THE DEVELOPMENT OF A CORRELATION TO PREDICT THE LEAN BLOWOUT OF BLUFF BODY STABILIZED FLAMES WITH A FOCUS ON RELEVANT TIMESCALES AND FUEL CHARACTERISTICS

Thesis

Submitted to

The School of Engineering of the

UNIVERSITY OF DAYTON

In Partial Fulfillment of the Requirements for

The Degree

Master of Science in Mechanical Engineering

By

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UNIVERSITY OF DAYTON

Dayton, Ohio

May, 2013

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ABSTRACT

THE DEVELOPMENT OF A CORRELATION TO PREDICT THE LEAN BLOWOUT OF BLUFF BODY STABILIZED FLAMES WITH A FOCUS ON RELEVANT TIMESCALES AND FUEL CHARACTERISTICS

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In many high-speed reacting flows, a bluff body is used to locally slow the velocity and stabilize the flame. Gas turbine engines, both in ground-based industrial settings, as well as in aviation settings, utilize bluff body stabilized flames, often running at lean fuel-air ratios to extend the equipment's lifetime or to meet emissions regulations. However, running the equipment at a lean condition also puts the system at risk for lean blowout, which can result in facility inefficiencies, hardware damage, and a catastrophic reduction in aircraft performance.

This thesis uses experimental data taken at the Air Force Research Laboratory, as well as data collected from a review of past literature, to develop a correlation to predict lean blowout using a least squares curve fit method. The laminar flame speed and ignition delay time were calculated for subsets of the data using the chemical kinetics software Cantera, and the results were incorporated into the correlations. The purpose of this effort was to provide an accurate, practical method of predicting lean blowout for designers and modelers, as well as to

provide insight into the critical parameters and timescales that govern the blowout process by examining the significance of each parameter included in the correlation and the physical and chemical processes it may affect.

The correlations presented in this thesis indicate that the lean blowout of bluff body stabilized flames is dependent on both the Damköhler number and the Lewis number. *U/D* is the inverse of the fluid mechanic timescale, likely that of the mixing time in the shear layer between the recirculation zone and the fresh reactants. Pressure, temperature, and the hydrogen to carbon ratio of the fuel all affect the reactivity of the mixture, contributing to the chemical timescale in the Damköhler number. The molecular weight of the fuel influences the mass diffusion, and thereby the Lewis number, of the fuel. As the Lewis number increases, various reaction rates, including the turbulent flame speed, decrease, also affecting the chemical timescale in the Damköhler number. The exact chemical timescale could not be determined from the laminar flame speed and ignition delay time data.

A major contribution of this work is establishing the role that fuel characteristics play in the lean blowout process. Very little work has been done in the literature on fuel effects in the lean blowout of bluff body stabilized flames, but the correlation developed clearly shows that both the molecular weight and hydrogen to carbon ratio of the fuel influence the process.

To my husband, George, and to my family and friends,

for their patience during this process

ACKNOWLEDGEMENTS

I would first like to thank my advisor, Dr. Scott Stouffer, for his guidance and encouragement, as well as the time he spent reviewing the text. His commitment helped make this work possible. I would also like to thank Dr. Jamie Ervin for graciously agreeing to serve on my committee, particularly at short notice.

Special thanks go to Dr. Barry Kiel for serving on my committee and for being a sounding board throughout this process. His expertise, enthusiasm, and mentorship have been instrumental in the completion this work.

I would also like to acknowledge everyone in the lab whose hard work and good humor have made some long days (and nights) seem much shorter: Amy Lynch, Drew Caswell, Dwight Fox, Harold Day, Jeff Monfort, Stan Kostka, and Steve Britton.

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LIST OF SYMBOLS AND ABBREVIATIONS

A, b, c	Experimentally derived constants
B	Blockage ratio
C	Carbon
D	Characteristic length scale
Da	Damköhler number
DeZ	DeZubay parameter
E	Activation energy
f	Characteristic shedding frequency behind a bluff body
η	Kolmogorov scale
H	Hydrogen
IDT	Ignition delay time
l	Integral length scale
λ	Taylor microscale
Le	Lewis number
MW	Molecular weight
n	Number of data points in correlation
n	Kinematic viscosity

p	Number of parameters in correlation
P	Pressure
ϕ	Equivalence ratio
R	Gas constant
R^2	R-squared value
Re	Reynolds number
S_L	Laminar flame speed
SS_E	Sum of the squares of the residuals
SS_T	Total sum of the squares of the dataset
St	Strouhal number
T	Temperature
τ	Characteristic timescale
Θ	Momentum layer thickness
Tu	Turbulence intensity
U	Velocity
u'	Turbulence intensity

CHAPTER 1

INTRODUCTION

Background and Motivation

In many high-speed reacting flows, a bluff body is used to locally slow the velocity and stabilize the flame. Both industrial and aviation gas turbine engines utilize bluff body stabilized flames. Bluff body flameholders are incorporated into designs for jet engine augmentors and ramjet and scramjet applications, and are used in both vitiated and non-vitiated flows. In many applications, the flame is kept below the stoichiometric fuel-air ratio, in the interest of extending the equipment's lifetime or meeting emissions regulations. When a combustion system operates in a lean condition, it can blow out more easily, especially if there are unpredictable fuel or airflow perturbations (Chaudhuri 2011). In order to avoid blow out, which can result in facility inefficiencies, hardware damage, and a catastrophic reduction in aircraft performance, two closely related challenges must be met. The first challenge is understanding the physical mechanism governing blowout; the second is being able to accurately predict and prevent blowout in a combustion system. This thesis will attempt to address both challenges.

In a bluff body flame, a high-speed, relatively cold, combustible mixture flows over a bluff body, as shown in Figure 1. The bluff body produces a recirculation zone behind it,

generating a region of low velocity. As the flame burns, hot combustion products are entrained into the recirculation zone. The flame "holds" in the wake of the bluff body, and a shear layer is formed between the recirculation zone and the combustible free stream. While Figure 1 depicts two opposing recirculation areas, shown in red, behind the bluff body, it is sometimes preferred to show this as one large recirculation area.

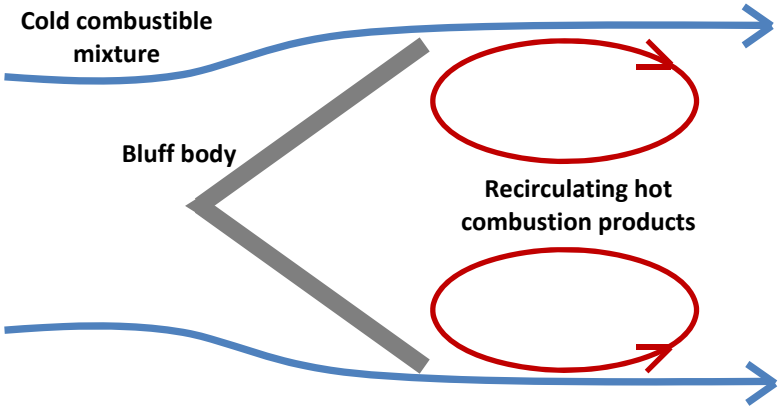

Figure 1. Schematic of bluff body flame stabilization – Reproduced from Law (2006)

Law (2006) contends that the limiting factor in stabilizing a flame on a bluff body is not the ignition process. It is commonly inferred that the reactants must ignite before they reach the end of the recirculation zone, and if their associated ignition delay time is longer than the time they spend mixing with the hot products, then the flame will not sustain itself. Law argues that the actual phenomenon of interest is the stabilization of an existing flame in the mixing layer, which is achieved through a balance between the local flow velocity and the flame velocity. This mechanism is quite different from a simple ignition problem, because the process is now affected by the stream-wise back-diffusion of heat and radicals from the existing flame.

The length and time scales for flame stabilization would then be much shorter than those for ignition.

Some of the first studies of lean blowout behavior in bluff body stabilized flames were conducted by Williams in the late 1940s and DeZubay in the 1950s. DeZubay's work, stemming from experiments conducted on disk-shaped flameholders, focused on correlating the fuel to air ratio at lean blowout with a parameter based on the inlet pressure and velocity and the characteristic diameter of the flameholder. In his original work, DeZubay did not vary the inlet temperature of the rig, so a modified DeZubay correlation that includes temperature dependence has become more widely used, with *T* representing the temperature parameter:

$$DeZ_T = \frac{U * 10^4}{P^{0.95} D^{0.85} T^{1.2}} \tag{1}$$

In this correlation, velocity (*U*) is in ft/s, pressure (*P*) is in psi, diameter (*D*) is in inches, and temperature (*T*) is in Rankine. Though DeZubay's experiment included both rich and lean blowout, the correlation is intended only for the lean region of the stability curve. Figure 2 shows the DeZubay curve as constructed from the data used for the present work.

While the DeZubay curve has been a well-known and popular correlation, Figure 2 demonstrates some of its faults. At a given DeZubay number, the equivalence ratio at lean blowout can vary greatly. For example, at a DeZubay number near 6000, the equivalence ratio at lean blowout ranges from 0.28 up to 0.75. In addition, there appears to be a fuel effect that the correlation does not capture. The propane data follows a curve reasonably well, as marked

by the black line in Figure 2. However, data from experiments run on JP-4, methane, gasoline, and jet fuels 7721, 6308, and 6169 follow different patterns.

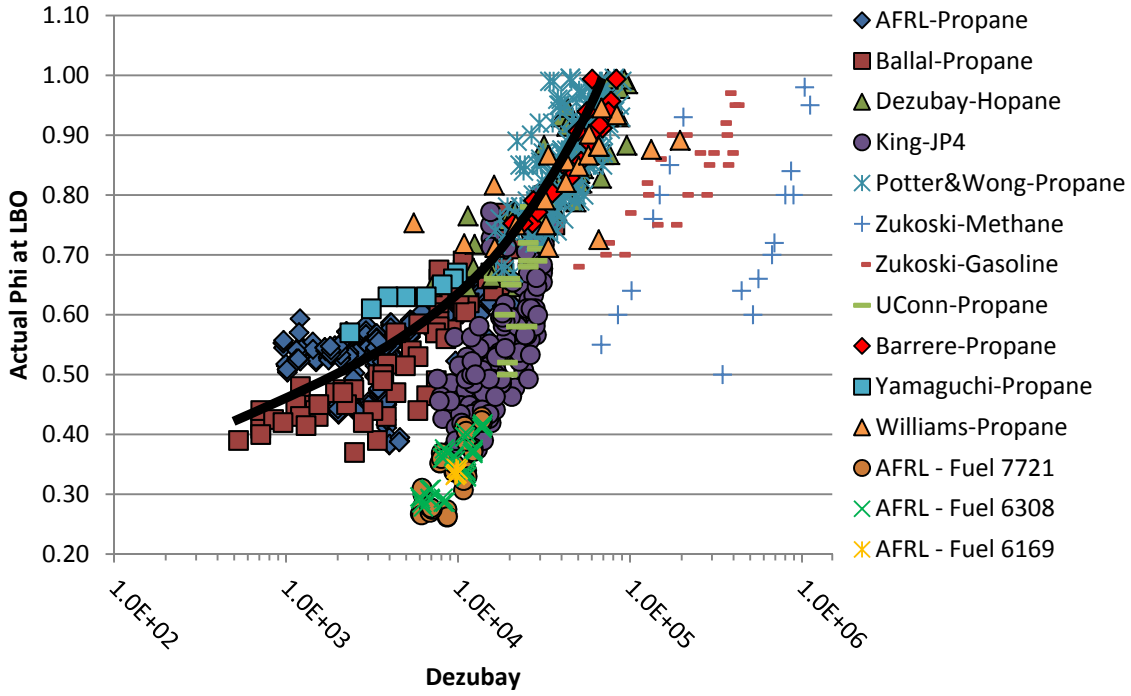

Figure 2. DeZubay curve constructed with data from the current work

Williams (1949) studied bluff-body flames over a range of inlet turbulence intensities, flameholder sizes and shapes, and fuel type. Williams found that the blowout velocity under steady flow conditions was affected primarily by the flameholder width and the properties of the incoming gases, and the flameholder shape was not a major influence. Williams also heated the flameholder, which increased the stability limits, and found that increasing inlet turbulence levels decreased the stability limits.

Lean blowout behavior of bluff-body stabilized flames continued to be studied in the following years by multiple researchers, including King (1957), Zukoski and Marble (1954, 1955),

Ozawa (1971), Ballal and Lefebvre (1979), and Plee and Mellor (1979). King (1957), using data taken on a v-gutter flameholder with JP-4 as a fuel, found that increased pressure and temperature and decreased velocity generally decreased the fuel to air ratio at lean blowout, but presented little discussion on the physical importance of his findings.

Zukoski and Marble (1955) conducted their lean blowout tests on flameholders of several shapes and sizes and used methane, hydrogen, and gasoline as fuel. They also injected a salt water solution into the flame in order to measure the length of the recirculation zone and attempted to measure the temperature of the recirculation zone using the sodium D-line reversal technique.

Zukoski and Marble proposed a flame stabilization mechanism for bluff-body flames, postulating that fresh gas from the free stream burns as it mixes with hot combustion products in the turbulent shear layer between the free stream and the recirculation zone. The length of the recirculation zone was found to depend only on the fluid dynamics of the system.

According to Zukoski and Marble, active combustion in the region of the recirculation zone is limited to its shear layer boundaries, with a portion of the hot products being re-entrained into the recirculation zone. In a stable flame, the fresh gas flowing past the bluff body is ignited before it reaches the end of the recirculation zone, propagating the flame. When the fresh gas fails to mix with the hot products in the recirculation zone for an adequate period of time, Zukoski and Marble theorize that the flame will blow off. They identified the time that the fresh gas spends in the shear layer and the ignition delay time as the critical timescales in the blowout process. They identified the ratio of the free stream velocity and the length of the

recirculation zone as representative of the time that the fresh gas spends in contact with the hot combustion products.

The critical timescales Zukoski and Marble identified can be configured into a Damköhler number, which is the ratio of a fluid mechanic timescale to a chemical timescale:

$$Da = \frac{L_{RZ}}{U\tau_{ign}} \tag{2}$$

L_{RZ} is the length of the recirculation zone and U is the free stream velocity.

The sodium tracer technique utilized by Zukoski and Marble was developed by Nicholson and Field, who attempted to characterize propane flames in 1949. The work was largely focused on expanding flame visualization techniques, though in doing so, it also documented particular flame phenomena near rich blowout. Pulsation of the flame at ignition and rich blow-off was observed, with frequencies dependent upon duct dimensions. "Horns of flame" appeared to develop at the flame edge during transient phases of ignition and blowout. Nicholson and Field proposed that flame stability may depend on a balance between the rate of dissipation of heat and radicals by eddy shedding and their production by combustion within the volume immediately behind the bluff-body.

Potter and Wong (1958) attempted to verify and build on the work of Zukoski and Marble by measuring the blowout velocities and recirculation zone lengths for cylinders of various diameters and at multiple fuel concentrations. The geometry of the duct in which the experiment was conducted was varied, as was the duct's pressure. Potter and Wong found that the influence of pressure varied with tunnel geometry and that the recirculation zone was

proportional to the square root of the flameholder diameter. They concluded that the critical fluid mechanic timescale was the ratio of the recirculation zone length to the blowout velocity.

Ballal and Lefebvre (1979) investigated the influence of multiple global parameters on lean extinction, including temperature, pressure, velocity, turbulence level, flameholder size, and flameholder blockage ratio. The correlation they derived is shown in Equation 3.

$$\phi_{LBO} = \left[\frac{2.25\left(1 + 0.4U\left(1 + 0.1Tu\right)\right)}{p^{0.25} T \left(e^{T/150} \right) D(1 - B)} \right]^{0.16} \tag{3}$$

U is the velocity in the plane of the maximum flameholder blockage, or the lip velocity, *Tu* is the turbulence level, *p* is the pressure, *T* is the inlet temperature, *D* is the flameholder diameter, and *B* is the blockage ratio. Units are standard SI. Ballal and Lefebvre concluded that the blowout was governed mainly by inlet air temperature and to a lesser degree by air velocity, turbulence level, and flameholder size. Despite its inclusion in their correlation, they found little to no dependence of the lean blowout on pressure.

Plee and Mellor (1979) developed a model to explain lean blowout based on the various timescales involved, including fluid mechanic and chemical times, as well as droplet evaporation time and fuel-injection mixing time in the case of heterogeneous mixing. The fluid mechanic timescale was taken to be a turbulent mixing time in the shear layer between the relatively cold incoming reactants and the hot burned gases in the recirculation zone. This timescale was approximated as the ratio of the flameholder width, which was also considered a measure of the size of the recirculation zone, and the velocity of the incoming gas at the lip of the

flameholder. The ignition delay time was taken as the critical chemical timescale, and approximated by Equation 4.

$$\tau_{chem} \approx \frac{e^{E/RT}}{\phi} \tag{4}$$

The model developed by Plee and Mellor successfully collapsed the lean blowout data from Ballal and Lefebvre (1979) to a straight line.

As more advanced diagnostics and high-speed imaging became available, researchers began to investigate the structure of the flame in more detail using techniques like schlieren imaging and chemiluminescence. In addition, the computing power available increased exponentially, making it possible to model both the fluid mechanics and the chemical reactions in the flame.

Yamaguchi, et al. (1985) investigated the extinction mechanism of bluff-body flames by measuring the fluctuating pressure gradient along the surface of the flameholder at the attachment point. Schlieren photography was also used to observe the structure of the flame. The experiment was unique in that it included flameholder configurations comprised of multiple bluff bodies while maintaining a constant blockage ratio. The authors concluded that the direct cause of blowout is the stretch of a weakly generated flame at the end of the recirculation zone.

Radhakrishnan et al. (1981) developed a correlation for the blowout velocity of premixed bluff body-stabilized turbulent flames by examining the relevant turbulent and chemical timescales, using the model of turbulence depicted in Figure 3, where small-scale structures are actually like tubes of vorticity.

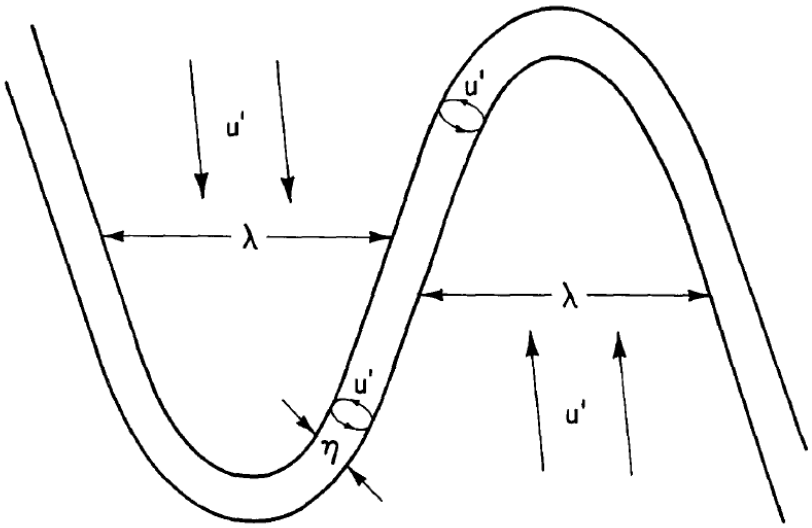

Figure 3. Turbulence model used by Radhakrishnan et al., where λ is the Taylor microscale, η is the Kolmogorov scale and u' is the turbulence intensity (Radhakrishnan 1981)

The Kolmogorov scale was taken to be the scale of the vortex tubes, while the Taylor microscale was defined as the average spacing of the randomly distributed vortex tubes. Radhakrishnan argued that the Taylor microscale is the scale across which the flame must propagate at the laminar flame speed, S_L , and for the flame to remain stable, the laminar flame propagation must occur in a time less than that of the characteristic fluid mechanic time. Based on previous studies, including those of Plee and Mellor, Radhakrishnan took the shear layer mixing time to be the critical characteristic turbulent timescale, rather than the residence time in the recirculation zone.

The chemical time was then defined as:

$$\tau_c = \lambda / S_L \tag{5}$$

The characteristic eddy time is defined in Equation 6.

$$\tau_e = l / u' \tag{6}$$

In Equation 6, l is the integral length scale. A ratio of the chemical timescale to the eddy timescale was proposed as the critical parameter by which blowout is governed. If the chemical timescale is substantially larger than the eddy timescale, the flame will not be able to propagate.

Assuming isotropic turbulence, and that u' is proportional to the velocity at the flameholder lip (U_{lip}), and that l is proportional to the length of the recirculation zone (L), τ_c/τ_e can be simplified as shown in Equation 7, where ν is the kinematic viscosity and S_L is the laminar flame speed.

$$\tau_c / \tau_e = \left(\frac{U_{lip} \nu}{L} \right)^{1/2} (S_L)^{-1} \tag{7}$$

Using Equation 7, as well as empirical correlations to estimate laminar flame speed, Radhakrishnan developed a model for the blowout velocity of bluff body-stabilized flames, which correlated well with experimental data taken on lean propane flames. It was found that the lip velocity was a better parameter for determining stability than the gas approach velocity. In addition, the recirculation zone length was found to be a more appropriate length scale than the flameholder size, though the authors acknowledged the difficulties in measuring the recirculation zone length (Radhakrishnan 1981).

Kariuki (2012) of the University of Cambridge has studied the blow-off behavior of swirl-stabilized premixed and spray flames, both as single and adjacent flames. Specifically, Kariuki utilized premixed methane and non-premixed heptane flames to examine blow-off limits, flame structure, and the average duration of the blow-off transient. OH* chemiluminescence imaging

showed that as the premixed flames neared extinction, the flame gradually moved further upstream into the recirculation zone, where the flame fragments survived for a time on the order of tens of milliseconds before finally extinguishing. The time for total blow-off to occur was calculated based on the time series of the OH* chemiluminescence signal. The blow-off event was found to be relatively long when compared to the fluid dynamic timescale *d/U*, suggesting that with adequate detection and control methods, blowout could be prevented in a system operating near the lean limit. It should also be noted that a longer or shorter blow-off transient did not necessarily translate into a higher or lower equivalence ratio at lean blowout.

Kariuki proposed the use of the parameter in Equation 8 to predict when lean blow-off will occur. This parameter was derived from a rearrangement of the turbulent premixed flame extinction theory originally proposed by Radhakrishnan et al.

$$\left[\left(\frac{U_b}{d}\right)\left(\frac{\nu}{S_L{}^2}\right)\right]^{1/2} \tag{8}$$

Kariuki plotted this value against the flame power and found that the scatter was "considerably smaller" than that usually observed in the literature. In theory, the parameter calculation should yield a value near unity. The values for the premixed flames studied by Kariuki ranged from 1.15 to 1.34.

In a 2003 study, Mehta and Soteriou investigated the vortex dynamics of bluff body-stabilized premixed flames through detailed modeling validated against experimental data. They found that the flame's wake was dominated not by the large asymmetrical Von Karman vortex shedding normally attributed to the wake behind a bluff body in a non-reacting

condition, but rather by symmetric shedding without any single dominant frequency. They attributed this shift in behavior to the dilatation caused by combustion heat release, as well as baroclinic vorticity. This work was continued by Erickson (2006), who used an unsteady, Lagrangian simulation technique to model bluff body-stabilized flames with varying temperature ratios ($T_{burned}/T_{unburned}$) across the flame. For relatively small temperature rises, Von Karman shedding appeared to dominate the flow, as seen in non-reacting flows. The strength of the Von Karman shedding diminished as the temperature ratio increased, until it was completely suppressed at high temperature ratios.

Research done in Tim Lieuwen's group at the Georgia Institute of Technology has focused on the mechanism of lean blowout and the timescales that may be critical to the process (Nair 2007, Husain 2008, Shanbhogue 2009). Nair et al. conducted laser sheet imaging studies and PIV (particle image velocimetry) velocity field measurements to determine the transient dynamics of near-blowout, bluff body-stabilized flames. They found that the first stage of blowout was characterized by localized "holes" in the flame sheet where the instantaneous stretch rate exceeds the extinction stretch rate. In theory, the flame could persist in this state indefinitely, and no large-scale alteration of the flame or wake dynamics was observed. As the equivalence ratio decreased from this condition, the duration and scale of these "holes" increased. As blowout was approached, the authors argue that the flame entered a second stage of blowout, where large-scale, violent flapping of the flame front was noted, similar to Von Karman-type shedding. The authors acknowledged that the first stage of blowout that they observed, with localized extinctions, may not be a necessary condition for the second stage to arise.

The authors also noted that the flame blew out much earlier than the point at which the average strain rate equaled the extinction strain rate, leading them to conclude that the blowout must be precipitated by a localized extinction event of large enough scale to cause blowout of the entire flame. They suggested that the possible mechanism for blowout could be the introduction of a "slug" of relatively cool, unreacted mixture into the recirculation zone by the large-scale dynamics seen in the second stage. This "slug" would then fail to ignite the incoming mixture, and the flame would blow out. Chauduri et al. (2011) noted a similar progression of flame behavior near blowoff, where shear layer extinction and recirculation zone burning are precursors to blowoff for premixed flames.

Husain (2008) attempted to develop a Damköhler number that could adequately model lean blowout in a large set of data obtained through past and recent literature, noting that almost every past researcher has concluded that a competition between some fluid mechanic timescale and a chemical timescale is critical to explaining the blowout process. Three chemical times were considered and calculated using CHEMKIN software: the minimum residence time of a well-stirred reactor for which a majority of the reactants are consumed (τ_{PSR}); the time related to the extinction strain rate of an opposed flame (τ_{ESR}); and the ratio of the premixed flame thickness and flame speed (τ_{pf}). The author found that both τ_{ESR} and τ_{pf} vary proportionally to τ_{PSR}, and so τ_{PSR} was used as the chemical timescale in the Damköhler number.

For the fluid mechanic timescale, Husain took *D/U*, where *U* is the lip velocity, and the characteristic length scale used was either the characteristic diameter of the bluff body or the estimated momentum layer thickness, defined in Equation 9.

$$\frac{\theta}{D} = \frac{35}{\mathrm{Re}_D^{0.5}} \tag{9}$$

Plotting the Damköhler number against the Reynolds number, Husain developed the correlation shown in Figure 4. The correlation that produced the smallest spread was with a Damköhler number calculated with the fluid mechanic timescale of D/U_{lip}.

Looking closely at the plot in Figure 4, it is of note that both the x and y axes are in a log scale, which causes the data to appear more closely grouped. In addition, while the authors claim a dependence on Reynolds number, if the blue lines on the plot are ignored, it becomes apparent that in actuality, the data fall on a mostly horizontal line, and the dependence on Reynolds number appears to be minimal for the dataset as a whole. Some individual data subsets, denoted by different symbols on the graph, do appear to have a clearer dependence on Reynolds number.

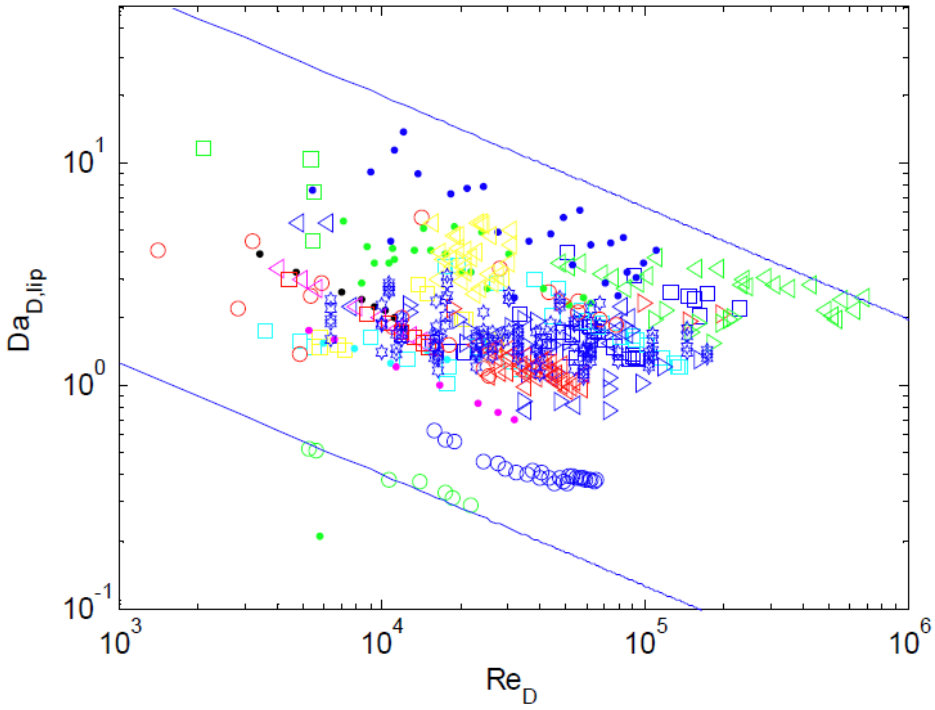

Figure 4. Correlation from Husain (2008)

Tuttle et al. (2012) investigated lean blowout behavior in vitiated and non-vitiated flames using chemiluminescence, both unfiltered and filtered for CH*, and simultaneous PIV and OH PLIF (planar laser-induced fluorescence). The PIV/OH PLIF measurements were evaluated to extract the aerodynamic stretch rates at the interface of the flame surface and the velocity field in both steady and blowout conditions. The researchers found that the flame blew off at lower equivalence ratios in vitiated flows than in non-vitiated flows and attributed this phenomenon to the generally higher temperatures of the vitiated flows. However, if the vitiation levels were increased, the effect of the higher temperature was mitigated by the decreasing oxygen concentration, and the reduction in equivalence ratio at lean blowout was more moderate.

For the temperature ratios studied by Tuttle et al., Von Karman vortex shedding dominated the flow field near lean blowout. The imaging data showed an increase in flame

stretch as blowout approached, which resulted in flame extinction on the periphery of the recirculation zone. In reviewing the results from their vitiated experiments, as well as the results from past non-vitiated experiments, the authors concluded that the final stage of blowout occurs when reactants are entrained and burned within the recirculation zone.

Gokulakrishnan et al. (2009) performed LES simulations to investigate the influence of chemical kinetics on bluff body-stabilized flames near blowout conditions using reduced kinetic models for propane and the Eddy Dissipation Concept (EDC) model to account for turbulence-chemistry interactions. In order to discern the effect that turbulence may have had on the model, simulations were also performed with a Laminar Chemistry (LC) model. When the LES was performed using the LC model, it predicted symmetrical Kelvin-Helmholtz type vortex shedding. When the model accounted for sub-grid scale turbulence-chemistry interactions, as in the EDC model, it predicted asymmetrical Von Karman vortex shedding. The LES-EDC simulations also predicted a blowout of the particular flameholder configuration at an equivalence ratio of around 0.6, which was near the actual experimental blowout of the configuration. The authors concluded that the interaction of turbulence and chemistry is important in determining the nature of the vortex shedding in a bluff body-stabilized flame, which may in turn influence the flame's stability.

While bluff body flames have been studied extensively for decades, there has not been a consensus on the physical cause of blowout. The conclusions of Shanbhogue et al. (2009) imply that the mechanism relies on ignition processes, which is disputed by Law (2006). Both Radhakrishnan (1981) and Kariuki (2012) had some success correlating blowout to flame speed, which would suggest that blowout is not governed by the ignition timescales. Shanbhogue et al.

also suggest that as the flame nears blowout, it develops a sinuous instability, which entrains cold reactants into the flame, disrupting the ignition process. However, it is unclear whether all bluff body flames exhibit this sinuous structure before blowout or whether it is a primary influence on the blowout. For example, Khosla et al. (2007) performed a Large Eddy Simulation analysis on bluff bodies with and without small tabs. The tabs effectively broke up the Von Karman vortex shedding, and yet both flameholders blew out at the same premixed equivalence ratio.

Chemiluminescence taken by Huelskamp et al. (2011) of flames stabilized on bluff bodies of various shapes showed that not all flames displayed sinuous shedding prior to blowout. The study also evaluated the effect that shape had on blowout by correlating the cold-flow Strouhal number to the equivalence ratio at lean blowout. The Strouhal number, which characterizes the shedding behavior behind a bluff body, is shown in Equation 10, where f is the characteristic shedding frequency behind the bluff body, U is the lip velocity, and L is the flameholder diameter.

$$St = \frac{fL}{U} \tag{10}$$

The Strouhal number was measured using hot wire anemometry, and the value varied with the shape of the bluff body. In this way, the shape of the bluff body could be assigned a numerical value, which could then be included in a correlation to predict lean blowout. The Strouhal number did not appear to have a first-order effect on lean blowout, indicating that the shape and the shedding behavior did not govern the mechanism of blowout.

The lack of a physical mechanism for lean blowout has made developing accurate prediction correlations very difficult. As discussed earlier, the DeZubay correlation predicts lean blowout of propane flames with some accuracy, but it begins to deteriorate when attempting to predict the blowout of flames fueled by other hydrocarbons. Because of the limitations in computing at the time, Radhakrishnan was forced to use empirical correlations to calculate flame speed, and so the correlation was as much a validation of the flame speed calculations as it was a prediction of blowout. The correlation developed by Husain was derived from physical principles, but results in a large spread of data. In addition, Husain's correlation relies on parameters that require computation on kinetics software, making the prediction cumbersome.

Overview of Present Work

This thesis will use experimental data taken at the Air Force Research Laboratory, as well as data collected from many of the papers reviewed above, to develop a correlation to predict lean blowout using a least squares curve fit method. The laminar flame speed and ignition delay time will be calculated for subsets of the data using the chemical kinetics software Cantera, and the results will be incorporated into the correlations.

This work will serve two purposes. The first is to provide an accurate, practical method of predicting lean blowout for designers and modelers. The second purpose of the correlation is to provide insight into the critical parameters and timescales that govern the blowout process by examining the significance of each parameter included and what physical and chemical processes it may affect.

CHAPTER 2

METHODS AND EXPERIMENTAL SETUP

Experimental Rigs

Experiments were performed in two combustion labs at the Air Force Research Laboratory (AFRL) on Wright-Patterson Air Force Base. Bluff body flameholding tests were performed in an atmospheric pressure combustion facility using propane as a fuel. The facility can deliver air inlet temperatures of up to 900°R with four electric heaters with a total power capacity of 358kW. Temperatures of up to 1800°R can be achieved with vitiation. Air is metered through orifice plates with an uncertainty within 2%, and coriolis meters measure the fuel flow within 0.35% of total flow.

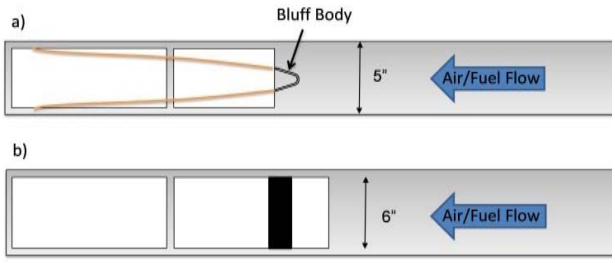

Figure 5. Schematic of bluff body rig showing optical access: a) top view b) side view

The available airflow to this facility can provide lip Mach numbers of up to 0.3 and lip Reynolds numbers up to 100,000 in a test section 6 inches high by 5 inches wide. Lip Reynolds number is calculated using the flameholder diameter and the velocity of the incoming gas as it passes over the flameholder. Figure 5 shows a schematic of the test rig with a v-gutter bluff body installed. The airflow is right to left and passes through a perforated plate, which provides

more uniform velocity and temperature profiles at the inlet of the test section. The flame holder trailing edge is 23 inches from the inlet of the test section. The flame holder spans the full height of the rig, and optical access through quartz windows is available for high-speed imaging. Gaseous propane is premixed with the air approximately 5 feet upstream of the test section. The fuel distribution was validated using acetone-seeded planar laser-induced fluorescence (PLIF). The fuel-air mixture is ignited with an ethylene torch behind the bluff body. Figure 6 shows the rig as it is installed in the facility.

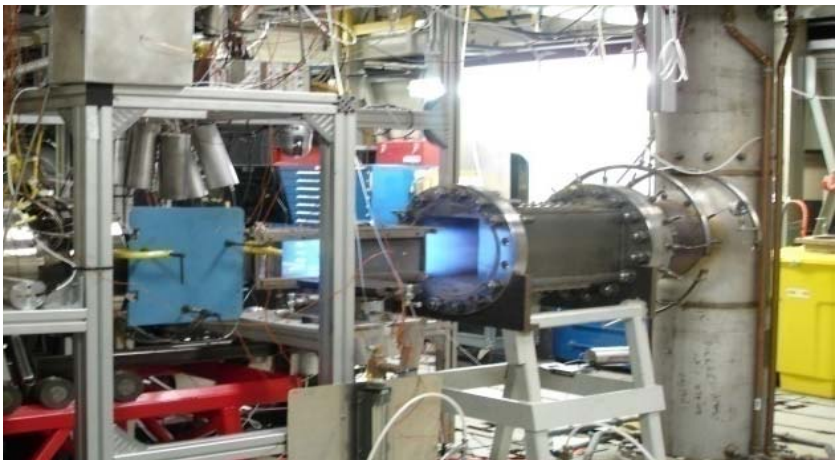

Figure 6. Rig as installed in the atmospheric pressure combustion lab

The High Pressure Combustion Research Facility also performed experiments for this work. Various jet fuels, including petroleum-derived JP-8, tallow-derived hydro-treated renewal jet (HRJ) fuel, and camelina-derived HRJ fuel, were combusted in a vitiated stream. The test section is 6 inches wide and 9 inches tall with a 1.5-inch wide v-gutter, and Mach numbers up to 0.3 can be achieved. This facility can vary the pressure in the test section from 5-20 psia. Heaters provide inlet air temperatures of up to 1200°R, and vitiation can raise the test section inlet temperature up to 1800°R. Oxygen levels of the gas entering the test section vary from 17-21%, depending on the chosen level of vitiation; for this study, the points chosen were taken at

an oxygen level of approximately 18%. The test section fuel is injected approximately 20 inches upstream of the flameholder through atomizing nozzles, providing a premixed, pre-vaporized fuel condition. The fuel distribution was verified using PLIF. The molecular weight of the jet fuels ranged from 153.9 to 161 g/mol, and the hydrogen to carbon ratio of the jet fuels ranged from 2.017 to 2.176.

Lean Blowout Data Collection and Correlation Setup

Lean blowout measurements were taken on four types of stainless steel bluff body flameholders: v-gutters with diameters of 0.375-1.5 inches, a cylinder, a plate, and a square cylinder. The cylinder, plate, and square cylinder were all 1.5 inches wide. Figure 7 depicts the cross-sections of these flame holders. Blowout was achieved by first reaching the desired inlet conditions and decreasing fuel flow until the flame was very near blowout, but stable. The fuel flow was then decreased slowly until the flame blew out, and a data point was recorded.

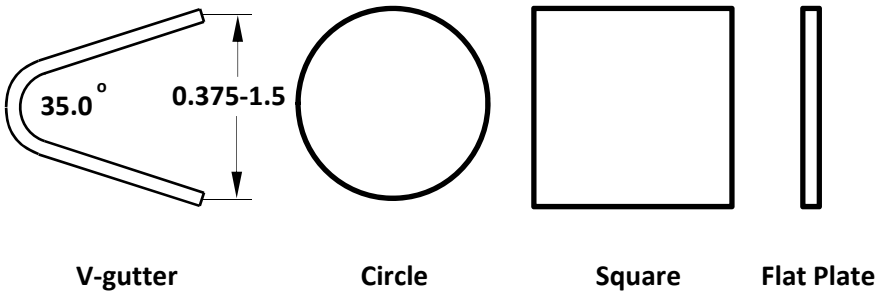

Figure 7. Various bluff body flameholders studied in this work

The data points from these experiments were combined with data points obtained through other authors' publications, including Ballal and Lefebvre (1979), DeZubay (1950), King (1957), Potter and Wong (1958), Williams (1949), Zukoski (1954), Chaudhuri (2011), Yamaguchi

(1985), and Barrere (1954). Table 1 is a summary of the experimental parameters from each study. Hopane, the fuel listed for the DeZubay work, contained 95% propane and 5% butane and/or ethane. An input file of over 1100 individual points included the relevant parameters from each study, such as inlet conditions and flame holder characteristics. All experiments were conducted using single-flameholder configurations. The least squares curve fit function in the Matlab optimization toolbox was used to find an optimal correlation. The desired equation form was selected before running the correlation code.

Table 1. Summary of experimental parameters from data used in this work

Author(s)	Lip Velocity (ft./s)	Flame holder Diameter (in)	Inlet Temp. (°R)	Inlet Pressure (psia)	Reynolds Number	Fuel Type
Huelskamp	21-171	0.375-1.5	523-1034	14.4	4800-86,000	Propane
Ballal and Lefebvre	34-497	0.8-4.92	540-1035	2.9-14.5	12,000-506,000	Propane
DeZubay	86-706	0.25-1	550	3-15	4200-345,000	Hopane
King	403-743	1.5	1260-1860	5.2-12.5	14,000-87,000	JP-4
Potter and Wong	79-765	0.375-1	540-550	3.7-13.8	7,300-260,000	Propane
Williams	29-353	0.1-0.51	540	14.7	1,400-89,000	Propane
Zukoski	81-1206	0.01-0.25	610-860	14.7	200-57,000	Hydrogen, Methane, Gasoline
UConn (Chaudhuri)	66-128	0.375	513-531	14.7	13,000-25,000	Propane
Yamaguchi	30-125	0.94	529	14.7	14,000-60,000	Propane
Barrere	39-157	0.20	522	14.7	4,000-16,000	Propane
AFRL	239-490	1.5	1318-1656	10	20,000-53,000	Jet fuels

Goodness of Fit Evaluation

In order to evaluate how various parameters improved or worsened the effectiveness of the correlation, the adjusted R-squared value for each correlation was calculated according to Equation 11.

$$R_{adj}^2 = 1 - \frac{SS_E/(n-p)}{SS_T/(n-1)} \tag{11}$$

In this equation, SS_E is the sum of the squares of the residuals, SS_T is the total sum of the squares of the original dataset, n is the number of data points, and p is the number of parameters used in the correlation.

The adjusted R-squared statistic is more appropriate for comparing correlations that contain varying numbers of parameters than is the traditional R-squared statistic. A least-squares curve fit algorithm will run until the residuals have been reduced as much as possible. If a parameter is introduced that is not relevant to the correlation, the curve fit will simply reduce its significance until it is negligible, and the change to the goodness of fit for that correlation will remain unchanged. If the parameter is relevant, it will be assigned the appropriate significance and the goodness of fit should improve. Because the least-squares algorithm will always reduce the residuals as much as possible, introducing a new parameter should never worsen the fit, and will therefore never decrease the traditional R-squared value. The adjusted R-squared statistic penalizes added parameters to correct for this bias, providing a better statistic for comparing correlations (Montgomery 2006). All R-squared statistics reported throughout this work will be the adjusted R-squared values.

In addition to calculating the R-squared statistic, the residual for each point was plotted against the predicted equivalence ratio at lean blowout to determine if trends were present within the residuals. If trends are present, it indicates that the model is inadequate, possibly due to phenomena that are not fully captured in the correlation (Montgomery 2006). An example plot is shown in Figure 8. For the correlations in this study, the residuals were generally randomly distributed over the range of predicted equivalence ratios, with the exception of some of the first correlation attempts with low R-squared statistics.

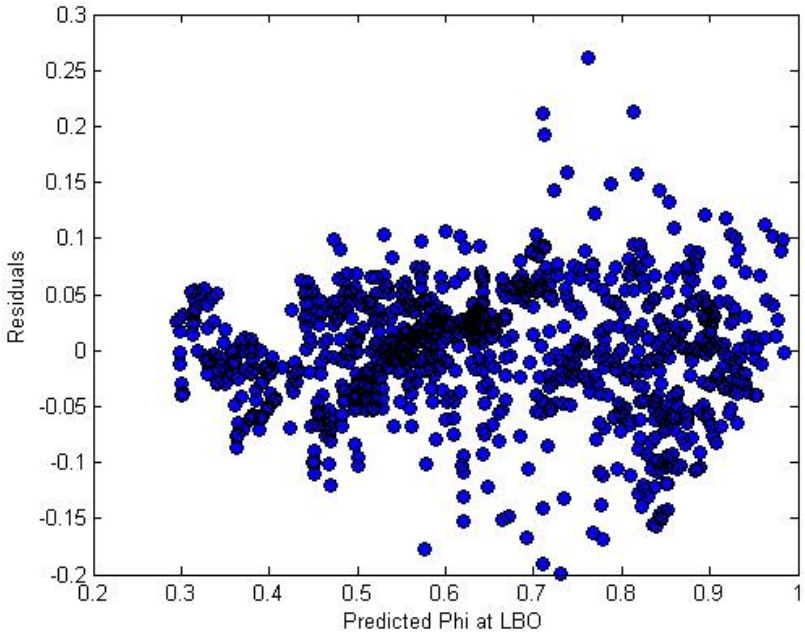

Figure 8: Representative residuals plot

Cantera Setup

Cantera, an open-source chemical kinetics software, was used to calculate the laminar flame speeds and ignition delay times for subsets of the data. 200 points over a range of pressures, temperatures, velocities, Reynolds numbers, and flameholder geometries were

selected from data points taken on propane and methane for the laminar flame speed data set. Propane and methane were chosen because chemical mechanisms that are validated at relevant conditions for these fuels are readily available. The GRI-Mech 3.0 mechanism was used for the methane chemistry, and a mechanism developed by Combustion Science and Engineering (CSE) in Columbia, Maryland was used for the propane chemistry. GRI-Mech 3.0 is an optimized mechanism designed to model natural gas combustion with 53 species and 325 reactions (Smith). CSE's reduced mechanism, consisting of 30 species and 114 reactions, has been validated against experimental data at the temperatures pertinent to the present study (300-650K), as shown in Figure 9 (Gokulakrishnan 2009).

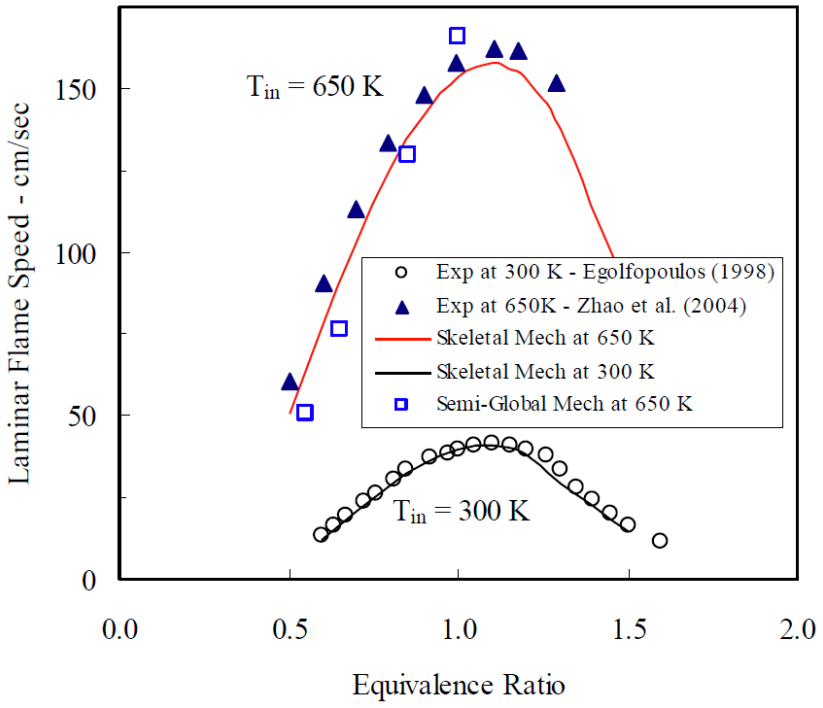

Figure 9. Validation of the CSE propane mechanism against experimental data (Gokulakrishnan 2009)

Using the inlet conditions at each data point, Cantera was used to calculate the laminar flame speed. For the data evaluated, the flame speeds ranged from 0.22 to 1.81 ft/s. This data was then processed through the Matlab optimization toolbox in a manner similar to that described in the Correlation Setup section.

The propane dataset used for the laminar flame speed calculations could not be used to study the effect of ignition delay time due to the extremely long ignition delay times of propane at atmospheric pressure and relatively low temperature (below 600K). Instead, the ignition delay dataset was comprised of data taken on various jet fuels for which chemical mechanisms are available. The chemical mechanism used with Cantera was developed by CSE. This mechanism uses a surrogate mixture for each jet fuel comprised of n-dodecane, n-decane, iso-octane, and propyl-benzene. The ratio of the various components is determined by matching the molecular weight, hydrogen to carbon ratio, derived cetane number, and threshold sooting index of the target fuel. Surrogates that mimic these relatively basic fuel properties exhibit very similar chemical kinetics-related behavior as the target fuels they are meant to emulate (Dooley 2010, 2012). Cantera calculated the ignition delay time of each point based on its inlet conditions. The oxidizer composition was calculated using a Matlab function relying on combustion chemistry and thermodynamic principles of equilibrium to calculate the chemical make-up of the inlet gases after vitiation. The Matlab least squares curve fit function then used the resulting data to find the desired correlation, as described earlier in the Correlation Setup section. For the data evaluated, the ignition delay times ranged from 412 to 5728 ms.

CHAPTER 3

CORRELATION RESULTS BASED ON INLET CONDITIONS

Correlation with Inlet Conditions

The Matlab correlation code was first run with the same parameters as those used in DeZubay's correlation: velocity, length scale, and inlet pressure and temperature. Figure 10 shows the correlation results with all of the available data, except the vitiated data from AFRL, which was excluded in the interest of determining the effect of various parameters without complicating the correlations with vitiation effects. The data is plotted with the predicted equivalence ratio (or phi) at lean blowout on the x-axis and the actual equivalence ratio at lean blowout on the y-axis. The equation resulting from the correlation is in the upper left corner of the plot. The black line running through the plot represents what would be a "perfect" correlation. The R-squared value from this correlation is 0.52.

Zukoski (1954) cites a Reynolds number of 10,000 as a transition point in the lean blowout behavior, and many of the outliers in the first correlation were points taken at low Reynolds numbers. Figure 11 shows the correlation results with all points taken at Reynolds numbers over 10,000. The filtered dataset improved the R-squared value from 0.52 to 0.77.

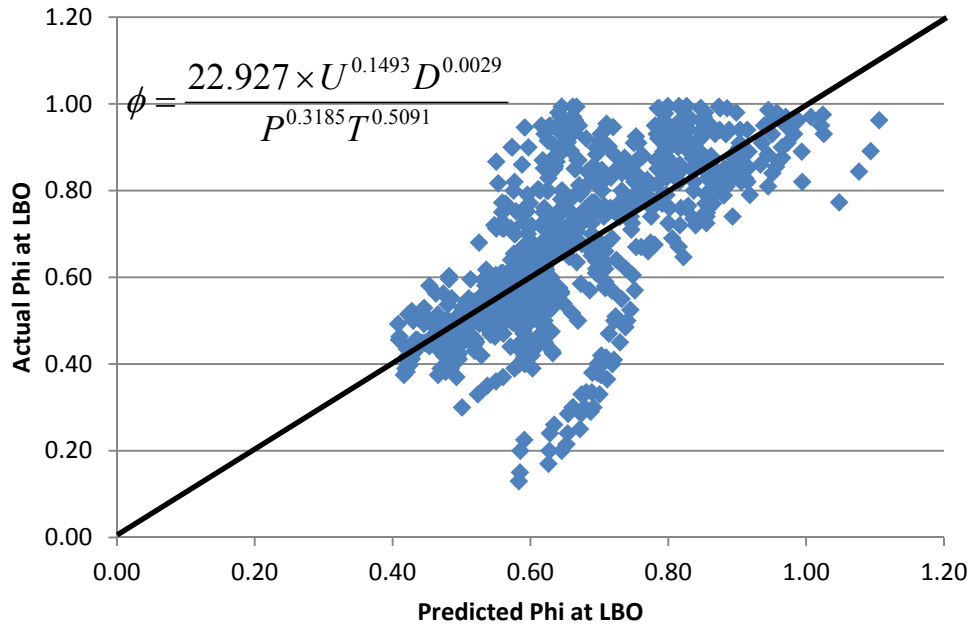

Figure 10. Correlation with all data, R^2=0.52

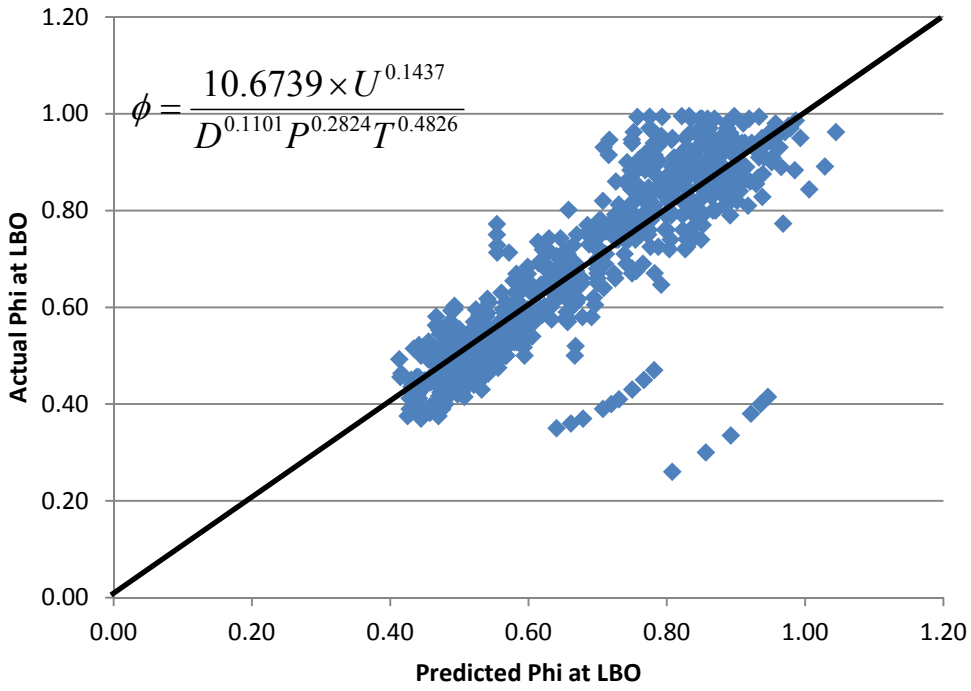

Figure 11. Correlation with data taken at Reynolds number of more than 10,000, R^2=0.77.

It is of note that the major outliers on this plot represent points taken from experiments that used hydrogen as a fuel. Hydrogen has very different physical and chemical properties, like diffusivity and flame speed, than the other fuels used in the dataset, and it is not unexpected that it would perform differently than the hydrocarbon fuels. When the hydrogen-fueled points are removed from the dataset, as in Figure 12, the R-squared value increases again, from 0.77 to 0.89.

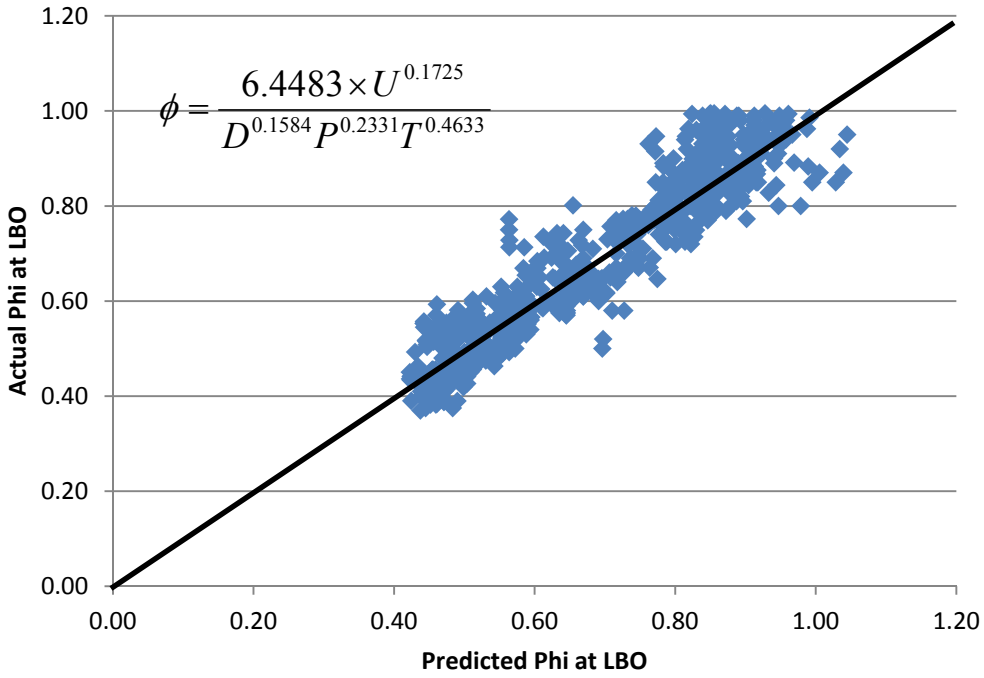

Figure 12. Data taken at Reynolds number of more than 10,000 without hydrogen data, R^2=0.89.

Filtering out only the hydrogen-fueled points, the correlation was performed again to include the previously excluded points that were taken at low Reynolds numbers. Including these points caused a slight reduction in the R-squared value of the correlation, but provided a larger dataset. The low Reynolds number points were included in subsequent correlations to

provide greater variation within the parameters used for the correlation. Figure 13 shows the correlation run without hydrogen experiments but with points taken at a Reynolds number below 10,000.

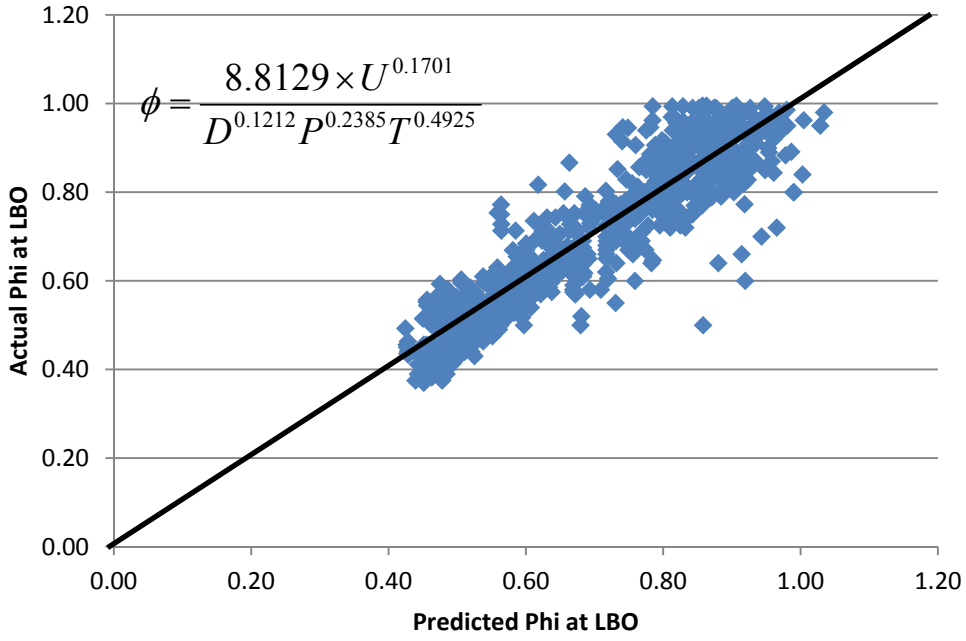

Figure 13. Correlation without data taken on hydrogen, R^2=0.86.

The exponents on the velocity and diameter parameters are similar. When these parameters are grouped together to form a single parameter, U/D, the resulting correlation equation, with an R-squared value of 0.85, is:

$$\phi_{predicted} = \frac{7.6918 \times \left(U/D\right)^{0.1387}}{P^{0.2684} T^{0.4442}} \quad (12)$$

The results, separated by source, are depicted in Fig. 14. The plot legend also indicates the fuel used in each experiment.

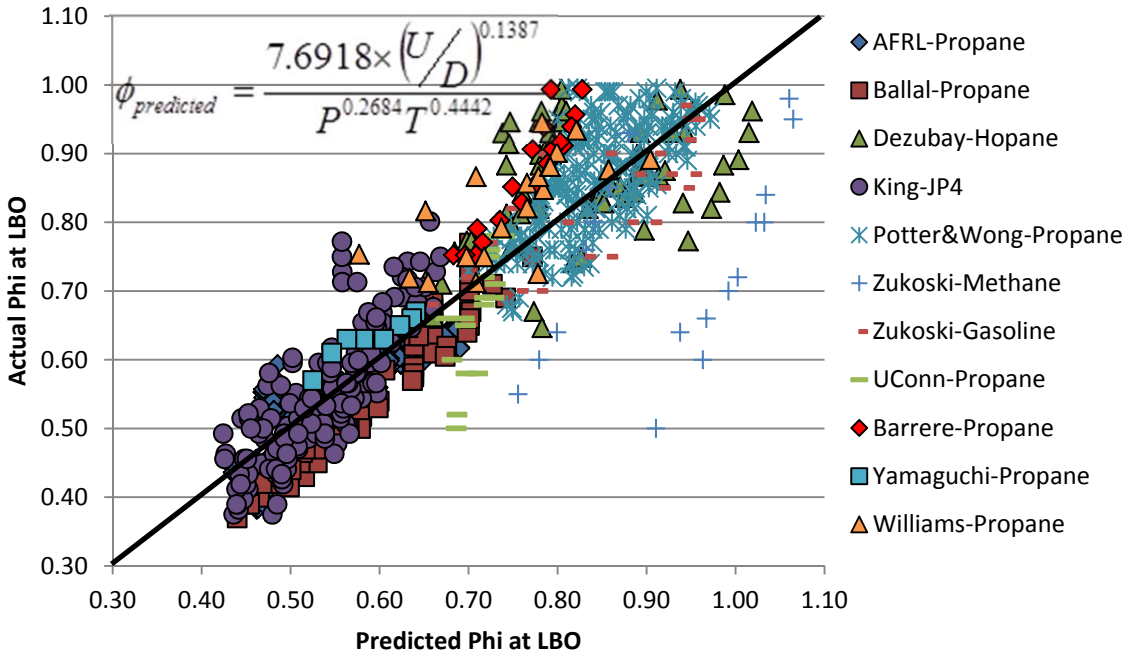

Figure 14. Correlation results with U/D as parameter, R^2=0.85.

Damköhler Number

The ratio of U/D is recognized as the inverse of a fluid dynamic timescale used in much of the reviewed literature to represent the time the reactants spend in contact with the recirculation zone. In addition, pressure and temperature are major influences in various chemical timescales, indicating that the correlations may be pointing to a global Damköhler number. As discussed earlier in the introduction, many previous researchers have also concluded that a Damköhler number governs lean blowout, though several timescales could be at work, including ignition delay time and laminar flame speed. It is possible that if the ignition delay time of the fresh reactants is longer than the associated fluid dynamic timescale, the reactants will not be able to ignite, causing blowout. This is the mechanism of blowout proposed by Marble and Zukoski. Other researchers have proposed that the chemical timescale

is the time required for the flame to propagate across the microscale eddies in the turbulent shear layer between the recirculation zone and the fresh reactants in the free stream (Radhakrishnan 1981).

For a given equivalence ratio, laminar flame speed can be curve fit in the form of Equation 13 (Liao 2004).

$$S_L \approx A \times P^b T^c \tag{13}$$

However, the ignition delay time follows a curve described more closely by Equation 14 (Plee 1979).

$$IDT \propto e^{A/T} \tag{14}$$

Due to the exponential influence of temperature on the ignition delay time, the form of the correlation equation was changed to provide an exponential form for temperature, in an effort to discern whether this would improve the correlation and therefore indicate that the chemical timescale may be ignition delay time instead of flame speed. The results are shown in Fig. 15.

Changing the form of the temperature portion of the equation had little effect on the R-squared value of the correlation, which remained near 0.85. Without a clear indication of the appropriate form of the temperature dependence in the equation, it is impossible to determine what timescale may be critical to the blowout process without further investigation. Due to this lack of clarity, both laminar flame speeds and ignition delay times were calculated for subsets of data and used in correlations for the equivalence ratio at lean blowout, as will be described in Chapters 5 and 6.

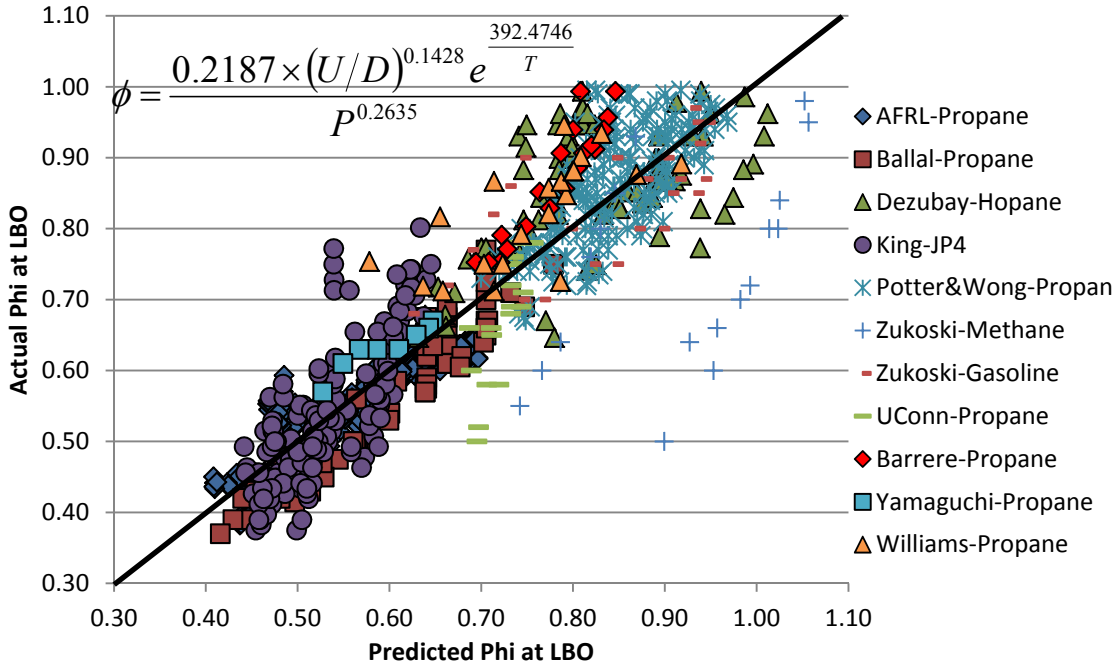

Figure 15. Correlation fit of data using an exponential for inlet temperature, R^2=0.85.

Though the chemical timescale could not be determined using only the inlet conditions of the gases flowing past the bluff body, it is reasonable to conclude that the equation found through the correlation represents a global Damköhler number. The U/D parameter is an indication of the fluid mechanical timescale, while the pressure and temperature carry the effect of the chemical timescale.

Despite the relatively good fit of the data to the correlation equation, some effects are visibly not captured. Closer examination of Figures 14 and 15 reveals that data points taken from experiments using fuels other than propane seem to either fall away from the "perfect fit" black line, as in the case of methane data, or to follow a slightly different slope on the plot, as in the case of the JP-4 data. This observation led to exploring the addition of fuel characteristics to the correlation.

CHAPTER 4

CORRELATION RESULTS BASED ON FUEL PROPERTIES

Background

As discussed in the experimental set-up, researchers have successfully developed surrogate jet fuel formulations based on molecular weight, hydrogen to carbon ratio, threshold sooting index (TSI), and derived cetane number (DCN) (Dooley 2010, 2012). Of these parameters, both molecular weight and hydrogen to carbon ratio are easily obtained for all of the fuels in the dataset for this work. In an effort to account for the fuel effects seen in Figures 14 and 15, the molecular weight and hydrogen to carbon ratios for each fuel were added to the correlation.

Initial Results

Figure 16 shows the results of the correlation using the same data as that used in Figures 14 and 15, but including molecular weight and hydrogen to carbon ratio in the correlation. The methane data is brought much closer to the perfect fit line, and the JP-4 data also appears to collapse more closely to this line. In addition, the R-squared value increases from 0.85 to 0.89. The exponents on both molecular weight and hydrogen to carbon ratio are relatively large, indicating that they are both important parameters.

Equation 15 shows the correlation equation with temperature in a power form (to fit flame speed curves), while Equation 16 shows the exponential form (to fit ignition delay curves).

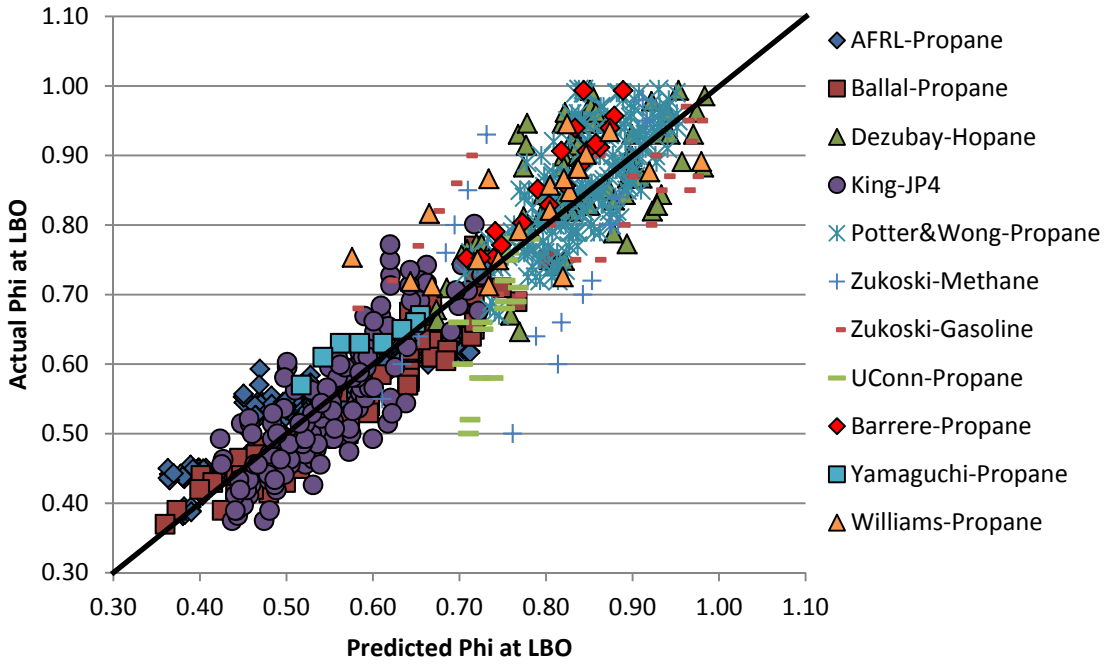

Figure 16. Correlation results with molecular weight and hydrogen to carbon ratio as parameters, R^2=0.89.

$$\phi = \frac{0.8598 \times \left(U/D\right)^{0.164} MW^{0.7093} \left(H/C\right)^{1.1964}}{P^{0.2281} T^{0.7537}} \tag{15}$$

$$\phi = \frac{0.0134 \times \left(U/D\right)^{0.1603} e^{\frac{570.366}{T}} MW^{0.4315} \left(H/C\right)^{0.6559}}{P^{0.2375}} \tag{16}$$

The R-squared statistic resulting from the correlation form in Equation 15 is 0.89, but is 0.87 from the correlation form in Equation 16. The higher R-square statistic associated with using an equation form that more closely matches that of flame speed than of ignition delay time may be an indicator that flame speed is more closely related to the timescales critical to the blowout process. In the correlation used to create Figure 16, and in subsequent correlations, the form used contains a power function for temperature.

Expanded Dataset

While Equation 15 adequately predicts blowout for data taken mostly on lighter, single-component fuels, many combustion systems of interest operate on diesel or jet fuel. In addition, some systems operate with vitiated inlet gases. In order to capture the effect that heavier, multi-component fuels may have, the dataset was expanded to include data taken on various jet fuels at vitiated conditions at AFRL. The conditions at which these points were measured are outlined in Table 1. The molecular weight and hydrogen to carbon ratios of these fuels were measured by Princeton University (Won 2013). Fuel 6169 is a petroleum-derived JP-8, Fuel 6308 is a tallow-derived HRJ fuel, and Fuel 7721 is a 50-50 blend of 6169 and a camelina-derived HRJ fuel. The vitiation levels, denoted by the percent of oxygen in the oxidizer, were calculated using a Matlab function based on combustion chemistry and thermodynamic principles of equilibrium. The vitiation levels are included to account for the change in reactivity that may take place with reduced oxygen content and increased levels of molecules from the combustion products.

Results with Vitiated Jet Fuel Data Points

Figure 17 shows the correlation with the jet fuel data added without taking into account the vitiation levels or the fuel characteristics. The R-squared value is 0.84. Again, the methane data falls off the perfect fit line, as does the newly introduced jet fuel data.

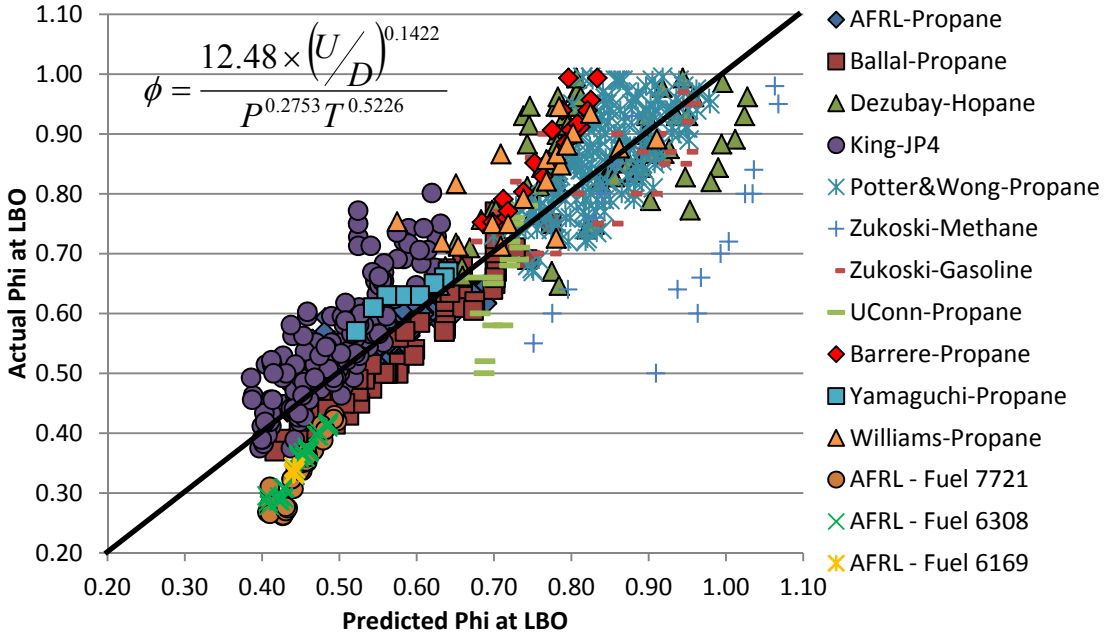

Figure 17. Correlation results with vitiated data, R^2=0.84.

The oxygen level was introduced as a parameter to account for the vitiation levels. For the AFRL jet fuel data, the oxygen level was near 18%. For the non-vitiated data, the oxygen level was assumed to be 21%, since the oxidizer in each experiment was air. The results of this correlation are shown in Figure 18. The AFRL jet fuel data now intersects the perfect fit line and the R-squared value has increased to 0.88.

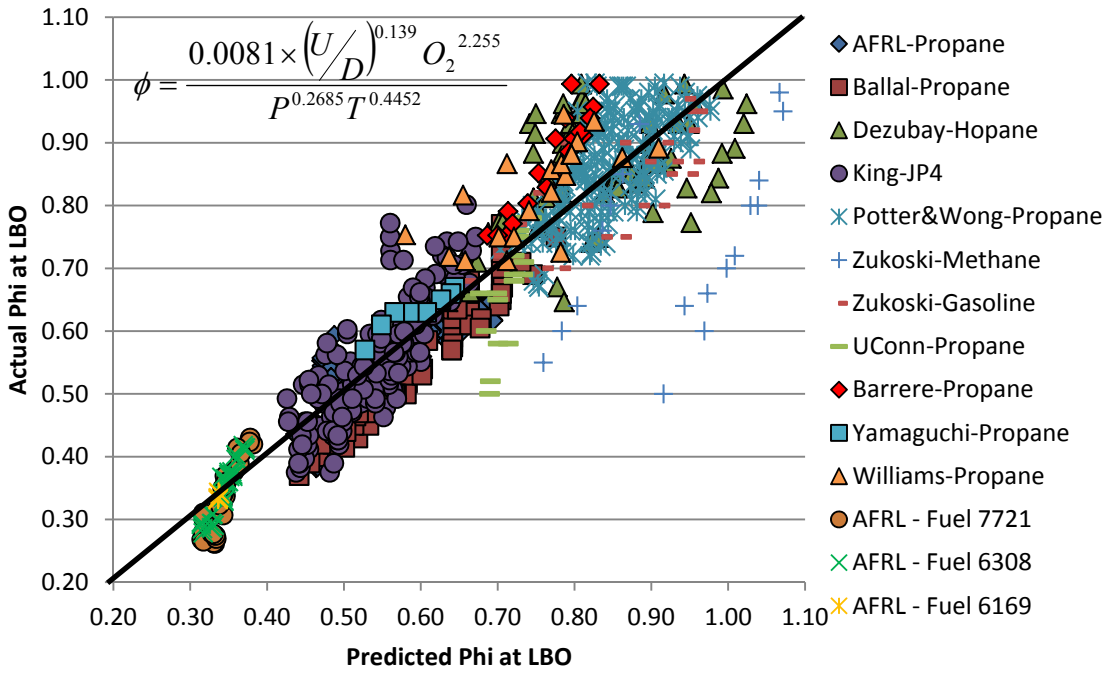

Figure 18. Correlation results with vitiated data and O_2 as a parameter, R^2=0.88.

Based on the findings in the dataset that did not include the AFRL jet fuel points, the fuel characteristics appear to play a major role in the lean blowout. When molecular weight and hydrogen to carbon ratio are included in the correlation with the jet fuel data, the R-squared value increases to 0.91. The plotted correlation is shown in Figure 19. The AFRL jet fuel data now fall very closely to the perfect fit line, and, as expected, the methane and JP-4 data also shift closer to this line. Equation 17 shows the correlation equation.

$$\phi = \frac{1.1 \times 10^{-6} \times \left(U/D\right)^{0.1642} MW^{0.7082} \left(H/C\right)^{1.1921} O_2^{4.4605}}{P^{0.2282} T^{0.7546}} \quad (17)$$

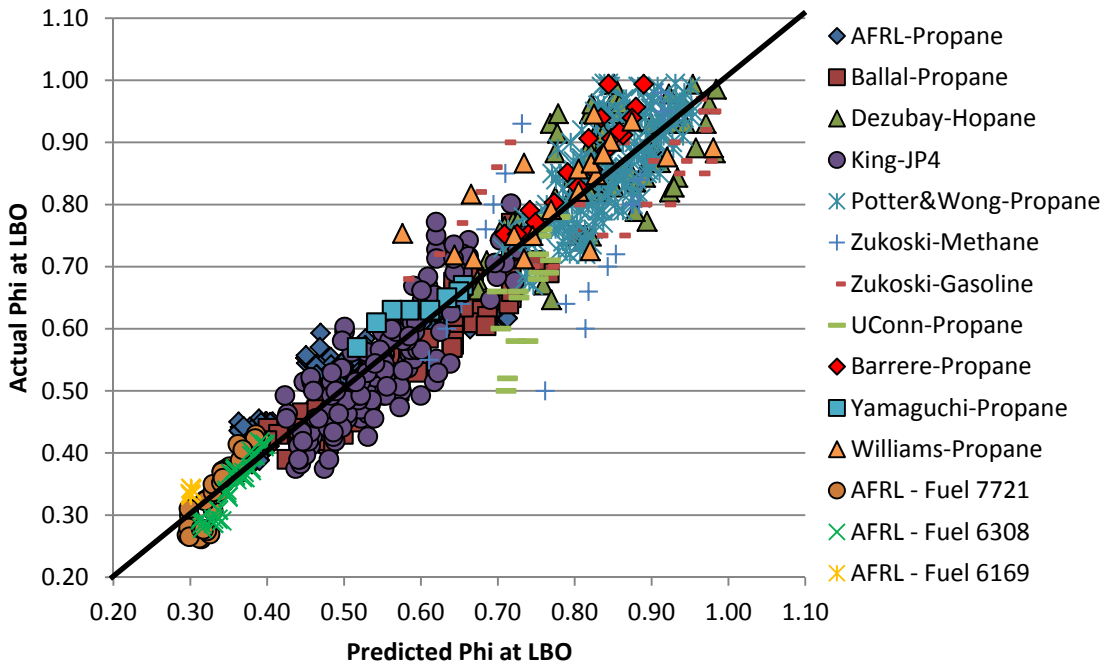

Figure 19. Correlation results with vitiated data and O_2 and fuel characteristics as parameters, R^2=0.91.

CHAPTER 5

CORRELATION WITH LAMINAR FLAME SPEED

Dataset and Cantera Calculations

Cantera was used to calculate the laminar flame speeds for 200 points taken on propane and methane over a range of pressures, temperatures, velocities, Reynolds numbers, and flameholder geometries. This data was then processed with the Matlab optimization toolbox to investigate the significance of laminar flame speed to blowout. Adjusted R-squared values were also calculated.

Cambridge/Radhakrishnan Parameter

As discussed in the Introduction, Kariuki et al. of Cambridge proposed the use of the parameter in Equation 18 to predict when lean blowout will occur. This parameter is derived from a rearrangement of the turbulent premixed flame extinction theory originally proposed by Radhakrishnan et al. In Equation 18, U_b is the bulk velocity, d is the flameholder diameter, S_L is the laminar flame speed, and ν is the kinematic viscosity of the reactants.

$$\left[\left(\frac{U_b}{d}\right)\left(\frac{\nu}{S_L^{\,2}}\right)\right]^{1/2} \tag{18}$$

Kariuki plotted this value against the flame power and found that the values for premixed flames were near unity. The dataset for which laminar flame speed was calculated in the current work was used to attempt to verify the previous researchers' results. Figure 20 shows the Cambridge/Radhakrishnan parameter plotted against the equivalence ratio at lean blowout. While the propane data do indeed produce a result near unity, especially past an equivalence ratio of 0.7, the methane data resulted in a parameter value of up to 10.

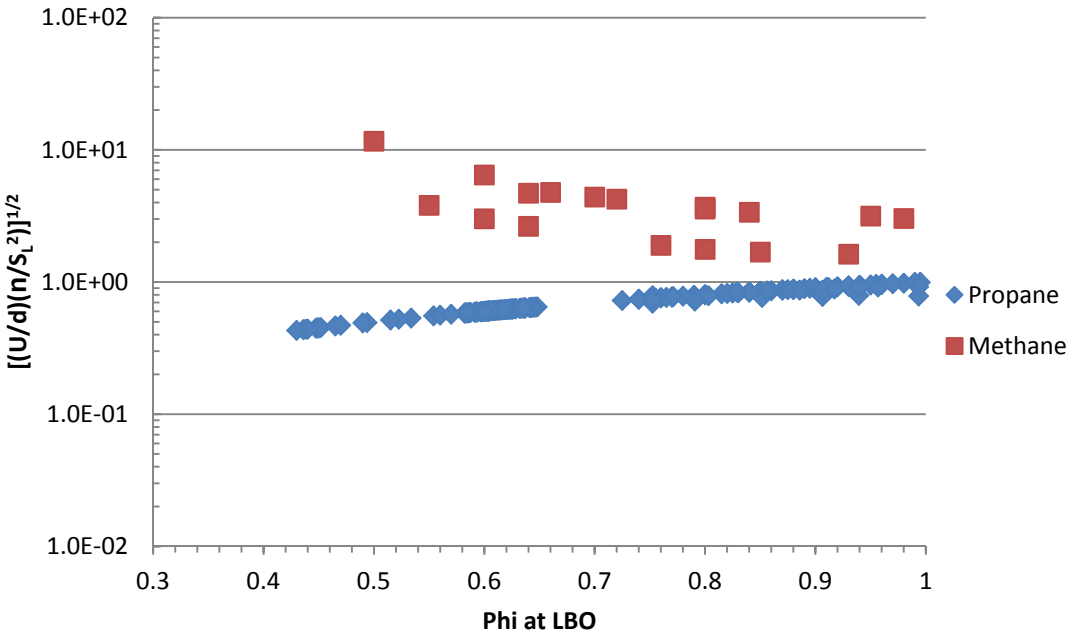

Figure 20. Cambridge/Radhakrishnan Parameter

Correlation Results with Laminar Flame Speed

Because the dataset was a smaller subset of the data, the correlation was first run using only the inlet conditions to establish a baseline comparison. The results are shown in Figure 21.

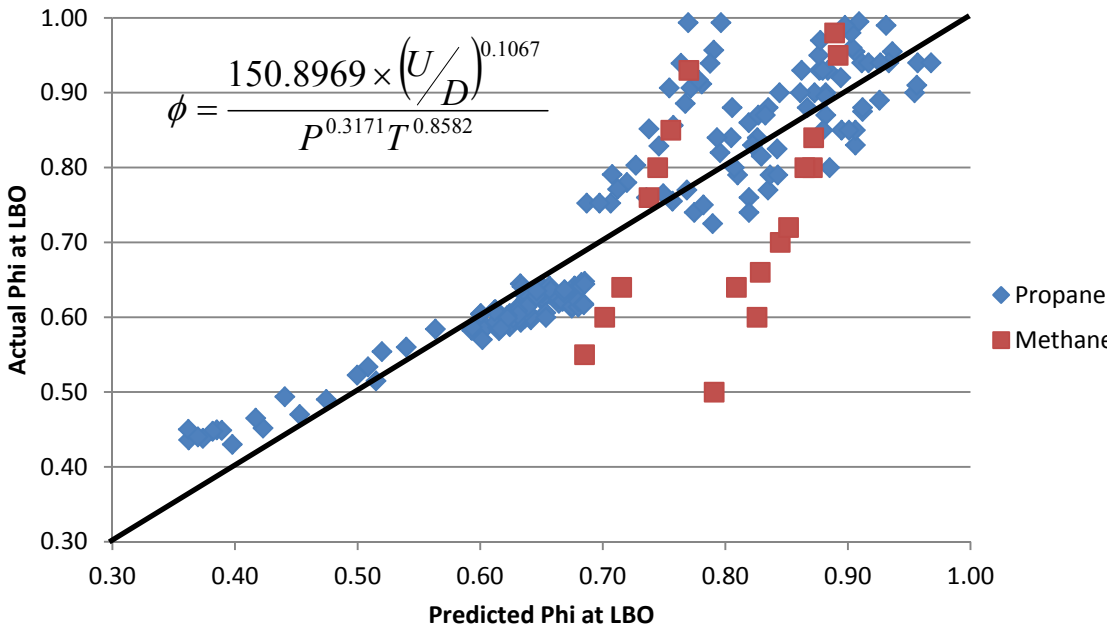

Figure 21. Correlation results with inlet conditions, R^2=0.80.

The methane data in Figure 21 clearly do not follow the same trend as the propane data. In addition, there appear to be two distinct curves within the methane data, each corresponding to a different U/D ratio.

Because laminar flame speed has been indicated by previous researchers, such as Radhakrishnan and Kariuki, as a critical parameter in blowout, it replaced the pressure and temperature in the correlation as the chemical "timescale", resulting in the plot in Figure 22.

Including laminar flame speed improved the R-squared value from 0.8 to 0.85. In addition, the methane data collapses very near the black perfect fit line, unlike the distinct methane lines in Figure 21. A cluster of data in Figure 22 in the lower actual equivalence ratio range falls to the right of the perfect fit line. Upon closer examination of the data, these points were all collected at elevated temperatures. Temperature was therefore added back into the correlation, as shown in Figure 23.

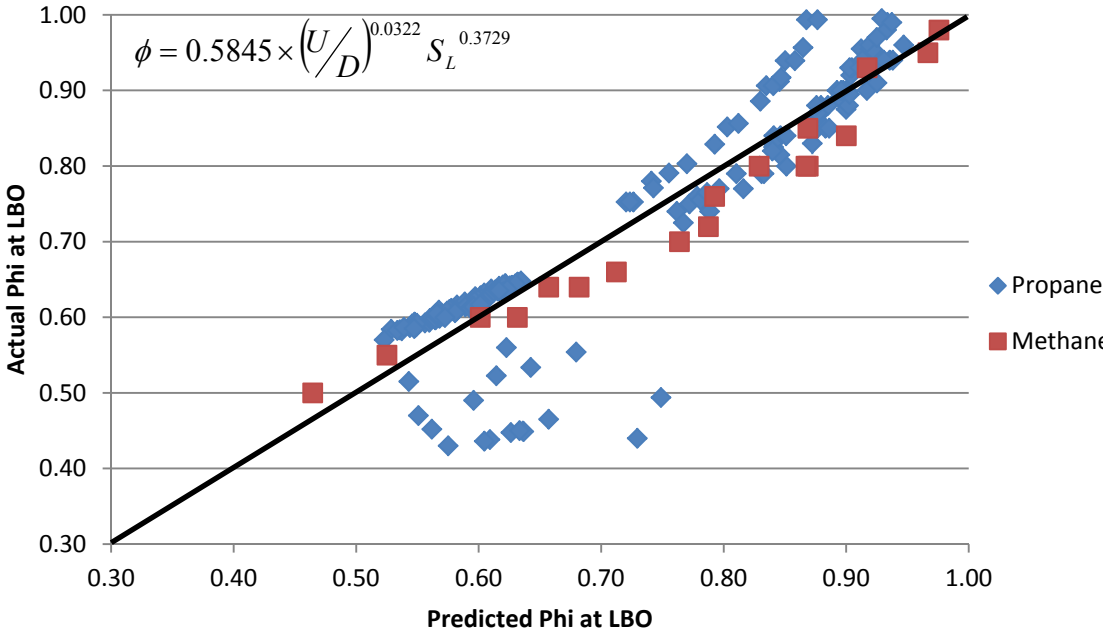

Figure 22. Correlation results with U/D and laminar flame speed, R^2=0.85.

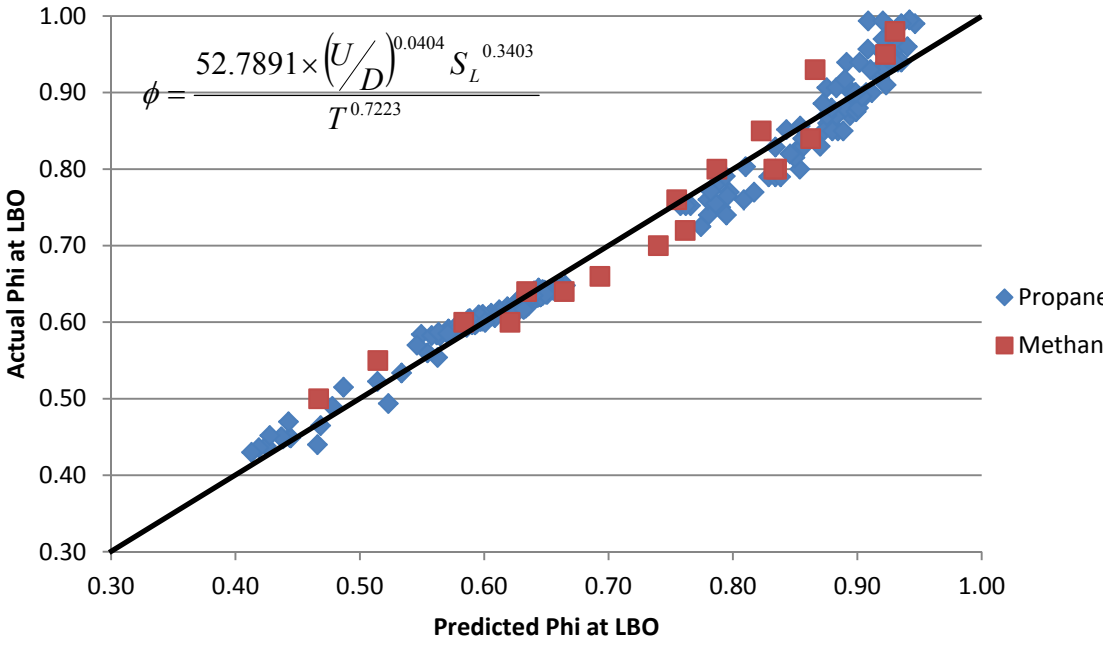

Figure 23. Correlation results with U/D, S_L and temperature, R^2=0.98.

The correlation with U/D, flame speed, and temperature resulted in a very strong prediction capability, with an R-squared value of 0.98. However, the equation lacks a robust physical explanation. The overall equation is not dimensionless, nor is flame speed really a timescale. The theories of Radhakrishnan provide a good possible physical explanation of the blowout phenomenon, and because viscosity varies with temperature, it seems logical that the parameters used by Radhakrishnan may capture the effects seen in the current dataset. Because the Radhakrishnan parameter is designed to return a value very near unity, it is not possible to correlate the lean blowout directly to the parameter as it is grouped together. There is not enough variability for the least squares curve fit algorithm to converge on a good fit. However, when the two groups *U/D* and n/S_L are used, the algorithm can find a good solution, as shown in Figure 24.

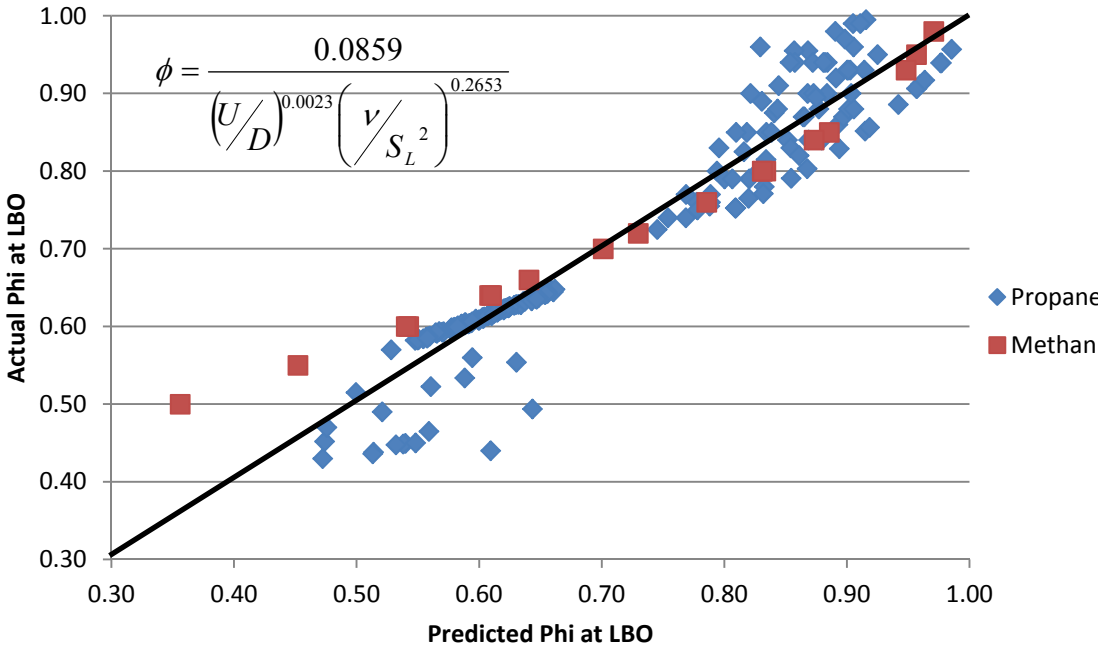

Figure 24. Correlation results with separated parameter, R^2=0.92.

Using the two timescale groups instead of individual parameters decreased the R-squared value to 0.92. The *U/D* parameter is now in the denominator of the equation, although with a very small exponent. The temperature effect to the right of the perfect fit line returns, indicating that the viscosity in the parameters used cannot fully capture the effect of temperature. Some of the lower-equivalence ratio methane data begin to fall off the line as well, perhaps as the curve fit attempts to correct for the temperature effect. These changes indicate that the temperature in the correlation is capturing an important effect that is not being conveyed with the two timescales, and should therefore be left in the equation.

Figure 25 shows that including temperature raises the R-squared value to 0.94 and brings the high temperature data back near the perfect fit line. The *U/D* parameter returns to the numerator, and the exponent on the temperature is relatively large, indicating a strong influence on the correlation.

When the parameters are further separated, as in Figure 26, the R-squared value returns to 0.98. Flame speed and temperature retain their significance in the equation, while both viscosity and *U/D* have very small exponents, implying that their influence on the lean blowout is trivial. Possible explanations for this finding are detailed in Chapter 7.

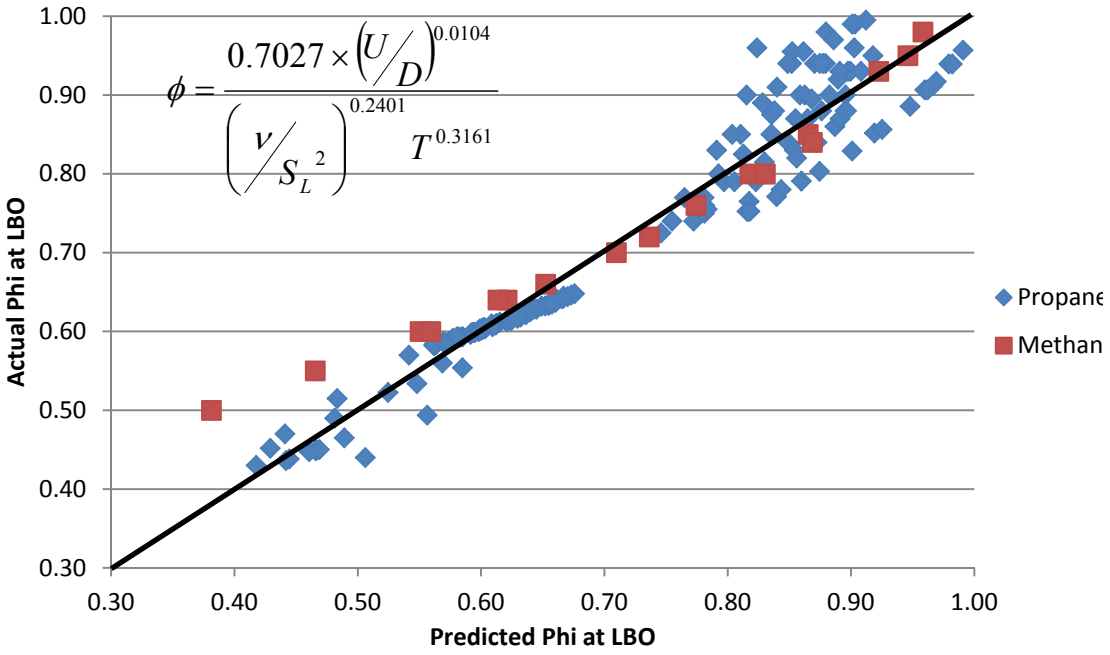

Figure 25. Correlation results with separated parameter and temperature, R^2=0.94.

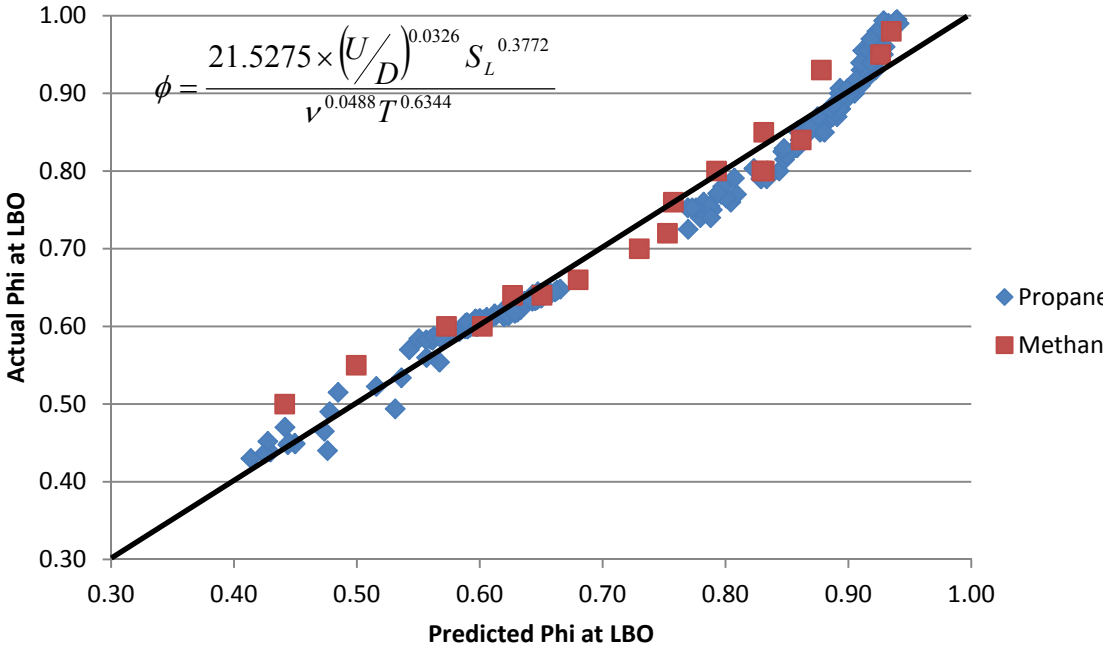

Figure 26. Correlation results with separated parameters and temperature, R^2=0.98.

CHAPTER 6

CORRELATION WITH IGNITION DELAY TIME

Dataset and Cantera Calculations

The propane dataset used for the laminar flame speed calculations could not be used to study the effect of ignition delay time due to the extremely long ignition delay times of propane at atmospheric pressure and relatively low temperature (below 600K). Instead, the ignition delay dataset was comprised of data taken on a petroleum-derived JP-8 and a tallow-derived HRJ fuel. The chemical mechanism used models each fuel using varying ratios of n-dodecane, n-decane, iso-octane, and propyl-benzene. Cantera calculated the ignition delay time for each of the 40 points in the dataset based on its inlet conditions. Because each of these points was taken on vitiated air, the oxidizer composition was calculated using a Matlab function relying on combustion chemistry and thermodynamic principles of equilibrium to calculate the chemical make-up of the inlet gases after vitiation. The Matlab least squares curve fit function was then used to find the desired correlation.

Correlation Results with Ignition Delay Time

The correlation was first run using only the inlet conditions to establish a baseline comparison. The data correlate quite well with only the inlet conditions, likely due to there

being less variation in the dataset than there would be with more data points. The pressure only varied by around 1 psia, and the temperature ranges from 1350 to 1640 R. In addition, all points were taken at AFRL's High Pressure Combustion Research Facility, eliminating any variability due to facility-related inconsistencies. The correlation is shown in Figure 27. The R-squared value is 0.94.

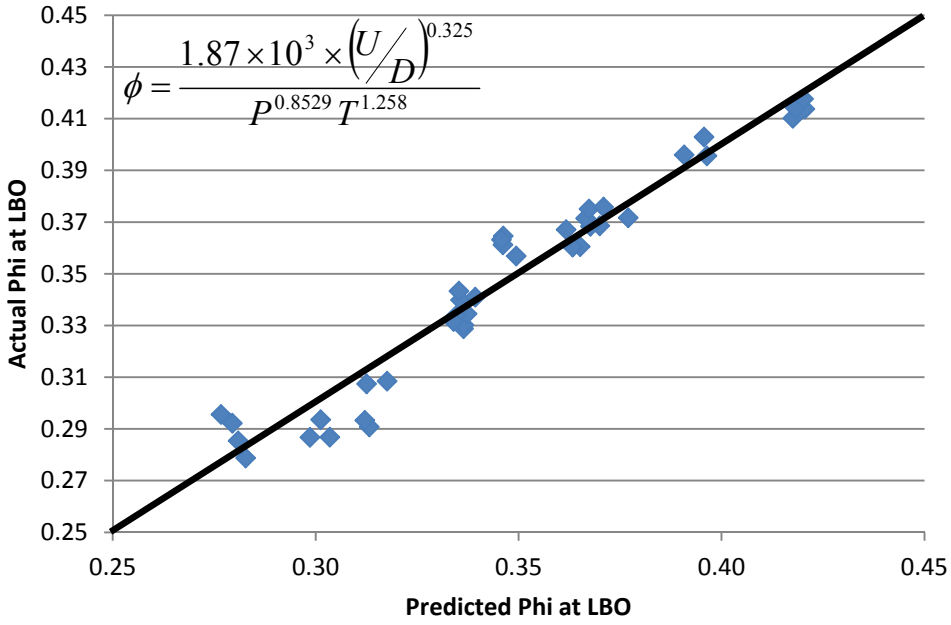

Figure 27. Correlation results with U/D, P, T, R^2=0.94.

As shown in Figure 28, the ignition delay time (IDT) was added to the correlation to investigate whether doing so would improve the correlation. The adjusted R-squared value decreased slightly, to 0.93. In addition, the exponent on ignition delay time is small, at 0.01, indicating that it is not a parameter of significance.

The exponents on pressure and temperature remain near those from the correlation in Figure 27, suggesting that these parameters carry the important chemical timescale effects

more than the ignition delay time. Further, when the ignition delay time replaces the pressure and temperature in the correlation, as shown in Figure 29, the R-squared value decreases to 0.91.

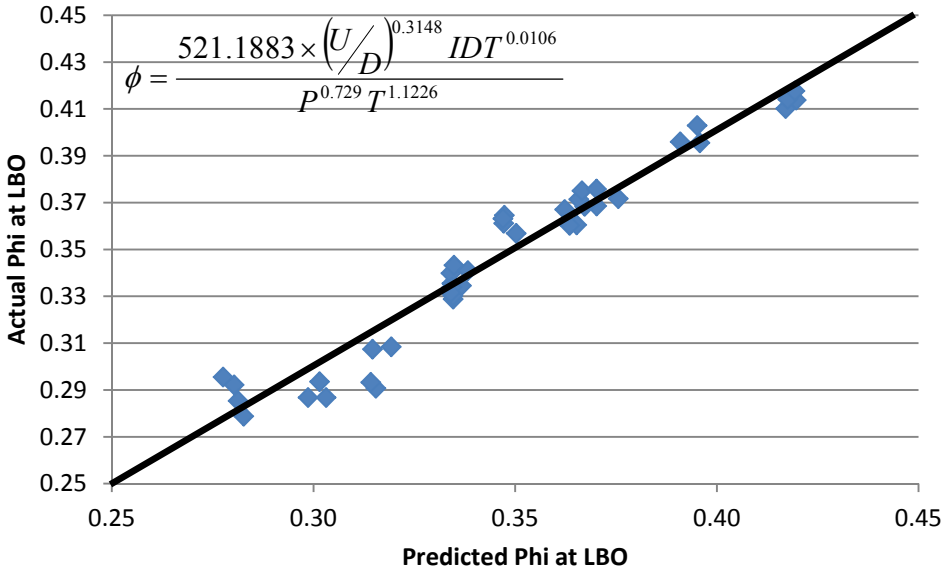

Figure 28. Correlation results with U/D, P, T, IDT R^2=0.93.

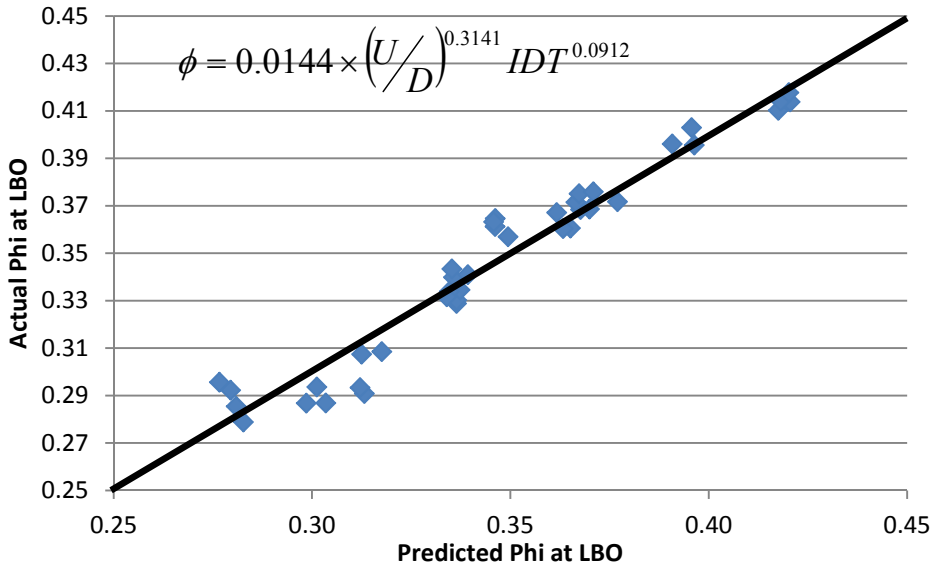

Figure 29. Correlation results with U/D, IDT, R^2=0.91.

While the prediction of blowout is still quite good, simply using the inlet pressure and temperature would result in a more accurate correlation, implying that while the ignition delay time is an adequate indicator of overall reactivity, it may not be the best parameter for capturing the chemical timescale critical for lean blowout.

CHAPTER 7

DISCUSSION

As stated earlier, this work serves two purposes; the first is to develop an accurate and practical correlation that predicts the lean blowout of bluff body stabilized flames. The second is to use the correlation results to develop a better physical understanding of the processes that govern blowout. While the correlation development was the focus of the previous chapters, a better understanding of why each parameter is in the correlation and its possible effects on the blowout process will be the focus of this chapter.

The "best fit" correlation equation using the inlet conditions and fuel properties is reproduced in Equation 19.

$$\phi = \frac{1.1\times10^{-6}\times\left(U/D\right)^{0.1642} MW^{0.7082}\left(H/C\right)^{1.1921} {O_2}^{4.4605}}{P^{0.2282}T^{0.7546}} \tag{19}$$

The exponent on the oxygen level, which is an inverse measure of the vitiation level, is unexpected. Past researchers have found that vitiation results in higher equivalence ratios at lean blowout due to decreased reactivity from reduced oxygen levels (Smith 2007). However, the correlation predicts lower equivalence ratios at lean blowout with increased vitiation. A closer examination of the data reveals that most of the vitiated data points were taken at high

temperatures and exhibited the lowest equivalence ratios at lean blowout of any of the data, resulting in a biased correlation. The algorithm only sees that the points taken at lower oxygen levels blow out at lower equivalence ratios. Therefore, no conclusions about the effect of vitiation on blowout can be drawn from this set of data, and the vitiated data were disregarded. The best correlation then reverts to the correlation with fuel effects and inlet conditions accounted for, reproduced below in Figure 30 with additional points for model validation, shown in yellow and discussed in the next section of this chapter. The correlation equation is shown in Equation 20.

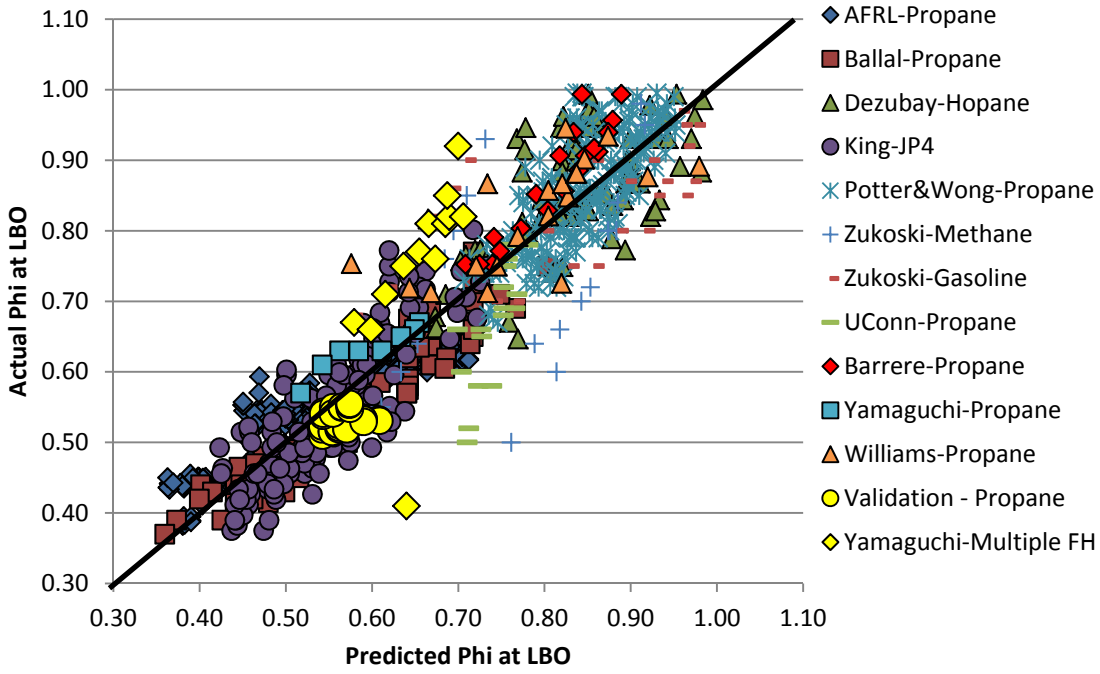

Figure 30. Correlation results with O_2 and fuel characteristics as parameters, R^2=0.89.

$$\phi = \frac{0.8598 \times \left(U/D\right)^{0.164} MW^{0.7093} \left(H/C\right)^{1.1964}}{P^{0.2281} T^{0.7537}} \qquad (20)$$

Correlation Validation

In order to assess the accuracy of the correlation, Equation 20 was used to predict the blowout of bluff body flames at an additional 44 conditions. The blowout points were selected from propane experiments run in the atmospheric pressure combustion lab at AFRL, as well from propane experiments done by Yamaguchi et al. Figure 30 shows a plot of the predicted points, shown in yellow, as well as the points used in the correlation.

The average error of the prediction within the validation dataset was 10.42%. The AFRL propane points lie very near the perfect fit line, and have an average error of 6.41%.

The Yamaguchi data also lies relatively near the perfect fit line, with the exception of an obvious outlier at an actual blowout of 0.4. This point was also something of an outlier in Yamaguchi's original data, and so may merit some disregard. Of particular interest concerning the Yamaguchi data is that flameholder configurations using multiple bluff-bodies were used. The blockage ratio of the experiment was kept constant by changing the flameholder diameter when the number of flameholders was changed (Yamaguchi 1985). When calculating the predicted equivalence ratio at lean blowout, only the actual diameter of the individual flameholders was taken into account. The correlation predicted the lean blowout at each point with an average error of 19.03%. If the outlier is excluded, the average error falls to 16.18%.

The average error in the predicted equivalence ratio for all points, including those used to form the correlation equations, was 6.59%. Excluding the outlier from Yamaguchi, the maximum error was 52.30%, which was the error on a point taken on methane. Methane points were generally associated with higher errors, with an average error of 16.06%.

Significance of the Correlation Parameters

Several of the parameters in the correlation shown in Equation 20 are logical extensions of the Damköhler number theories presented in previous literature. *U/D* appears to be the inverse fluid mechanic timescale, where *U* is the lip velocity and *D* is the flameholder diameter. This finding supports the conclusions of many researchers in the past, like Zukoski and Marble, Plee and Mellor, and Husain, and implies that the mixing time in the shear layer between the hot products in the recirculation zone and the fresh reactants flowing past the flameholder is an important timescale. As the fresh reactants flow past the recirculation zone, they mix in the shear layer with hot combustion products. If the reactants do not mix and react sufficiently in the amount of time that they spend in the shear layer, the flame cannot propagate. Because the dimensions of the recirculation zone generally scale with the width of the flameholder, the width of the flameholder can be substituted for the recirculation zone length, though it introduces some variability to the correlation.

Pressure and temperature both contribute to the chemical timescale in the Damköhler number. In the correlation equation shown in Equation 20, the equivalence ratio at lean blowout decreases as pressure and temperature increase. In general, as the pressure and temperature of a combustible mixture increase, the reactivity of that mixture increases. If the reactivity of the mixture in a bluff body flame increases, the chemical timescale should decrease, resulting in a flame that should be able to propagate in more adverse flow conditions.

The fuel characteristics of molecular weight and hydrogen to carbon ratio are also included in the correlation equation shown in Equation 20. As each of these fuel parameters increases, the correlation predicts that the equivalence ratio at lean blowout will also increase.

In the case of molecular weight, this response can be explained by the effect of molecular weight on diffusion.

As the molecular weight of a gas increases, the mass diffusivity of the gas decreases (Incropera 2007). The mass diffusivity of the gaseous fuel is important as it relates to the Lewis number of the fuel. The Lewis number is the ratio of the thermal diffusivity to the mass diffusivity of one substance into another. In reacting mixtures, the diffusivities are often based on the limiting or deficient reactant; in the case of lean flames, the diffusivities would be based on the fuel concentration. As the mass diffusivity of the fuel decreases, the Lewis number will increase, indicating that more thermal energy is being lost in the reaction compared to the chemical energy being gained through the fuel addition. Inversely, if more chemical energy is provided through higher mass diffusivities than thermal energy is lost, local enthalpy, burning rate, and propagation speed increase (Lipatnikov 2005). Work done by Kido et al. (1989) found that fuels with lower Lewis numbers exhibited higher turbulent burning velocities, even as the turbulence intensity increased, as shown in Figure 31. Also of note in Figure 31 is the trend of increasing Lewis number as the molecular weight increases.

The higher equivalence ratios predicted by Equation 20 with high molecular weight are indicative of a slower propagation rate in the blowout process. With high molecular weight, the mass diffusivity of the fuel will decrease, increasing the Lewis number. At higher Lewis numbers, flame speeds will decrease in the turbulent shear layer, increasing the timescale required for the flame to propagate successfully and reducing the flame stability.

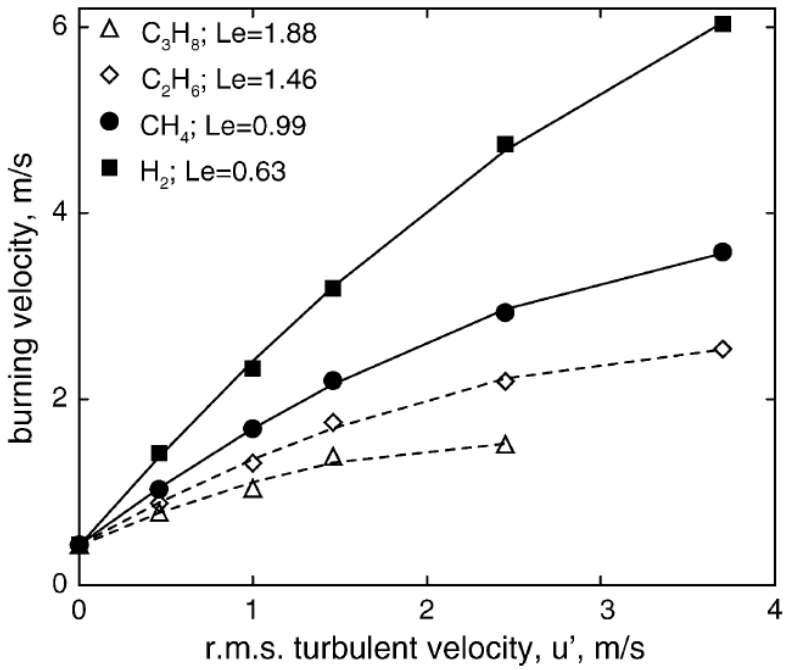

Figure 31. Burning velocities measured by Kido et al. for fuel/oxygen/nitrogen/helium mixtures where S_L=0.43 m/s

The equivalence ratio at lean blowout also increases with increasing hydrogen to carbon ratio. This effect can be explained by the bond energies and stabilities within the fuel molecules. For straight-chain aliphatic compounds, the hydrogen to carbon ratio decreases as the chain lengthens. In addition, longer chains will have more secondary C—H bonds, which are bonds where the carbon atom is bonded to two additional carbon atoms and two hydrogen atoms. These bonds are generally weaker than primary C—H bonds, where the carbon atom is bonded with one carbon atom and three hydrogen atoms. These bond types are illustrated in Figure 32, below. In straight-chain alkane combustion, the C—H bond is critical, because the fuel is often first broken down through an H-abstraction reaction, where a hydrogen atom is stripped off of the molecule (Law 2006).

As the hydrogen to carbon ratio increases, the number of weaker secondary bonds is decreased, causing the reactivity of the fuel to decrease. With lower reactivity, the flame is less stable, resulting in higher equivalence ratios at lean blowout, as predicted in Equation 20.

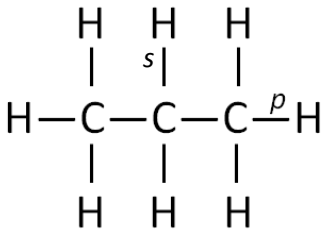

Figure 32. Secondary and primary C—H bonds; secondary bonds are denoted with an s, primary with a p

While bond strength explains why the hydrogen to carbon ratio affects the blowout in straight-chain alkanes, the bond stability may be another factor in the multi-component fuels, as well as in alkenes. Alkanes are generally more stable than alkenes, because the carbons prefer the single-bond structure to the double-bond structure, and so the double bond is susceptible to attack from both O and OH radicals. H-abstraction reactions are not necessary for the molecule to be oxidized (Law 2006). While jet fuels have generally low levels of alkenes, high alkene levels would increase the reactivity of the fuel. Alkenes have generally lower hydrogen to carbon ratios for a given number of carbons. If relatively large numbers of alkenes were present in a fuel, it could drive up the reactivity while decreasing the hydrogen to carbon ratio, which would increase the stability of the flame. This increased stability would be reflected in a lower equivalence ratio at lean blowout, which is predicted by the correlation shown in Equation 20.

Correlation with Laminar Flame Speed

The correlation with the highest R-squared value with the laminar flame speed is shown in Equation 21.

$$\phi = \frac{21.5275 \times \left(U/D\right)^{0.0326} S_L^{\ 0.3772}}{\nu^{0.0488} T^{0.6344}} \tag{21}$$

Equation 21 states that as the laminar flame speed increases, the equivalence ratio at lean blowout should also increase. This relationship contradicts the idea that as the chemical timescales needed for stable combustion decrease, the flame should become less prone to lean blowout. In addition, this correlation assigns a very small significance to the *U/D* parameter that represents the fluid mechanical timescale, indicating that it is not an important parameter for lean blowout. Outside of disregarding nearly every theory regarding the mechanisms that govern lean blowout, the logical conclusion is that the correlation is not actually predicting lean blowout. Instead, the correlation is essentially creating a laminar flame speed curve. Laminar flame speed increases with equivalence ratio when the flame is lean, as demonstrated previously in Figure 9. The correlation algorithm recognized this, and simply correlated the flame speed to equivalence ratio. If more data were available where the flame speeds differed substantially at the same equivalence ratio, the equivalence ratio/flame speed link may be broken, and the correlation could be run to predict lean blowout. Because that data is not currently available, the correlation shown in Equation 21 must be disregarded for lean blowout prediction.

Correlation with Ignition Delay Time

Equation 22 shows the correlation with ignition delay time and the inlet conditions, which resulted in an R-squared value of 0.93. The exponent on ignition delay time is very small, and the inclusion of the ignition delay time in the correlation did not improve the R-squared value.

$$\phi = \frac{521.1883 \times \left(U/D\right)^{0.3148} IDT^{0.0106}}{P^{0.729} T^{1.1226}} \tag{22}$$

While the ignition delay time did appear to capture the general trend of the chemical timescale when it replaced the pressure and temperature in the correlation, using the inlet conditions themselves resulted in a better R-squared value.

The dataset used for the ignition delay time correlation was relatively small. All points were taken in the High Pressure Combustion Research Facility at AFRL within a fairly small range of inlet conditions and fuel properties. Because the data lacks a lot of variation, the correlation does a very good job of predicting blowout without specifically identifying a chemical timescale, and it is difficult to discern whether including ignition delay time would have a more significant impact in a larger dataset. However, for the dataset used in this work, the ignition delay time did not appear to improve the correlation, indicating that it may not be the most representative chemical timescale for lean blowout.

CHAPTER 8

CONCLUSIONS AND FUTURE RESEARCH

The correlations presented in this thesis indicate that the lean blowout of bluff body stabilized flames is dependent on both the Damköhler number and the Lewis number. The best correlation is reproduced in Equation 23.

$$\phi = \frac{0.8598 \times \left(U/D\right)^{0.164} MW^{0.7093} \left(H/C\right)^{1.1964}}{P^{0.2281} T^{0.7537}} \tag{23}$$

U/D is the inverse of the fluid mechanic timescale, likely that of the mixing time in the shear layer between the recirculation zone and the fresh reactants. Pressure, temperature, and the hydrogen to carbon ratio of the fuel all directly affect the reactivity of the mixture, contributing to the chemical timescale in the Damköhler number. The molecular weight of the fuel influences the mass diffusion, and thereby the Lewis number, of the fuel. As the Lewis number increases, various reaction rates, including the turbulent flame speed, decrease, also affecting the chemical timescale in the Damköhler number.

The exact chemical timescale could not be determined from the laminar flame speed and ignition delay time data. From the review of past literature, the timescale from

Radhakrishnan (1981) appears to be rooted in a plausible physical model, where in order for the flame to be stable, it must be able to propagate within the turbulent shear layer. The fact that Lewis number influences the lean blowout seems to support this theory, as the Lewis number affects the turbulent flame speed.

A major contribution of this work is establishing the role that fuel characteristics play in the lean blowout process. Very little work has been done in the literature on fuel effects in the lean blowout of bluff body stabilized flames, and from Equation 23, it is quite apparent that both the molecular weight and hydrogen to carbon ratio of the fuel influence the process.

While this study provides a practical, accurate correlation for predicting lean blowout in bluff body flames, the correlation has several limitations. It cannot account for vitiation effects, and it is less accurate for methane flames. It is only valid within the parameter ranges specified in Table 1, with the exceptions that the smallest flameholder in the final dataset was 0.025 inches in diameter and the correlation does not account for hydrogen combustion. The highest molecular weight was that of JP-4, at 119 g/mol, so heavier hydrocarbons may not correlate well.

Future Work

Possible future work includes incorporating vitiation effects into the equation and investigating the plausibility of creating a correlation with the laminar or turbulent flame speed. In order to incorporate vitiation effects, more data will need to be collected over a greater range of equivalence ratios and vitiation levels. Using such a dataset should prevent the bias seen with the currently available data.

In order to create a correlation that includes laminar flame speed but does not simply correlate the dependence of flame speed on equivalence ratio, flame speeds must be included with greater variations at a given equivalence ratio. In order to vary flame speed in such a manner, more data taken on different fuels must be included in the correlation. Because the turbulent flame speed may be a more accurate representation of the flame propagation in the shear layer, it should also be calculated. In order to do so, the turbulence intensity in the shear layer must be measured, which may be possible using PIV techniques.

The fluid mechanic timescale could also be further refined by measuring the recirculation zone length and using it as the length scale in the correlation instead of the flameholder diameter.

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