Comprehensive JP-8 Mechanism for Vitiated Flow

Validation of Model

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July 31, 2009

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Abstract

The overall objective of the entire commissioned project is to develop a computer model of the micro-level kinetics in JP-8 combustion occurring in the afterburner in jet engines. Validation of the computer model in a combustion environment is done by sampling gas species reacting in a counter-flow burner that mimics afterburner conditions and comparing the sampled species with the predicted ones.

Since validation of the computer model requires accurate experimental data obtained from the flame, this project has focused on both isokinetic sampling for accurate species measurement and achieving a stable flame in order to have a well defined combustion environment for modeling. Experiments thus far have shown that sampling probe inner diameter, sampling probe location in the flame and sampling velocity are important factors in precise species determination.

Introduction

The Air Force currently uses JP-8 jet fuel to power their air fleet. Once combusted, JP-8 can produce high amounts of soot, a major pollutant. In an ongoing effort to reduce atmospheric pollution, the Air Force wants to minimize potentially hazardous emissions in the jet engine afterburner as well as improve afterburner operation.[1] Afterburner design can be modified to minimize soot formation; however this cannot currently be done due to the lack of information on important chemical reactions occurring in JP-8 combustion systems at afterburner conditions.

Due to the limited understanding of the chemical kinetics of JP-8, there is an initiative by the Air Force to understand the chemical kinetics of JP-8 combustion. The Air Force has contracted a small business, Innovative Energy Solution (IES), in cooperation with the University of Illinois at Chicago (UIC), to develop a program which will model the micro-level kinetics of JP-8 combustion in an afterburner environment. Once developed, the kinetic model will be incorporated into a computational fluid dynamic (CFD) package for delivery to the Air Force. The contract with the Air Force involves two validations of the chemical kinetics. The first is using a shock tube at low pressures to study the basic fuel decomposition characteristics of the surrogate components of JP-8 fuel. A surrogate fuel is one that can reasonably represent the performance and emissions behavior of jet fuels[1]. It is necessary to understand the behavior of each individual component before the complex interactive kinetics of the jet fuel can be understood. For this reason, m-xylene is evaluated independently in this study. The second validation technique is using a counter-flow burner to produce a diffusion flame of the surrogate components at afterburner conditions- high temperature and minimal oxygen. The flame is then sampled at varying combustion conditions and analyzed via gas chromatography. The data from the counter-flow diffusion flame will be compared to data generated using CFD. This project is

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the second validation, using surrogate fuels to produce a diffusion flame in a counter-flow burner.

Counter-flow burners have been used frequently to evaluate the oxidation of jet fuel surrogates[2, 3]. Previously the team attempted to validate the CFD package using a co-flow burner, however results only showed carbon monoxide and carbon dioxide, which are erroneous as more species are expected. The lack of other combustion products required a new setup in order to obtain representative samples. Because of the obstacles encountered using the co-flow burner and due to success of previous experiments using counter-flow burners, it was decided that a counter-flow burner would be the most accurate way to model afterburner conditions. In addition, software is readily available that models counter-flow diffusion flames; no such commercially available software exists for co-flow flames.

While there have been recent studies analyzing counter-flow diffusion flames of jet fuel surrogates, these fuel streams consisted of highly combustible gases, such as methane or ethylene, doped with the surrogate[2, 3]. The fuel stream in this experiment consists of the surrogate diluted with an inert carrier gas, nitrogen. By studying the surrogate directly, rather than through doping, the resulting concentrations of combustion products should give a more accurate representation of JP-8 behavior.

In order to obtain the most precise concentration profiles of combustion products, sampling extraction via probes must be minimally invasive. If the probe disrupts the flame and skews flow, the sample will not represent actual flame concentrations. The effects of various sizes and shapes of quartz probes has been well documented[4, 5] and they are considered to be a dependable tool to sample combustion species. Tapered tips have been found to be the most effective for sampling because they decrease soot deposits on the inner walls of the probe[4] and

minimize flame perturbation[5]. The inner diameter of the tip varies depending on the size of the

particles being collected. For large particles, such as soot, probe tip inner diameters can be as

large as 20 mm[6]. Smaller particles, such as methane combustion products, require a much

smaller collection probe with an inner diameter of 170 μm[3]. For the purposes of this experiment,

smaller probes are necessary to ensure that only combustion products are sampled.

Materials and Methods

The experimental setup consists of a counter-flow burner in which fuel and the oxidizing gases are released from opposing sides to produce a non-premixed diffusion flame. Oxidizing gases are passed through a ceramic honeycomb and wire mesh and released from the top portion of the burner. Fuel is passed through a ceramic honeycomb and wire mesh and released from the bottom portion of the burner. Both the fuel and oxidizer nozzle outlets have a diameter of 22.4 mm. A nitrogen sheath with outer diameter 66.3 mm shields the flame from room draft and ensures that the fuel is oxidized in a controlled environment. There is a 15 mm space between the opposing nozzle outlets. Figure 1 shows a schematic of the experimental setup and a schematic of the counter-flow burner[3]. Figure 2 shows the actual burner used for experimentation.
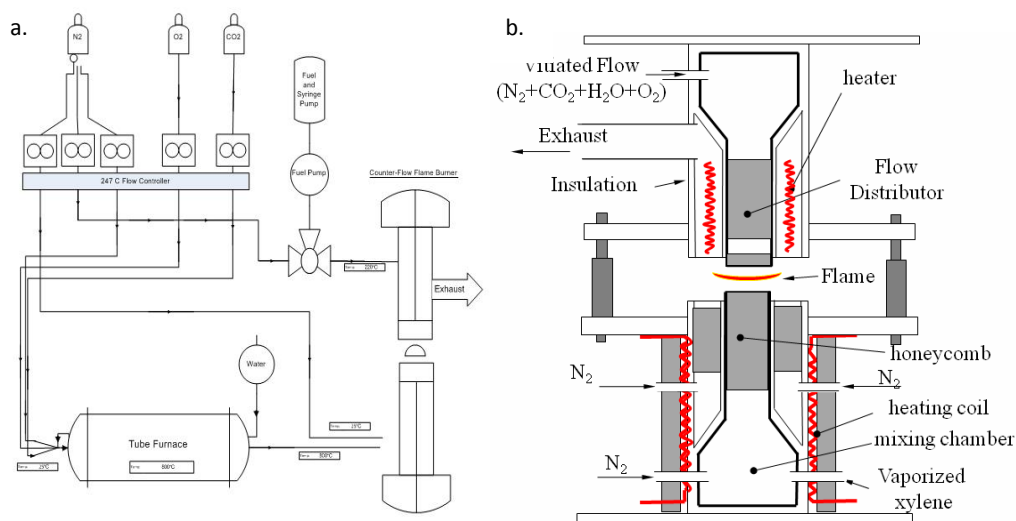
Figure 1: a) A schematic displaying the experimental set-up, b) a schematic displaying the counter-flow burner[7]. Copied from P. Berta Ph.D. Thesis.

Figure 2: The counter-flow burner

Fuel and Oxidizer Heating

Reaching complete fuel vaporization is critical when dealing with heavier hydrocarbons, like m-xylene and 1, 3, 5 - trimethyl benzene, since condensation of the fuel could occur in the lines leading to the burner. To ensure complete fuel vaporization, the fuel is provided by a syringe pump to a vaporizer that heats it above 412 K, the boiling point of m-xylene. The temperature is monitored using thermocouples. The fuel is highly diluted with nitrogen to assist flow of the surrogate fuel.

To mimic high temperatures of afterburner conditions, the oxidizing gases are passed through a furnace, which is kept above 1000 K, before being released into the counter-flow burner. At this stage in the study, the oxidizer stream consists of oxygen diluted with nitrogen. Ultimately, the oxidizer stream will consist of nitrogen, oxygen, carbon dioxide and water vapor, as is found in a jet afterburner. For this reason, the furnace is also equipped with a syringe pump to inject water. The water will be subject to two rotations through the furnace: the first rotation vaporizes the water, while the second rotation allows water vapor to mix with the other oxidizing

gases. All tubing is heated with heating tape and insulated with fiberglass cloth and aluminum sheets to maintain temperature and atomization and prevent any species from condensing out.

Flow Rates

The flow rates of both the fuel and oxidizing gases greatly affect flame stability, which is directly proportional to the flame strain rate, the amount of flame deformation over time due to stress. A high strain rate is required for accurate, repeatable sampling. In fuel flow rates with high concentration of the surrogate gas, it is easy to obtain a stable flame; however, in order to mimic after-burn conditions, the fuel stream needs to have a dilute concentration of the surrogate gas. The ideal oxygen content of the oxidizing stream is 6%, but at this stage, the oxidizing stream contains 29% oxygen. For the reported experiments, the following flow rates were used: m-xylene, 15 mL/hr; nitrogen carrier, 1.20 L/min; nitrogen oxidizer, 1.20 L/min, oxygen oxidizer, 0.500 L/min; and nitrogen sheath, 10.1 L/min. M-Xylene flow was controlled by a syringe pump, while other flows were controlled using a model 247C flow controller with a 4-channel display. Figure 3 is a picture of the flame with high oxygen content in the oxidizer stream.

Figure 3: The flame with 50% Oxygen content in oxidizer stream

Flame Stability

Several factors affect the stability of the flame including temperature, strain rate and stream concentrations. Maximum strain rate yields optimal flame stability[8] REF. The following is the equation for strain rate with the strain rate, a, relating to the distance between the nozzles, L, velocity, V_a and V_f, and density, ρ_a and ρ_f, of the air and fuel streams respectively:

$$a = \frac{2V_a}{L} \left\{ 1 + \frac{V_f \sqrt{\rho_f}}{V_a \sqrt{\rho_a}} \right\}$$

(1)

The equation shows the direct proportionality of both air and fuel velocity to strain rate.

Sampling

Samples of the flame are taken using a quartz probe along the center line of the flame at varying vertical positions. Each probe tapers from 6.35 mm at the connection to the gas chromatograph (GC) to an inner diameter at the tip ranging from 6.35 mm to 80 μm. The inner diameter of the probe can affect the observed concentrations of combustion species. For this reason, four different probes with varying tip inner diameters were tested: 6.35 mm, 310 μm, 110 μm, and 80 μm. In order to accurately sample the flame, the sample needs to be taken at a velocity equal to the radial velocity at the stagnation plane. This sampling technique is called isokinetic sampling[8]. Flame samples are extracted at varying velocities to achieve a velocity that minimizes disturbance visually in the flame. The extraction flow is manipulated using a flow meter valve at the entrance of the GC.

Results

     During experimentation, gas samples were analyzed using a mass spectrometer in order to determine the m-xylene combustion products. Three main components were identified: benzene, toluene and phenyl-acetylene. Figure 4 displays a GC graph with these products labeled.
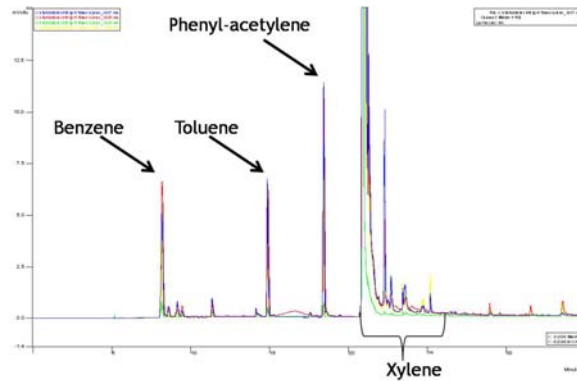

Figure 4: GC results with main combustion components and m-xylene labeled

     Experimentation shows that probe inner diameter is an important factor in determining the species resulting from fuel combustion, as well as the relative concentrations of these products, probably because it affects the degree of isokinetic sampling. The measurements of the inner diameter of the tip opening of probes A, B, C and D are 310 μm, 110 μm, 80 μm and 6.25 mm, respectively. The flame was sampled four times at four specific velocities with each probe. The following figures display the resulting FID graphs from GC analysis of samples taken.

     Each graph in figure 4 contains data from probes A-D at specific sampling velocity. The velocities are recorded with full unobstructed flow defined as 100 % and a completely closed valve as 0%. For the four velocities sampled, Probe A shows the most species peaks as well as the highest species peaks of any probe. While the presence of many species in a GC output

could be indicative of sampling from too wide a volume, this is highly unlikely; if the sampling area was too broad, the concentrations of the combustion products would be diminished by dilution. Because Probe A shows high concentrations of benzene, toluene and phenyl-acetylene, it is likely that Probe A samples the most appropriate volume. In addition, at the 100% velocity sample, Probe A was the only one to collect heavier hydrocarbons as can be seen by the peaks in the 25 - 35 minute range.
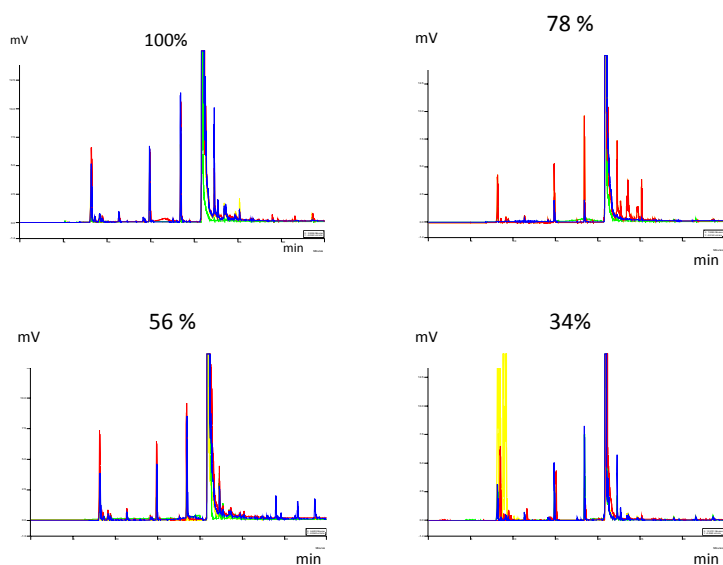

Figure 4: GC results for samples collected by probes A-D at four different velocities. Probes A, B, C, and D are colored red, green, yellow and blue, respectively.

Figure 5 shows that sampling velocity is also a factor in the observed relative concentrations of combustion products. A sampling velocity that is too slow results in a limited sample lacking key combustion products because not enough sample material is collected. It is evident that the 34% sampling velocity (yellow) is too slow and excludes important species, as can be seen by the lack of yellow peaks in figure 5. The 34% sampling velocity also produced

the most inconsistent results. Alternatively, a sampling velocity that is greater than the flame speed results in extraneous species from the fuel and oxidizing stream being detected by the GC, ultimately minimizing the relative concentrations of significant combustion products. At the 100% sampling velocity (blue), heavier hydrocarbons appearing in the 25 - 35 minute range were undetected.
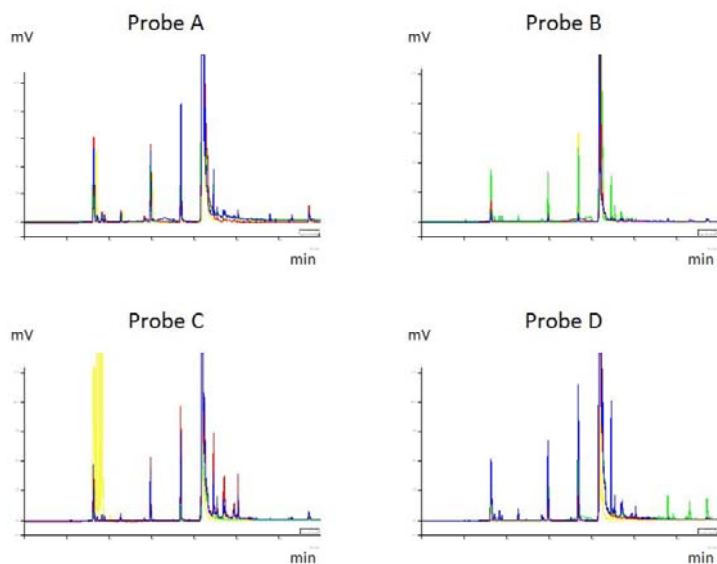

Figure 5: GC results for samples collected at velocities ranging from 34%-100% using 4 different probes. Velocities of 34%, 56%, 78% and 100% are colored yellow, green, red and blue, respectively.

Figure 6 shows that the vertical position of the probe in the flame greatly affects the observed concentrations of resulting species. Placing the probe close to the oxidizer outlet results in a sample containing minimal levels of expected combustion products. This trend is evident by the lack of peaks when the probe was placed 1.19 mm (blue) from the top of the flame. Placing the probe at the opposite extreme, close to the fuel outlet, results in a sample containing high amounts of fuel with low amounts of combustion products. This trend is evident

by the large m-xylene peak (21 minutes) and lack of peaks prior to m-xylene when the probe was

placed 7.14 mm (aquamarine) from the top of the flame.
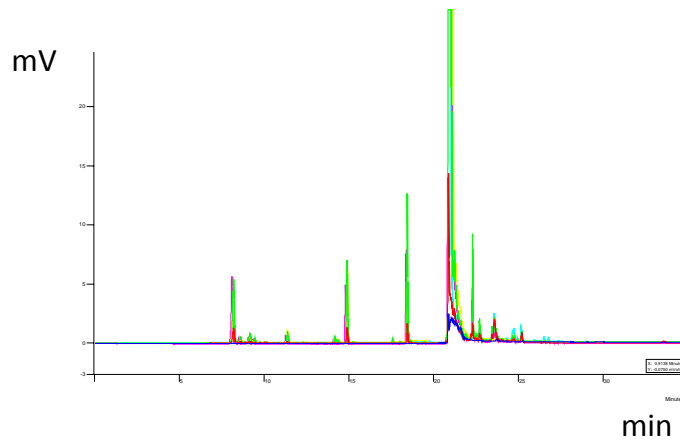
Vertical Position

Figure 6: GC results for samples collected with Probe A at 64% velocity at vertical positions ranging from 1.19 mm-7.14 mm from the top of the flame. Displacements of 1.19, 2.38, 3.57, 4.76, 5.95 and 7.14 are colored blue, red, green, yellow, fuchsia and aquamarine, respectively.

Discussion and Conclusions

It appears that Probe A (inner diameter, 310 μm) yields the most quantitative results (the most species peaks as well as the highest species peaks). Probe C (inner diameter, 80 μm) also displayed strong quantitative results in terms of peak size, though the very small tip opening seems to have affected the number of species collected during sampling. Probe D (inner diameter, 6.35 mm) also produced quantitative results with regards to peak size, but important species, particularly larger hydrocarbons, were missing completely from the resulting FID graphs. The inner diameter of probe D is so large in comparison to the flame, which results in a large sample volume. It is likely that large hydrocarbons were present in the sample, but did not appear on the graph because their concentrations were diluted by the sample volume size. Probe B (inner diameter 110 μm) gave the least quantitative results, which is somewhat surprising because the tip inner diameter is between that of probes A and C, which had moderate to high success in sampling. Probe B's failure could possibly be caused by the shape of the tip, which was more tapered than any of the other probes, possibly causing a loss of species on the probe surface. The face was not flat, which would have affected gas collection. In the future, probe shape should be standardized to ensure that it does not negatively affect sampling.

Samples were taken at four different velocities. The resulting graphs at each velocity represent the flame contents moderately well. Nitrogen, oxygen, carbon monoxide, carbon dioxide, benzene, toluene, and m-xylene were all accurately represented at each velocity – the discrepancy appears with heavier hydrocarbons, which appear in smaller concentrations. At 100% velocity, all species appear with decent peak height. However, peaks for heavier hydrocarbons were somewhat undersized. This lack of peaks is due to the fact that at a high

velocity, or super-isokinetic sampling, the probe 'sucks in' the gas rather than allowing it to flow

normally. Light species are carried into the probe, while the inertia of heavier species causes
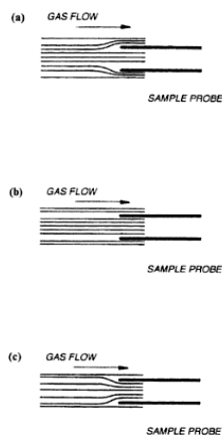
them to miss the probe[9] (Figure 7, c).

Figure 7: Sub-isokinetic sampling (a),
isokinetic sampling (b) and super-
isokinetic sampling (c)[9]. From
Environmental Analytical Chemistry.

The best velocity appears to be 78%. There are a wide range of species with acceptable

peak heights across the graph. The lower velocities, 56% and 34%, both have significant faults.

The hydrocarbon peaks are completely omitted from these graphs. This is most likely due to a

sampling velocity that is slower than the actual flame velocity species, or sub-isokinetic

sampling, which omits some species from the sample[9] (Figure 7, a).

Because of the large affect that sampling velocity has on sample quality, it will be

necessary to identify the optimal velocity for collecting JP-8 combustion products. The ideal

sampling velocity is equal to the velocity of the flame, as molecules do not 'back up' or get

'sucked in' at the probe opening (Figure 7, b). In order to ensure a collection speed equal to that

of the flame, the flame velocity must first be measured. The most accurate method to measure

flame speed is using a laser doppler velocimeter (LDV). However, such technology is not accessible by the lab. The method adopted uses a pitot tube to measure pressure difference, which can be used to calculate velocity.

A pitot tube (Figure 8) measures pressure at two points: the opening at the end of the tube (P2) measures total pressure, and the smaller inlets placed radially on the tube (P1) measure static pressure (the pressure of the stagnant gas)[10].
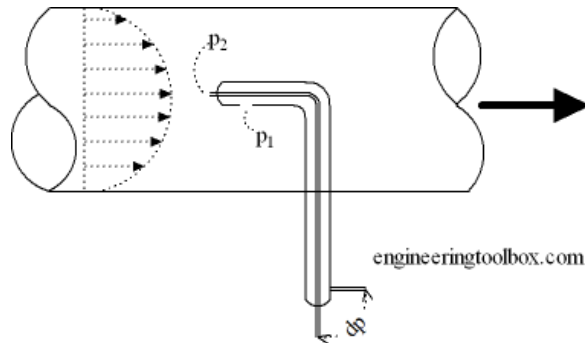

Figure 8: A schematic of a pitot tube measuring gas flow through a larger annulus[10]. From www.engineeringtoolbox.com.

A manometer connected to the pitot tube measures the dynamic pressure, the difference between total pressure and static pressure. Equation 2 can be used to calculate the velocity, v, using the determined dynamic pressure, P_d, and density of the gas, ρ.

$$v = \sqrt{\frac{2P_d}{\rho}}$$

(2)

The ideal sampling location in the flame is at the stagnation plane, the place at which the fuel and oxidizer meet and the gas flows out radially. In an opposed flow diffusion flame, the flame is located on the oxidizer side of the stagnation plane[11]. The only way to measure the exact location of the stagnation plane is by first determining velocity, as flame speed is highest at the

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stagnation plane. Since flame velocity is still unknown, concentrations of combustion products were taken at different vertical positions in the flame in an attempt to locate the stagnation plane. Samples taken near the oxidizer and fuel nozzles were inaccurate and left out major components of the flame. The best area to sample was determined to be in the center of the two nozzles, however the exact location of the stagnation plane could not be determined from these trials alone. Further investigation is needed to accurately locate the stagnation plane in order to obtain the most representative concentration profile.
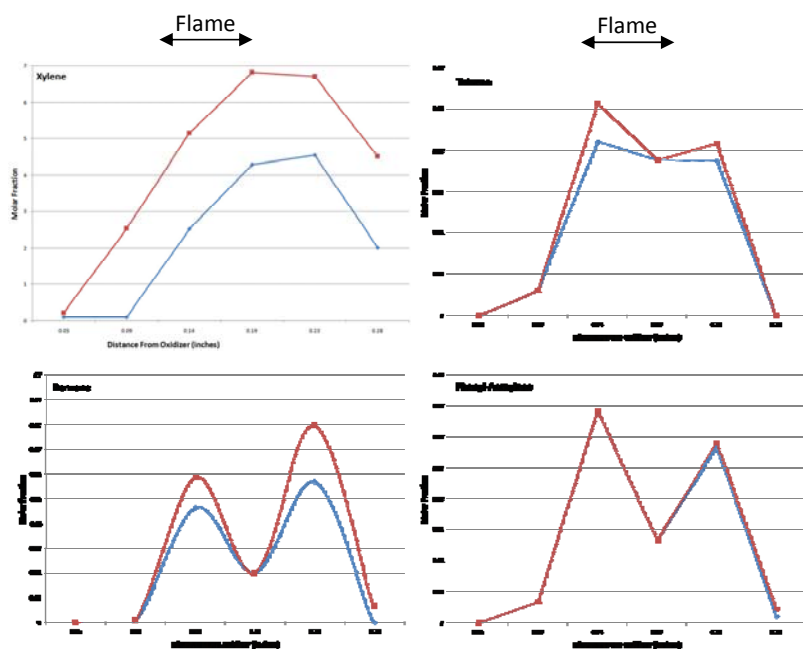

Figure 9: The mole fraction versus distance from the oxidizer for xylene, benzene, toluence and phenylacetylene. Probes A and C are colored red and blue respectively.

Since the exact location of the stagnation plane is not known, concentrations were measured as a function of distance from the oxidizer nozzle, similar to those in figure 6. As can be seen in figure 9, the relative concentrations of hydrocarbons as a function of height are complex. The concentration profiles of two different probes, sampled at the same heights were

compared. While the concentrations are different, they follow the same trends. The trends for benzene, toluene and phenylacetylene are all bimodal. This trend can also be seen from similar experiments run by other groups[12]. The team is unsure of the cause of the dip in the data in the center of the flame, and this is a subject that will be examined in future work. Future work must also include a full concentration profile from the oxidizer outlet to the fuel outlet. The existing concentration profile measures from the oxidizer to the bottom of the flame, thereby giving an incomplete profile of the concentrations of species across the burner.

The overall goal of the project is to simulate the conditions in jet fuel afterburners in order to develop a comprehensive mechanism for JP-8 combustion. The goal of the validation portion of the project was to determine the species generated by fuel combustion in addition to the relative concentrations of these products in order to later confirm the mechanism. While not all species have been identified, the team has an initial idea of what species are produced by m-xylene combustion. In addition, the team has developed an effective sampling system for future use when examining other surrogate fuels. Concentration profiles resulting from these and future tests can then be compared to results from numerical simulations.

Acknowledgements

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Afterword

The Research Experience for Undergraduates (REU) Program is a program funded by the National Science Foundation (NSF). It provides undergraduate students the opportunity to work at a prestigious research university alongside graduate and post-doc students. Each student is assigned an individual project in which they assist an over-seeing professor. This summer I participated in the REU program at the University of Illinois at Chicago in the Department of Mechanical Engineering in the Energy Systems Laboratory.

My experience as an REU student afforded me the opportunity to get a first hand experience of what graduate school would entail. Furthermore, it allowed me to expand my education by exposing me to another engineering field. Working with a mechanical engineering group, more specifically a combustion group, allowed me the opportunity to strengthen the engineering concepts I had previously learned in my classes. Prior to my enrollment in the REU program, I was very unsure if I wanted to pursue a doctorate in chemical engineering, however after experiencing another facet within engineering I have developed a new desire to continue my engineering education.

Participating in the REU program this summer has not only inspired me to pursue a graduate degree in engineering, but has shed light on the material I have learned in the classroom. Before this summer, most of the concepts taught in class were exactly that, concepts. I now understand the logistics that make these concepts possible. For example, a thermocouple is the piece of equipment in many of my engineering problem statements, however until this summer I had never understood what a thermocouple actually was. The hands-on experience I

gained this summer has increased my understanding of engineering applications and will

continue to enhance my classroom education in the future.