

# DETERMINATION OF SOOT VOLUME FRACTION AND PARTICLE SIZING IN FARNESANE-KEROSENE WICK-FED DIFFUSION FLAMES

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Abstract. The whole world is concerned about running out of petroleum in the future. There is also the concern about the emissions to the environment, caused by the combustion processes, which are responsible for about 90% of all primary energy produced in the world. The renewable biofuels are currently seen as good alternatives, which may be able to address both concerns. One of the most promising biofuels, to be used in the world transportation sector, on ground and in air, is the Farnesane  $(C_{15}H_{32})$ , an hydrocarbon produced by adding Hydrogen to the Farnesene, extracted from yeast-fermented sugar cane. Among the air pollutants emitted by any combustion process, the particulates are the most harmful to the environment. The ones which size is lower than 100 nm are known as soot and their formation is associated with hydrocarbons cracking reactions that generate solid condensed cores, mainly under rich combustion and at high temperatures. The soot emission is not only harmful to the environment but also represents a loss of useful energy, negatively affecting the efficiency of any combustion process. This work provides a comparison of the soot volume fraction and particle sizes on wick-fed diffusion flames from mixtures, in different proportions (0, 5, 10, 20, 50, 75 and 100%), of Aviation Kerosene, also known as aviation turbine fuel or simply Jet Fuel, with Farnesane, using the Laser Induced Incandescence (LII) technique, in order to evaluate the effects of the presence of the Farnesane in the Aviation Kerosene combustion. The results demonstrate that the maximum concentration of soot is located 11 mm above the burner and that the addition of Farnesane to the Kerosene causes the soot concentration to decrease. Concerning the soot particle diameters, they present low axial variation for fuel blends with low quantities of Farnesane. The soot particle sizes decrease at fuel blends with higher proportions of Farnesane, and for all fuel blends the lowest soot particle sizes are observed at 11 mm above burner, same height as the highest soot volume fractions.

Keywords: Soot, Farnesane, Incandescence, Combustion, Emissions

## 1. INTRODUCTION

The combustion processes are involved in more than 90% of all primary energy produced in the planet, according to the International Energy Agency, on its 2011 Key World Energy Statistics. The dependency of mankind with such processes leads to two main concerns: the availability of fuel and the emission of air pollutants, which are harmful to the environment and to the humans' health. Regarding the first concern, the transport sector is still widely dependent on petroleum based fuels, which reserves are finite, forcing the countries to look for other alternatives, preferably the renewable ones. About the second concern, the world population growth causes the demand for energy to increase, leading consequently to an increase on the emissions to the environment.

Therefore, developing fuels that, not only come from renewable sources, but also which combustion products are less harmful to the environment are a key factor for the future of the planet. These new generation of fuels, from renewable sources and environmentally friendly, are commonly called biofuels.

The main pollutants resulting from the combustion processes are the sulfur dioxide ( $SO_2$ ), the mono-nitrogen oxides ( $NO_x$ ), the carbon monoxide (CO), the Unburned Hydrocarbons (UHCs) and the particulates. This last is the most harmful to the environment and the ones which size is lower than 100 nm are known as soot. Its formation is associated with hydrocarbons cracking reactions that generate solid condensed cores, mainly under rich combustion and at high temperatures.

The soot particles are formed mainly in the primary zone of diffusion flames, where, in general, the combustion occurs without enough oxygen. However, if the mix between the combustion reagents is not adequate, the soot formation can occur anywhere in the flame. The majority of the soot produced in the primary region of the flame can be consumed in the secondary region of it, which is a region where the oxygen concentration is higher, if the temperature is sufficiently high. Therefore, from the soot formation standpoint, the flame can be divided into two distinct regions:

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the primary region, which governs the soot production rate; and the secondary region, which defines the soot consumption rate. The presence of soot in the combustion products depends on the balance between these two regions.

The emission of soot particles on a combustion system affects its irradiative characteristics and influences the global energetic aspects of the reactions. Concerning the thermodynamic aspects, the soot formation causes loss of energy associated with the incomplete combustion process. Regarding the environmental aspects, the soot formation represents a large portion of the total particulate material present in the atmosphere of big and highly industrialized cities, being directly associated with respiratory diseases and even deaths.

# 2. THE FARNESANE

The Farnesane is currently one of the most promising biofuels in the world, to be used in the transport sector. It is an hydrocarbon produced by adding Hydrogen to the Farnesene ( $C_{15}H_{24}$ ), extracted from yeast-fermented sugar cane, which transforms it in the  $C_{15}H_{32}$ , as illustrated on Fig. 1. Besides the fact that the Farnesane comes from a renewable source, the CO<sub>2</sub> released from the combustion of it is captured during the sugar cane growth process.



Figure 1. Farnesane Formation

The Farnesane has the potential to become a fuel with same characteristics as the Aviation Kerosene, keeping the same performance, which leads to the necessity of investigating its emissions, in order to cover all the current world concerns.

### 3. LASER INDUCED INCANDESCENCE (LII)

The LII technique is based on the capture of blackbody radiation emitted by the soot particles, when shot by a high energy pulsed laser. When the soot is hit by the laser beam, it is heated up to its vaporization temperature. The duration of each laser pulse is in the order of 10 ns or less and the energy density is greater than 0.2 J/cm<sup>2</sup>. When the laser energy is increased, the LII signal increases while the soot particle is being heated. At a certain energy level, subsequent increases in the laser energy will practically not affect the LII signal anymore. This happens because at this point the soot particle has reached its vaporization temperature, which is about 4000 to 5000 K, and the LII signal becomes almost constant, not being anymore influenced by the laser energy density.

The soot incandescence signal is captured by a photomultiplier, which converts it into a voltage signal that can be read through an oscilloscope. This voltage signal, captured in the oscilloscope, represents the soot particle heating and subsequent cooling, within the control volume measured.

According to Boiarciuc, *et al.* (2004), the signal captured by the oscilloscope shows a steep ramp-up, which lasts a few nanoseconds, in the order of the laser pulse duration, followed by a smooth decay curve, lasting a few hundreds of nanoseconds.

Based on Melton (1984), the captured signal intensity is proportional to the soot volume fraction, while the decay curve is directly related to the average soot particle diameter, meaning that the larger the particle slower is its cooling.

Therefore, the LII technique can be used to determine both the soot particle size and the soot volume fraction at any point of a flame. The Fig. 2 illustrates a typical LII signal with its regions of interest.



Figure 2. Typical LII Signal with Regions of Interests

### 3.1 Determination of soot volume fraction

The application of the LII technique adopted on this work, to determine the soot volume fractions, followed the methodology known as "Auto-Calibration Technique", developed by Smallwood, *et al.* (2002). It consists in capturing the incandescence signal in two different detection wavelengths in order to determine the temperature reached by the soot particle, heated by the laser. In order to capture the LII signal in two distinct wavelengths, two monochromators, coupled with two photomultipliers, were used. Having determined its temperature, the soot volume fraction may be determined.

According to Vander Wal (2000), high intensity ultraviolet laser pulses produce unwanted photochemical processes in soot containing flames, adding a spurious signal that will likely be unrelated to the soot concentration. Therefore, Vander Wal (2000) proposes the use of long-wavelength irradiation, such as 1064 nm, since in general it is energetically incapable of generating the referred processes while still capable of producing soot incandescence.

Also, the detection wavelength, adjusted in the monochromator, shall be such that it does not coincide with any spectral interference associated with the combustion process or with the flame luminosity.

For the experiments that supported this work, the monochromators used were the Shoeffel 1118 lines/mm, model GM 250, adjusted to 410 nm and the Optometrics LLC, model MC1-01, adjusted to 600 nm. The laser cannon was the Quantel, model Twin, adjusted to a wavelength of 1064 nm and a frequency of 10 Hz. The Fig. 3 shows a simplified schematic of the experimental set-up.

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Figure 3. Simplified Experimental Set-up

The first step in the calculation of the soot volume fraction is the determination of the soot particle temperature. In order to determine it, a calibrated temperature source, which spectral radiance at a certain distance be known, is required. A 32 V, and 200 W power, calibrated quartz tungsten halogen lamp has been used on this work. The position of this calibrated source in regards to each monochromator shall be the same as the wick-fed lamp during the experiments. This way, the calibration factor, which is the relation between the signal captured in the oscilloscope from the calibrated source, through the two photomultipliers,  $S_{SOURCE}(\lambda 1)$  [V] and  $S_{SOURCE}(\lambda 2)$  [V], and the known spectral radiance at each one of the detection wavelengths,  $R_{SOURCE}(\lambda 1)$  and  $R_{SOURCE}(\lambda 2)$  [W/m<sup>3</sup>Sr], may be determined as shown on Eq. (1).

$$\eta(\lambda) = \frac{S_{\text{SOURCE}(\lambda)}}{R_{\text{SOURCE}}(\lambda)}$$
(1)

The calibration factor is assumed to be also valid with the LII signal, which means that the relation between the signal captured in the oscilloscope from the soot incandescence,  $S_{LII}$  [V], and its unknown spectral radiance,  $R_{LII}(\lambda)$ , is assumed to be the same as the one determined with the calibrated source. Therefore, the LII spectral radiance may be determined through Eq. 2.

$$R_{LII}(\lambda) = \frac{S_{LII(\lambda)}}{\eta(\lambda)}$$
(2)

Based on Smallwood, et al. (2002), the temperature reached by the soot particle may be determined via the Eq. (3).

$$T = \frac{h.c}{k} \cdot \left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right) \cdot \frac{1}{\ln(\frac{S_{LII}(\lambda_1).\eta(\lambda_2).\lambda_1^6.E(m)_{\lambda_1}}{S_{LII}(\lambda_2).\eta(\lambda_1).\lambda_2^6.E(m)_{\lambda_2}})}$$
(3)

where *h* [J.s] is the Planck Constant, *k* [J/K] is the Boltzmann Constant, *c* [m/s] is the speed of light and E(m) is the complex refraction index function of the soot. According to Snelling, *et al.* (2000), E(m) measurements performed by several researchers demonstrated that they almost do not depend on the type of fuel nor on the detection wavelength, in the range of 400 to 800 nm. Therefore, considering that  $\lambda_1$  and  $\lambda_2$  have been defined within this range (410 nm and 600 nm), the relation between  $E(m)_{\lambda_1}$  and  $E(m)_{\lambda_2}$  may be approximated to 1, disappearing from the Eq. (3).

After the soot particle temperature has been determined, the soot volume fraction may be found, using the Eq. (4).

$$f_{v} = \frac{S_{LII}(\lambda).\lambda^{6}}{\eta(\lambda).d_{b}.12.\pi.c^{2}.h.E(m)_{\lambda}} \cdot \left(e^{\frac{h.c}{k.\lambda.T}} - 1\right)$$
(4)

where  $d_b$  [m] is the laser beam diameter.

According to Schuocker (1998),  $d_b$  may be determined with the Eq. (5).

$$\boldsymbol{d}_{\boldsymbol{b}} = \boldsymbol{\theta} * \boldsymbol{F}_{(5)}$$

where  $\theta$  [rad] is the laser beam divergence and *F* [m] is the lens focus, represented on Fig. 3 as LENS 1. According to the laser cannon manual, its laser beam divergence is 0.006 rad while the LENS 1 focus is 0.2 m.

The E(m) value chosen for the soot volume fraction calculations of this work was 0.30, as communicated by Snelling, *et al.* (2000), for a 1064 nm wavelength laser.

#### 3.2 Determination of soot particle diameter

Vander Wal, *et al.* (1999) observed two important aspects of the LII signal, which are the basis for the soot particle diameter determination method proposed here. The first aspect concerns the fact that the LII signal decay, shown dashed in the Fig. 4, can be represented, with a very good level of agreement, by a double-exponential curve, as detailed on Eq. (6).



Figure 4. LII Signal Decay Mathematical Function Fit

$$LII(t) = Ae^{\frac{-t}{\tau_1}} + Be^{\frac{-t}{\tau_2}}$$
(6)

The second important aspect observed by VANDER WAL, *et al.* (1999) refers to the two time constants  $\tau_1$  and  $\tau_2$ , which reflect different timescales associated with the different soot particle cooling mechanisms. Assuming  $\tau_1 < \tau_2$ , using the lower time constant  $\tau_1$  (fast decay rate) did not give a monotonic relation with increasing primary particle size, while the greater time constant  $\tau_2$  (slower decay rate) did produce and therefore may be used to build a calibration curve.

From the LII acquisitions, as well as the TEM (Transmission Electron Microscopy) measurements performed by VANDER WAL, *et al.* (1999), the Tab. 1 was produced, where *K* is  $1000/\tau_2$ , the inverse of the greater time constant (slower decay rate), multiplied by 1000 in order to ease its representation and manipulation along the work.

(7)

Fuel	TEM Soot Primary Size (nm)	K (ns <sup>-1</sup> )
Methane (CH <sub>4</sub> )	14.2±1.5	5.9
Ethane $(C_2H_6)$	20.4±1.9	4.2
Ethylene ( $C_2H_4$ )	33.3±3.2	3.5
Acetylene ( $C_2H_2$ )	59.7±3.9	1.8

Table I. Primary Soot Particle Size and Decay Rate	Table 1.	. Primary	Soot	Particle	Size	and Decay	Rates
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The data shown on Tab. 1 allowed the construction of a polynomial, as shown on the Eq. (7), which provides a correspondence between K and D.

 $D(K) = 0.0051K^{6} - 0.1353K^{5} + 1.2961K^{4} - 5.3193K^{3} + 9.39K^{2} - 21.745K + 88.651$ 

# 4. THE WICK-FED DIFFUSION FLAMES

The combustion environment inside a gas turbine is very complex, with several parameters that affect the soot formation varying, driven by the different engine operating regimes, such as: the equivalence ratio in the primary zone of the combustion chamber; the fuel injection conditions; the fuel atomization; etc. Therefore, since the addition of a biofuel to the Aviation Kerosene, also known as Aviation Turbine Fuel, would affect all these parameters, individual experimental investigations involving just one of these parameters, are required.

Inside the combustion chamber of a gas turbine engine, the two kinds of flame conditions, the pre-mixed and the diffusive ones, can be found.

In the present work, the experiments focused on the diffusion flames. In order to allow the comparison of different blends of Aviation Kerosene with Farnesane, concerning the soot volume fraction, as made by Tran et al. (2012) with soybean based biofuel-diesel mixes, all the experiments have been performed with the flames below the smoke point condition, which was defined by Olson et al. (1985) as being the combustion condition with maximum smoke-free laminar diffusion flame height and has been used as a relative measurement of the tendency of fuels to produce soot since the 1930s.

The methodology to determine the flame smoke point, before quantifying the soot volume fraction through the LII technique, followed the procedure defined by the American Society for Tests and Materials (ASTM), document number D1322-12 (2012). The method basically consists of using a wick-fed lamp equipped with an adjustable height wick, where the longer the wick, the higher the fuel flow and the higher the fuel flow, the higher the flame height. The Fig. 5 presents different stages of the flame during the determination of the smoke point.



Figure 5. Different Stages of the Flame during the Smoke Point Determination

## 5. RESULTS AND DISCUSSIONS

The following fuel blends were evaluated: B0 (pure Kerosene), B5 (5% of Farnesane), B10, B20, B50, B75 and B100 (pure Farnesane). The smoke point experiments revealed that the pure Aviation Kerosene has the lowest smoke point, 23 mm and that the addition of Farnesane to it causes the smoke point to increase, almost linearly, reaching the

maximum value of 55 mm, for the pure Farnesane. Therefore, in order to make sure that all the experiments would be performed below the smoke points, the flame length adopted for the LII measurements on all fuel blends was 20 mm.

The soot emissions were measured on the center of the flames, at 6 mm, 8.5 mm, 11 mm, 13.5 mm and 16mm of HAB (Height Above Burner). At each test point, 200 LII measurements have been performed. The Fig. 6 presents the results, concerning the soot volume fractions for all fuel blends. Each point of the plotted curves already represents the mean of the 200 LII measurements mentioned above. The margin of error of the soot volume fractions determined was 15%.



Figure 6. Soot Volume Fractions at Center of Flames

The results show that the highest concentration of soot is located at 11 mm of HAB and also that the addition of Farnesane to the Kerosene causes this concentration to decrease. Some blends with less Farnesane seem to produce less soot than others with more Farneane, however, most of them are within the margin of error, which means that applying the error, the order of the values could be inverted or could even be the same.

Regarding the soot particle diameters, they have been determined based on the same LII signals captured for the soot volume fraction determinations. For each test point the resulting signal from the same 200 measurements has had the decay region isolated and then approximated to a second order exponential decay curve, revealing the slower decay time constant that, after converted to K, it has been inputted on the Eq. (7) which result was the soot particle diameter on that point of the flame. The Fig. 7 presents the results for all fuel blends.

It can be observed that for fuel blends with lower quantities of Farnesane the variation of soot diameters along the flame is lower. At 6 mm above burner, the soot diameter appears on the plot as being zero because, as observed on Fig. 6, the soot volume fractions at this height are very close to zero as well. Besides the fact that soot particle sizes seem to vary more for fuel blends with more Farnesane, these blends present lower particle sizes. Finally, for all fuel blends, the lowest soot particle sizes are located exactly at 11 mm above burner, where the highest concentrations of soot have been observed.

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Figure 7. Soot Particle Diameters at Center of Flames

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