R&T Center, CS 80112, 78722 Magny-Les-Hameaux, France

<sup>2</sup> Institut Pprime, CNRS, ISAE-ENSMA, Université de Poitiers, F-86962 Futuroscope Chasseneuil, France

<sup>3</sup> Institut Pprime, CNRS, Université de Poitiers, ISAE-ENSMA, F-86962 Futuroscope Chasseneuil, France

## 1 Introduction

For many years, aeronautical industry has favored heavy fuels due to their safety characteristics and storage and transport simplicities. Pollutant emissions are actually a major issue in the design of current turbo-engines. Environmental international bodies as ACARE for Europe (Advisory Council for Aviation Research and Innovation in Europe) require more and more drastic objectives in terms of pollutant emission and consumption reduction [1]. To reach these objectives, innovative solutions with technological breakthrough are in development, as constant-volume combustion which promises a 10% to 20% consumption reduction in comparison to current engines [2]. As a first step, a better understanding, characterization and control of combustion process of kerosene-air mixtures during constant-volume combustion is necessary. Indeed, knowledge on the basic premixed combustion properties of kerosene/air mixtures still has to be improved. This is the case especially for the flame front propagation in laminar adiabatic conditions. Laminar flame speed is one of the most essential physical properties [3] related to both constant-volume combustion process and gasoline piston engines. Although laminar burning velocity were extensively studied over the last decades with various techniques, only a few recent publications deal accurately with these essential data for liquid jet fuels. In parallel, there is considerable interest in the scientific community to develop kinetic models better representing the combustion processes of kerosene. Commercial jet fuel is composed of hundred components, and its composition depends on its production place [4]. In order to obtain reproducible experiments, the laboratory experiments are often performed with a surrogate fuel representing kerosene. It is composed of a few species and most studies uses from one to about ten components. The present study focuses on laminar flame speed of a *n*-decane/*n*-propylbenzene/*n*-propylcyclohexane surrogate, measured using a new spherical combustion chamber in high temperatures and pressures. The experimental set-up is first validated with a *n*-decane/air mixture. Experimental results are detailed in sections below, for initial temperatures ranging from 400 K to 470 K, initial pressures of 0.1 MPa to 0.5 MPa and equivalence ratios varying between 0.6 to 1.5. Results are compared to numerical

simulations and to previous studies. This surrogate is selected because its reduced kinetic mechanism is employed in aeronautical industry. Nevertheless, to the knowledge of the authors, only a recent paper reports experimental data for this surrogate in terms of flame velocity and Markstein length [5], and is based on another technique of flame velocity measurement (Bunsen burner). Moreover, the reduced kinetic mechanism employed to represent the surrogate was only validated to model molar fraction profiles in perfectly stirred reactor and ignition delays in shock tubes [6]. This highlights the relevance of a validation work concerning laminar burning velocities.

## 2 Experimental methodology

### 2.1 Experimental set-up

The experimental set-up is a stainless-steel spherical combustion chamber with a 4.2 L inner volume (0.2 m in diameter), fitted with 2 UV-sapphire windows with a 0.07 m diameter (Fig. 1). The vessel can be heated up to 470 K and is designed for initial pressures reaching up to 10 bar. The walls of the chamber and the feeding lines are regulated in temperature by 24 cartridges heaters and 4 K-thermocouples (2 fixed on the vessel, and 2 fixed on the feeding lines). The vacuum is performed with a rotary-vane pump until reaching a pressure lower than 200 Pa. Chamber pressure variation during combustion is measured by a piezoelectric dynamic pressure transducer (Kistler 6054AR 0-250 bar) protected with a silicone layer of 2 mm in thickness, and used with a Kistler ICAM amplifier (Type 5073A). Combustion is initiated with an electrical discharge of approximately 20 mJ deposited between two pin to pin tungsten electrodes with a 1 mm diameter by an inductive ignition circuit. The gap between the electrodes is adjustable and set to 1 mm for this study.

The flame propagation is monitored by a Schlieren visualization system using a high speed camera Photron FASTCAM SA5 at a frame recording rate of 7 kHz. Pictures resolution is 1,024\*1,024 pixels<sup>2</sup>. The light source is a collimated LED. The camera recording and the pressure measurements are synchronized with the onset of the spark between the two electrodes thanks to a TTL signal. These synchronized signals allow to control that all the measurements occur at constant pressure.

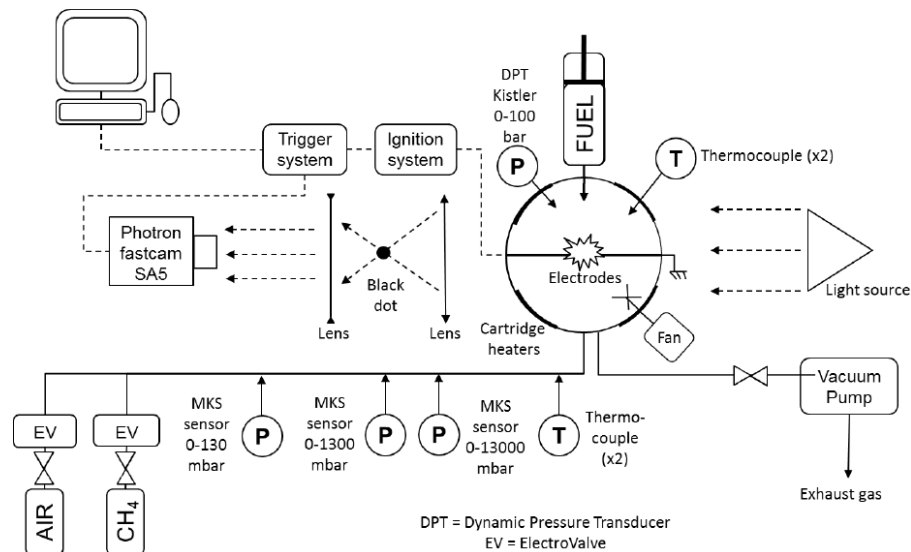


Figure 1. Schematic of the experimental set-up

## 2.2 Mixture preparation

Particular attention is paid to the preparation of the mixture: a difference between expected and real conditions (temperature, pressure, equivalence ratio, ...) can skew the results [7] [8]. The mixture preparation is automatically carried out by the method of partial pressures. Two injection lines are used for gas and a low-pressure automotive injector is used for liquids. The pressure of injected gas into the combustion chamber is regulated by two multiplier dome pressure regulators without automatic decompression. The pressures are controlled by three absolute pressure transducers (MKS Baratron Type 631) calibrated with different full scales: the first on 0-100 torr (heated transducer), the second on 0-1000 torr (heated transducer), and the last one on 0-10,000 torr (non heated transducer) to reach the higher tested pressures ( $P > 1.5$  bar). These different scales provide a good accuracy on the equivalence ratio of the mixture for a large panel of fuels (uncertainty on equivalence ratio lower than 1.5 %).

The jet fuel surrogate is prepared with high purity grade commercial chemicals: *n*-decane (Merck,  $\geq 99$  %), *n*-propylbenzene (Merck,  $\geq 98$  %), *n*-propylcyclohexane (Sigma-Aldrich,  $\geq 98.5$  %). The Dagaut surrogate chemical composition employed in this study is a mixture of 76.7 % *n*-decane, 13.2 % *n*-propylbenzene and 10.1 % *n*-propylcyclohexane in mass fraction, and the average chemical formula is  $C_{9.74}H_{20.05}$  [9]. Mixtures are completed with synthetic air prepared with high purity oxygen and nitrogen (both 99.99 % pure) with molar ratio of  $N_2:O_2 = 3.76$ .

## 2.3 Laminar flame speed measurements

The time-evolution of the flame radius  $R_f(t)$  is extracted frame per frame from the Schlieren records using a Matlab program (Fig. 2). Pictures are binarized and the flame edge is determined automatically. Area of the flame is then calculated along with the equivalent radius.

The propagation speed  $S_b$  is calculated from the radius time-evolution with a second-order centered scheme. The stretch rate  $\kappa$  is also evaluated in order to extrapolate the unstretched laminar burning velocity of burnt gases  $S_b^0$  and the Markstein length  $\mathcal{L}_b$  with the non-linear model of Kelley and Law (model which best represents the flame evolution) (Eq. 1) [10].

$$\left(\frac{S_b}{S_b^0}\right)^2 \cdot \ln\left(\frac{S_b}{S_b^0}\right)^2 = -\frac{2 \mathcal{L}_b \kappa}{S_b^0} \quad (1)$$

The unstretched laminar burning velocity  $S_u^0$  and unburnt Markstein length  $\mathcal{L}_u$  are finally determined with the expansion factor  $\sigma = \rho_u/\rho_b$ , where  $\rho_u$  and  $\rho_b$  are respectively the unburnt and burnt gas density. Their values are calculated for an adiabatic combustion with the help of CANTERA [11] and the chemical kinetic mechanisms [6] and [12] presented in section 3. Only frames without cells on flame are used to extrapolate the flame speed. Sometimes, cells can appear during combustion phenomenon but outside the range of radii employed for extrapolation of laminar burning velocity. These instabilities are due to hydrodynamic and thermodiffusive effects, generate a flame front acceleration and appear increasingly rapidly with increasing pressure and equivalence ratio.

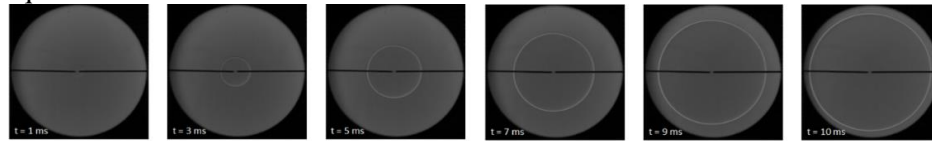


Figure 2. Time-evolution of flame radius for a *n*-decane/air mixture at initial temperature  $T_0 = 400$  K,  $P_0 = 0.1$  MPa and equivalence ratio  $\Phi = 1.0$ .

### 3 Numerical simulations

Experimental results are compared with numerical simulation performed with CANTERA chemical kinetic software [10]. The code simulated the free propagation of a one-dimensional unstretched adiabatic flame using chemical kinetic mechanisms and the associated transport and thermodynamic data. *n*-Decane/air flames are simulated using the JetSurf 2.0 detailed chemical kinetic mechanism (348 species/2163 reactions) [12] and jet fuel surrogate/air flames are simulated using the reduced Luche chemical kinetic mechanism (91 species/991 reactions) [6].

## 4 Results

### 4.1 Experimental set-up validation with *n*-decane/air flames

The first measurements of laminar burning velocities with liquid fuels were performed using *n*-decane/air mixture to validate the experimental set-up measurement and the Matlab post-processing algorithm, in comparison with data from literature and numerical simulations. *n*-Decane/air flames were tested at initial temperature  $T_0 = 400$  K, initial pressure  $P_0 = 0.1$  MPa and equivalence ratios range of  $\Phi = 0.7 - 1.5$ . These first results can be observed in Fig. 3. The maximum estimated uncertainty for the unstretched laminar burning velocity is less than 3 cm/s. This uncertainty also takes into account the uncertainty on extrapolation according to the York method. The experimental results shown are in excellent agreement with those of literature [13, 14] using the same method for measuring laminar flame speeds, namely the spherical bomb method. Indeed, on average, differences of 0.7 % over the lean side and of 2.6 % over the rich side are observed in comparison with the results of Comandini et al. [14]. The experimental set-up can be considered as validated for liquid fuels. In addition, calculations with JetSurf 2.0 mechanism are also in very good agreement, although the maximum of the unstretched laminar burning velocity is slightly underestimated. Differences between our measurements and these calculations are respectively evaluated at 2.1 % and 3.5 % on the lean and the rich side.

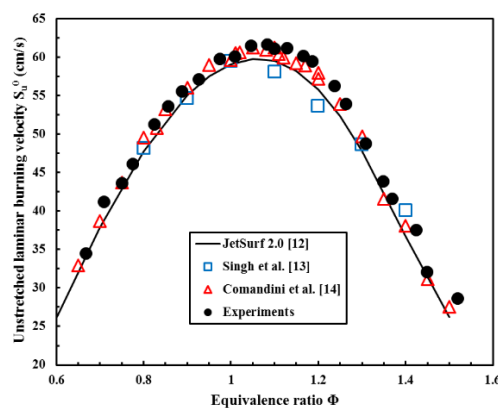


Figure 3. Unstretched laminar burning velocity  $S_u^0$  plotted against equivalence ratio  $\Phi$  for a *n*-decane/air mixture at  $T_0 = 400$  K and  $P_0 = 1$  bar.

### 4.2 Results for Dagaut jet fuel surrogate/air flames

This section presents the experimental and numerical results obtained for the Dagaut jet fuel surrogate for various initial temperatures, pressures and equivalence ratios. The influence of initial temperatures is first studied at an initial pressure  $P_0 = 1$  bar in Fig. 4.a. The observed trends are typical of hydrocarbons fuels:

the unstretched laminar flame speed is maximum for a slightly rich mixture ( $\Phi \approx 1.12$ ) and the velocity decreases abruptly as soon as one moves away from this optimum equivalence ratio. Increasing the initial temperature boosts the unstretched laminar burning velocity of the jet fuel surrogate. On the contrary, increasing the initial pressure causes a decrease in laminar burning velocity (Fig. 4.b and Fig. 4.c). The Luche reduced kinetic mechanism is able to aright represent the measurements: a very good agreement is obtained on the lean side with a maximum difference on the average of 3.5 % between measurements and calculations. The rich side is also correctly represented with a maximum difference of 6%. The Luche reduced kinetic mechanism can be considered as validated for laminar burning velocities.

Unburnt Markstein length can be easily obtained with spherical flames although a good precision is hard to obtain for this parameter. In Fig. 5.a, temperature seems to have no effect on its evolution. For an initial pressure  $P_0 = 1$  bar, the Markstein length is decreasing with increasing equivalence ratio and becomes negative at  $\phi \approx 1.35$ . At this equivalence ratio value and beyond, the flame is unstable and the diffusion instabilities are prevalent. These instabilities create wrinkles on the flame edge at an earlier stage of the flame propagation. Fig. 5.b shows that increasing pressure makes the flame unstable at a lower equivalence ratio ( $\phi \approx 1.20$ ).

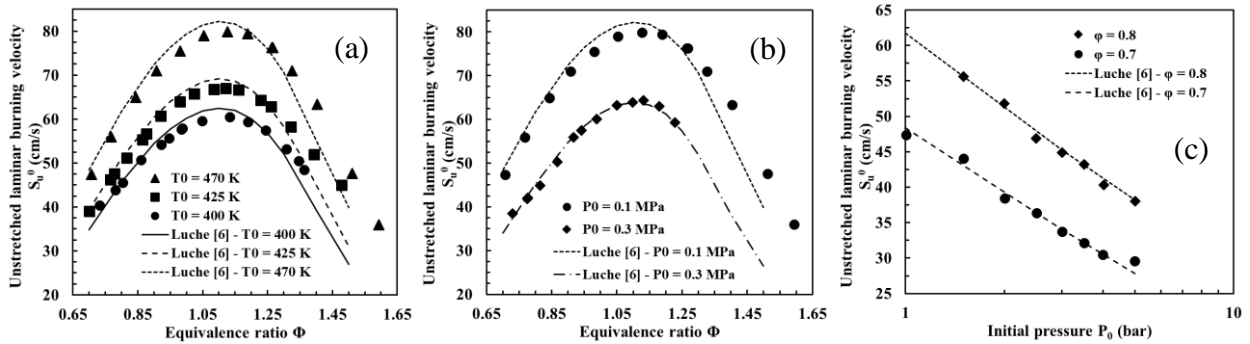


Figure 4. Unstretched laminar burning velocity  $S_u^0$  plotted against equivalence ratio  $\Phi$  for a Dagaut jet fuel surrogate/air mixture at (a)  $P_0 = 0.1$  MPa (b)  $T_0 = 470$  K (c)  $T_0 = 470$  K.

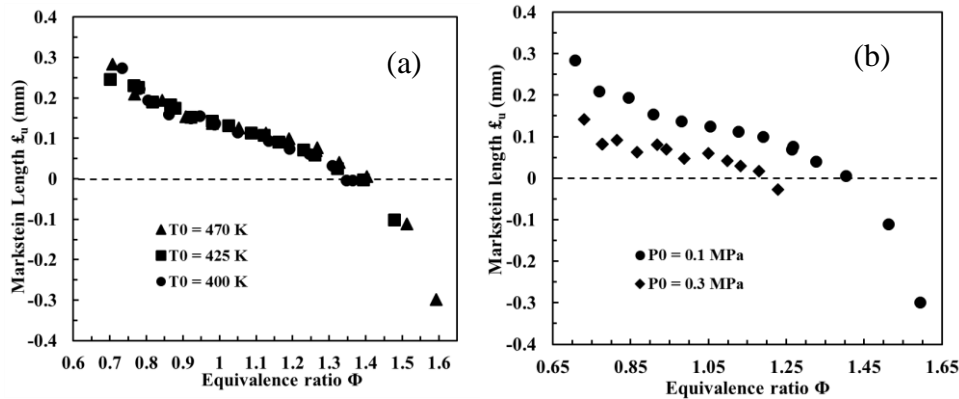


Figure 5. Markstein length  $L_u$  plotted against equivalence ratio  $\Phi$  for a Dagaut jet fuel surrogate/air mixture at (a)  $P_0 = 0.1$  MPa (b)  $T_0 = 470$  K.

## 5 Conclusion

The laminar flame speeds of single- and multi-components jet fuel surrogates have been measured in this study using a new spherical bomb chamber (developed at Institut PPRIME). A non-linear extrapolation method was used for various conditions of initial temperatures, initial pressures and equivalence ratios. The technique was first validated measuring laminar burning velocities of *n*-decane/air flames and comparing with data from the literature. The measurements were then performed for a more complex surrogate of kerosene: *n*-decane/*n*-propylbenzene/*n*-propylcyclohexane. Both pressure and temperature have influence on laminar burning velocity. The Luche reduced kinetic mechanism was able to represent the data for the different tested conditions. Although this mechanism was not initially developed to represent laminar burning velocities, the validation for this parameter can be considered as effective. Markstein lengths of the three-components jet fuel surrogate were also measured. As expected, pressure has a strong influence on the flame stability. But contrary to flame velocity, temperature has no effect.

## Acknowledgements

This work was financially supported by Safran, MBDA and ANR in the framework of the CAPA Chair project on innovative combustion modes for airbreathing propulsion. The authors would also thank E. Mazanchenko for providing her knowledge in experimental support.

## References

- [1] Flightpath 2050 Europe's vision for aviation – Report of the high level group on aviation research. Technical report, Advisory Council for Aviation Research and innovation in Europe (ACARE), 2011.
- [2] Wintenberger E, Shepherd JE. (2006). Thermodynamic cycle analysis for propagating detonations. *J. Prop. Power* 22:694-698.
- [3] Shy SS, Liu CC, Shih WT (2010). Ignition transition in turbulent premixed combustion. *Comb. Flame* 157:341-350.
- [4] Violi A, Yan S, Eddings EG, Sarofim A. (2002). Experimental formulation and kinetic model for JP-8 surrogate mixtures. *Comb. Sci. Tech.* 174:399-417.
- [5] Wu Y, Modica V, Grisch F (2015). Laminar flame speed measurement of multicomponent Jet A-1 and LUCHE kerosene surrogate fuels in elevated pressure and temperature conditions. *Proc. of the European Combustion Meeting 2015*.
- [6] Luche J. (2003). Elaboration of reduced kinetic models of combustion. Application to a kerosene mechanism, PhD Thesis. LCSR Orléans.
- [7] Chen Z. (2015). On the accuracy of laminar flame speeds measured from outwardly propagating flames: Methane/air at normal temperature and pressure. *Comb. Flame* 162:2442-2453.
- [8] Beeckmann J. (2015). Uncertainties in spherical flame measurements: a collaborative study. 2<sup>nd</sup> Workshop on Laminar Burning Velocity, Rouen, France.
- [9] Dagaut P, El Bakali A, Ristori A. (2006). The combustion of kerosene: Experimental results and kinetic modelling using 1- to 3-component surrogate model fuels. *Fuel* 85:944-956.
- [10] Kelley AP, Law CK. (2009). Nonlinear effects in the extraction of laminar flame speeds from expanding spherical flames. *Comb. Flame* 156:1844-1851.
- [11] Goodwin DG, Moffat HK, Speth RL (2016). Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. <http://www.cantera.org>, Version 2.2.1.
- [12] Wang H, Dames E, Sirjean B, Sheen DA, Tangko R, Violi A, Lai JYW, Egolfopoulos FN, Davidson DF, Hanson RK, Bowman CT, Law CK, Tsang W, Cernansky NP, Miller DL, Lindstedt RP. (2010). A high-temperature chemical kinetic model of *n*-alkane (up to *n*-dodecane), cyclohexane, and methyl-, ethyl-, *n*-propyl and *n*-butyl-cyclohexane oxidation at high temperatures, JetSurF version 2.0.
- [13] Singh D, Nishiie T, Qiao L. (2011). Experimental and kinetic modeling study of the combustion of *n*-decane, Jet-A, and S-8 in laminar premixed flames. *Comb. Sci. Tech.* 183:10:1002-1026
- [14] Comandini A, Dubois T, Chaumeix N. (2015). Laminar flame speeds of *n*-decane, *n*-butylbenzene, and *n*-propylcyclohexane mixtures. *Proc. Combust. Inst.* 35:671-678