Laminar Flame Speed and Laser Absorption Measurements of Conventional and Alternative Kerosene-Based Liquid Fuels

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1 Introduction

Kerosene-based fuels continue to be among the primary energy sources for the world. However, there are still gaps in the fundamental combustion research for these fuels, and additionally there is also a push to study alternative and synthetic liquid fuels. The overall composition of these synthetic fuels is believed to be very similar to the conventional kerosene fuels, with the primary difference being how (and from where) the fuel is produced. Therefore, the chemical kinetics of the conventional and synthetic fuels are also assumed to be similar, and combustion research into both should be conducted together. The study of these fuels is complicated because these they are blends of hundreds to thousands of different hydrocarbons. As such, either the average chemical formula for a batch of fuel or a surrogate fuel is used as the baseline for analysis. While an average chemical formula might provide more-accurate results for a particular batch of fuel, it is not necessarily transferable to the next batch of fuel produced. This average chemical formula will change, sometimes significantly, from one batch of fuel to the next. A surrogate fuel can provide a good approximation for the fuel properties and provide consistency when comparing several different batches of fuel. However, the preferred surrogate of choice changes over time and from research group to research group, leading to similar problems to using the average molecule for a particular batch of fuel. Both methods could lead to variations in experimental results even within the same batch of fuel.

Three conventional and two synthetic fuels were investigated in this study. These fuels were Jet-A, RP-1, Diesel Fuel #2, Syntroleum S-8, and Shell GTL (Gas-to-Liquid). However, unlike the other fuels in this study, Diesel Fuel #2 was only investigated at lean, stoichiometric, and slightly

rich conditions. This smaller range of equivalence ratio was due to noticed condensation of the fuel inside the vessel while attempting richer mixtures. No condensation of fuel was noticed for any of the other fuels over the range of equivalence ratios investigated in this study. Research-quality samples with the average chemical formula of all fuels were sourced through the Air Force Research Laboratory (AFRL) in Dayton, OH. Like all fuels distributed by AFRL, each of these fuels was identified by a POSF number, which is a sequential identification number assigned to the fuel by AFRL when it is received from the manufacturer, as noted by Edwards [1]. This number along with detailed information about the composition (average molecule, etc.) are passed on to researchers. This methodology helps to establish a baseline for comparison between different data sets. This comparison is based on a clear identification as to what batch of fuel was used.

The Jet-A used in this study was identified as POSF 10325 with an average chemical formula of $C_{11.4}H_{22.1}$. The RP-1 used was POSF 5235, which has an average chemical formula of $C_{12}H_{24.1}$. The Diesel Fuel #2 was POSF 12758 with an average chemical formula of $C_{13.1}H_{24}$. The S-8 used was identified as POSF 5018 with an average chemical formula of $C_{11.8}H_{25.6}$, and the GTL was POSF 5729 with an average formula of $C_{11}H_{23}$. These average molecules were used throughout the study to determine fuel equivalence ratio. The molecular class breakdown of these fuels by weight is shown in Table 1. These are average percentages that have been rounded off so the values do not always add up to 100%. Presented in the sections below is a summary of the experimental setup and procedures, followed by the results of the laminar flame speed experiments.

% Weight					
Molecular Category	Jet-A (POSF 10325)	RP-1 (POSF 5235)	#2 Diesel Fuel (POSF12758)	S-8 (POSF 5018)	Shell GTL (POSF 5729)
Alkylbenzenes	12.90	0.15	14.41	0.16	0.26
AlkyInaphthalenes	2.33	-	-	<0.01	<0.05
Cycloaromatics	3.43	0.04	10.61	0.03	0.02
iso-Paraffins	29.45	35.07	22.10	75.88	55.1
n-Paraffins	20.03	0.46	12.77	23.37	44.0
Monocycloparaffins	24.87	40.41	23.33	0.50	0.59
Dicycloparaffins	6.78	21.66	11.52	0.05	0.07
Tricycloparaffins	0.21	2.19	<0.01	<0.01	-
Diaromatics		<0.01	4.92		
Triaromatics			0.35		

Table 1. Molecular Class Composition of the fuels included in this study.

2 Experimental Setup and Procedures

All experiments were conducted in the high-temperature, high-pressure stainless steel constantvolume vessel at Texas A&M University. A full description of this experimental setup is available in Krejci et al. [2]. The vessel was outfitted with a heating jacket with temperature control to raise the temperature to the desired experimental condition of 403 K. The vessel was designed for a maximum initial temperature of 600 K. The mixtures were prepared using the partial pressure method. The liquid fuel was injected directly into the vessel via a syringe and septum. The liquid fuel quickly vaporized in the heated vessel. The partial pressures for the fuel in this data set ranged from about 8 Torr for lean experiments to 15 Torr for rich experiments. The partial pressure of the fuel was measured with a 0-100 Torr pressure transducer mounted just off of the vessel. The portion of the fill lines exposed to the liquid fuel was wrapped with heating tape and fiberglass insulation to prevent any cold spots in the system where fuel could condense and alter the composition of the overall mixture. After the pressure had stabilized, the vessel was closed off, and the fill lines were vacuumed and flushed with atmospheric air at least twice to ensure there was no fuel left in the line. The oxidizer components of O_2 and N_2 were added while carefully observing for any signs of condensation.

Experimental data were collected using a schlieren setup and a high-speed camera. The frame rate of the camera was set at 10,000 frames per second. This speed allowed for at least 100 frames to be available for data analysis for each experiment. Images were then analyzed using a MATlabbased edge detection program as outlined in Sikes et al. [3]. The unburned, unstretched laminar flame speed and burned-gas Markstein length were determined using the appropriate non-linear equation as outlined by Chen [4].

The procedure for filling the flame speed bomb was verified using an *in-situ* laser absorption technique. This additional measurement was done to limit and verify uncertainties in the equivalence ratios of the tested mixtures. To this end, a 3.39-µm HeNe laser used in conjunction with Beer's Law (Eq. 1), was used to verify fuel mole fraction, leading to the equivalence ratio.

$$\frac{I}{I_0} = exp\left[-\sigma_v \frac{X_i P}{R_u T} L\right] \tag{1}$$

The only two species-dependent terms in the equation above are the absorption cross section, σ_v , and the mole fraction, X_i . Since O₂ and N₂ do not absorb at 3.39 µm, the only mole fraction of concern is the fuel mole fraction, X_{FUEL} . The transmitted intensity, I, and incident intensity, I_0 , of the laser are the two measured parameters in the equation. The pressure, P, and temperature, T, are experimentally measured parameters, and R_u is the ideal gas constant. The only term that is adjustable is the tested area path length, L. It was desired to have I/I_0 in the range between 40 and 70%. Based on the absorption cross section for Jet-A obtained by Klingbeil et al. [5], this required the path length for the absorption measurement to be significantly. The optical path length used for schlieren imaging through the vessel is 28 cm, and would have resulted in I/I_0 being over 90%, and was therefore too long. To achieve the required short path length through the vessel, the electrodes were removed and rods with windows on the ends were installed. The path length between these two windows of 3.75 cm was measured. Accurately knowing this distance was necessary to measure and predict the intensity ratio. Unfortunately, this setup prevented flame data from being collected at the same time. Figure 1 shows the setup. Experimental mixtures were prepared in exactly the same manner as for a laminar flame speed experiment. Once the full mixture was prepared and the vessel stabilized at 760 Torr, the laser readings were recorded every 3 to 4 minutes for about 25 minutes. The average and standard deviation of these readings were then calculated.



Figure 1. Diagram of setup for laser absorption experiments.

Figure 2a shows the results for I/I_0 versus equivalence ratio for Jet-A/air mixtures. These mixtures were prepared in the manner described above. The laser absorption values shown are the average values over a period of about 20 minutes. As expected, I/I_0 decreased as the mixture became richer, as the greater amount of fuel absorbed more of the laser. The results for Jet-A are reasonably close to the results of [5]. Similar results were seen for RP-1 and Diesel Fuel #2.

During experiments for all three fuels, it was found that I/I_0 values would stabilize over time. As seen in Fig. 2b, a reading of the sensors taken immediately after filling the vessel would return a value almost 20% higher than the actual value. It is believed this result is due to fuel condensing as air was added to the vessel. The fuel would then vaporize within about 5 minutes, returning the mixture to the expected equivalence ratio and corresponding laser transmission intensity.



Figure 2. a) Laser absorption data compared to results from the literature for Jet-A at 403 K and 1 atm; b) Laser Absorption data over time for three sample mixtures. Dashed lines indicate average values for I/I₀.

3 Results

Laminar Flame Speed results for the five fuels are shown in Fig. 3. All fuels except Diesel Fuel #2 were tested over a range of equivalence ratios from around 0.8 to 1.6. Diesel fuel #2 was limited to the lean and slightly rich conditions due to noticed condensation of the fuel when richer mixtures were attempted. All Fuels have a peak flame speed between $\varphi = 1.2$ and 1.3, with the synthetic fuels showing a slightly faster peak value. The differences amongst the fuels are normally within 2 cm/s. The peak flame speed for Jet-A was 58.1 cm/s, while RP-1 had a peak flame speed of 56.3 cm/s. Shell GTL had a peak flame speed of 59.8 cm/s, while S-8 peaked at 58.4 cm/s. Experimental points proved to be repeatable at both lean and rich conditions, with repeated points at both extremes with less than 1 cm/s difference in flame speed.

The largest uncertainty in kerosene-based fuel experiments is the equivalence ratio. This uncertainty can be seen in both the laser absorption measurements and in the laminar flame experiments. The 4.2% uncertainty in absorption cross section noted in [5] results in a variation of $\varphi = \pm 0.05$. This uncertainty accounts for the horizontal error bars seen in the previous graphs. The results for all five fuels appear to be reasonably repeatable. The laminar flame speeds are very similar to each other, typically within about 6%. This similarity is not surprising given that the average molecule and H/C ratio of each of these fuels is very similar.

The Markstein lengths for these fuels are shown in Fig. 4. For all fuels, the Markstein length follows a generally decreasing path as the mixture becomes richer. The Markstein length switches to negative values around $\varphi = 1.4$ for Jet-A. This trend indicates that the flame is becoming more unstable at rich conditions. However, the Markstein length for RP-1 remained positive throughout all the conditions investigated. Both S-8 and Shell GTL saw an almost linear trend to the Markstein length as conditions became richer, with the Markstein length going negative only at the richest conditions investigated.



Figure 3. a) Laminar flame speed results for conventional fuels: Jet-A, RP-1, and Diesel Fuel #2 at initial conditions of 403 K and 1 atm. b) Laminar flame speed results for alternative fuels: S-8 and Shell GTL at initial conditions of 403 K and 1 atm.



Figure 4. a) Burned gas Markstein length results for conventional fuels: Jet-A, RP-1, and Diesel Fuel #2 at initial conditions of 403 K and 1 atm. b) Burned gas Markstein length results for alternative fuels: S-8 and Shell GTL at initial conditions of 403 K and 1 atm.

4 Conclusions

New laminar flame speed experiments have been presented for conventional and alternative liquid fuels. Laser absorption measurements for Jet-A, RP-1, and Diesel Fuel #2 were used to verify the experimental methods for introducing the liquid fuels into the test vessel, showing no sign of condensation that would affect equivalence ratio in the system. This filling technique was then used during laminar flame speed experiments for these three fuels plus S-8 and Shell GTL. Overall, the results for the three fuels appear to be similar. Results are repeatable, within about 6% with the largest uncertainty being from the mixture equivalence ratio. This uncertainty corresponds to the known absorption cross section as verified during laser absorption measurements.

5 References

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