The effect of elevated water content on ethanol combustion

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THE EFFECT OF ELEVATED WATER CONTENT ON ETHANOL COMBUSTION

A Thesis

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Master of Science in Mechanical Engineering

In

The Department of Mechanical Engineering

By
Baine Breaux
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TABLE OF CONTENTS

ACKNOWLEDGEMENTS........................................................................................................ii

ABSTRACT............................................................................................................................v

INTRODUCTION....................................................................................................................1
Motivation for Research........................................................................................................1
Ethanol as a Potential Solution.............................................................................................3
Present Study.......................................................................................................................4

LITERATURE REVIEW.........................................................................................................5
Combustion Classification....................................................................................................5
Combustion Characteristics.................................................................................................7
Industrial Combustion Devices and Flame Stabilization Schemes.......................................13
Investigative Combustion Devices.....................................................................................19
Hydrous Ethanol as a Potential Fuel...................................................................................19
Theoretical Considerations and Predictions for Hydrous Ethanol.......................................25

TEST APPARATUS.................................................................................................................37
Combustor Design................................................................................................................37
Fuel Injection System..........................................................................................................42
Air Supply System...............................................................................................................44
Ignition System.....................................................................................................................51
Thermocouple Probe..........................................................................................................55
Exhaust NOx Analyzer..........................................................................................................56
High Speed Camera.............................................................................................................56
Photodiode...........................................................................................................................58
Gas Chromatograph.............................................................................................................59
Hot-Wire Anemometer.........................................................................................................62
Data Acquisition System......................................................................................................63

TESTING AND MEASUREMENT PROCEDURES................................................................68
Test Conditions.....................................................................................................................68
Fuel Mixing..........................................................................................................................69
Combustor Operation and Data Collection Procedures.....................................................69
Reaching Steady State and Ensuring Repeatability..............................................................70

RESULTS AND DISCUSSION.............................................................................................73
Pre-Study: Hot-Wire Anemometry and Ignition Study.........................................................73
Hot-Wire Anemometry.........................................................................................................73
Ignition Study.......................................................................................................................76
Sub-Study 1: Flame Structure, Lean Blow Out Limit, Flame Temperature, Exhaust
Temperature, and Exhaust NOx..........................................................................................78
Flame Structure...................................................................................................................78
Lean Blow Out Limit............................................................................................................80
<table>
<thead>
<tr>
<th>Sub-Study 1: Combustion Efficiency and Emission Reduction</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flame Temperature</td>
<td>82</td>
</tr>
<tr>
<td>Exhaust Temperature</td>
<td>86</td>
</tr>
<tr>
<td>Exhaust NOx</td>
<td>87</td>
</tr>
</tbody>
</table>

**Sub-Study 2: Flame Imaging, Spatial Distribution of Heat Release, Time Dependence of Heat Release**

- Time-Averaged CH* Images: 90
- Time-Averaged OH* Images: 93
- Spatially-Averaged Time-Averaged CH* Intensity: 94
- Spatial Distribution of Time-Averaged CH* and OH*: 95
- Time-Dependent Chemiluminescence Data: 97
- Photodiode Data: 99

**Sub-Study 3: Gas Composition Analysis**

- Data Collection Method: 100
- Exhaust Oxygen Concentration: 100
- Exhaust Carbon Dioxide Concentration: 102
- Exhaust Methane and Carbon Monoxide Concentration: 103

**Sub-Study 4: Flame Tip Temperature and CH* Intensity**

- Flame Tip Temperature: 104
- Flame Tip CH* Intensity: 108
- System Performance and Life-Cycle Savings: 108

**SUMMARY AND CONCLUSIONS**

- General Conclusions: 111
- Future Work Recommendations: 112

**REFERENCES**

- 113

**VITA**

- 116
Ethanol is currently being considered as a potential alternative to traditional fuels. However, the fuel offers a low return in terms of energy output per dollar invested when compared to fossil fuels. More than 1/3 of the cost associated with bio-ethanol production is devoted to distillation and water removal. This study seeks to validate the use of hydrous ethanol as a practical fuel to be used in lieu of fossil fuels or anhydrous ethanol. Success would reduce the production cost associated with ethanol fuel. Hydrous ethanol was burned in a swirl-stabilized combustor, air is introduced at a constant flow rate through a dump diffuser, and fuels ranging from 0%-40% water by volume was tested for practicality. A stable flame was achieved with up to 35% water and the Lean Blow Out limit was determined for these fuels. Fuels ranging from 0% to 20% water were tested in greater detail. This included thermal mapping of the flame, exhaust temperature measurements, exhaust NO\textsubscript{x}, CO\textsubscript{2}, and O\textsubscript{2} measurement, as well as CH* and OH* imaging of the low-flame region. Equivalence ratio was varied to include test points at 0.6, 0.8, 1.0 and 1.1. This range provides insight into flame behavior at extremely lean, lean, stoichiometric, and rich test conditions. Results revealed that exhaust heat rate, combustion efficiency, and combustor thermal efficiency were not affected negatively by elevated water content. However, flame temperature decreased as a result of water addition, particularly in the low flame region. CH*/OH* emissions in the low-flame region were also reduced due to the parasitic heat load of water vaporization and local quenching. The practical consequence of burning hydrous fuel was reduced exhaust temperature. This negative consequence, coupled with the desirable consequence of increased mass flow rate, did not appreciably affect the net exhaust heat rate. Reduced peak temperatures lead to exhaust NO\textsubscript{x} reductions. In conclusion, this study reveals that ethanol with proof as low as 140 behaves as a practical fuel and is recommended as a means of increasing the economic return when using ethanol as fuel in situations where increased volumetric consumption of the fuel is acceptable.
INTRODUCTION

Motivation for Research

Global use of fossil fuels has been steadily growing since the resource was discovered as a source of energy. The use of these fuels is spreading internationally as the standard of living increases in across the world. As a larger population steps into the ‘first world’ they demand dependable and regular access to electricity and transportation resources. Global electricity generation is very heavily dependent upon coal, natural gas, and fuel oil combustion processes. The fossil fuel consumption for transportation is almost entirely dependent upon conventional liquid fossil fuels. Figure 1 shows the increase in oil consumption over the past 45 years. The data for this plot was taken from the BP Statistical Review of World Energy [BP, 2011].

![Global Oil Consumption and Production](chart.png)

**Figure 1: Global Oil Consumption and Production over the Last 50 Years [BP, 2011]**

From this plot it can be observed that global oil consumption has followed global oil production rather closely over the past 45 years. Another study suggests that world energy demand is expected to grow 1.8% annually over the next 30 years [Energy Information Administration, 2009]. However, it is known that there is only a finite amount of fossil fuel reserves available on the planet. Fossil fuels are actually organic matter (once living) that has been decomposing slowly for millions of years. Some fossil resources, such as coal, have been forming for over 300 million years [Fossil Energy Office of Communications, 2008]. If oil consumption continues to increase, or even remains constant, consumption will eventually exceed production and mankind will eventually consume all of this nonrenewable resource. The dates and rates of this ‘peak oil’ phenomenon are debated; but its existence is obvious if the trends remain unchanged. Similar phenomena will occur with the resources of natural gas and coal. Simple foresight requires that alternatives to traditional fuels be developed before conventional resources become scant.

The limited nature of the oil supply is motivation enough to look into alternative fuels, but additional motivations also exist. Fossil fuel use often has negative effects on the terrestrial environment and on atmospheric health. Incidents such as the BP Horizon Oil Spill and phenomena such as smog development in urban areas are known negative consequences caused by fossil fuel consumption. Emissions from hydrocarbon combustion include carbon monoxide (toxic), carbon
dioxide (global warming contributor), unburned hydrocarbons (toxic and smog forming), particulate matter (respiratory distress causing), oxides of nitrogen (smog forming, acid rain, ozone forming), and water vapor. If the fuel is a residual fuel, as is commonly burned in land-based turbines for power generation, fuel sulfur can result in sulfur oxide formation which also contributes to sulfuric acid present in the atmosphere and results in acid rain. Reduction of these harmful emissions is always a target for engine designers. Government regulations dictate maximum concentrations of NOx and SOx emissions and advocate the use of “Best Available Control Technology” to limit environmental effects of fossil fuel combustions [Environmental Protection Agency, 2006]. Power producers and engine designers in part meet these requirements through engine modifications, but emissions can also be improved by selecting a fuel that has burning properties that tend towards cleaner emissions. Natural Gas produces much less soot, particulate matter, and SOx than coal. Similarly, there may be alternative non-fossil fuels that are capable of improving combustion efficiency and effectiveness and reduce pollutant formation.

Furthermore, developed nations like the United States are heavily dependent upon oil consumption for both transportation and power generation. These nations may not necessarily have access to the oil reserves needed to support their economy and it becomes a matter of national security that these nations develop alternative fuel resources. Figure 2 shows the distribution of proven oil reserves in the world [BP, 2011]. Despite being a major consumer of oil (Figure 1) North America possesses only a very small portion of the proven reserves. This limited access to petroleum supply can result in political tensions and geographic interdependence.

Figure 2: Distribution of Proved Oil Reserves [BP, 2011]

The development of fossil fuel alternatives promotes local economic growth. The variety of potential alternatives is large. Each geographic region has unique set of alternative energy resources. While no particular alternative power supply will likely prove itself as the ‘holy grail’ replacement for fossil fuels, the effective use of all resources has the potential to provide a stable energy supply. Local resources may include wind, tidal, geothermal, biomass, and agricultural resources. Each of these resources exhibits diversity under its umbrella. For instance, biomass may include municipal waste, industrial sawdust or pulp waste, or agricultural waste such as bagasse (sugar cane waste). Every local economy will be able to provide a unique combination of alternative resources and effective utilization of these resources will result in local economic growth. Through this diversification in energy supply
the energy portfolio can become more robust and the shortcomings of any one particular resource can be effectively balanced by additional components of the portfolio.

Local and federal governments have recognized these motivations for investing in petroleum alternatives. Stringent emissions requirements, renewable energy requirements, and, in some cases, even carbon dioxide caps have been integrated into law, requiring the energy industry to develop additional resources in order to meet government regulations. In addition, the general public provides pressure to the energy industry, consumers are requesting ‘green’ alternatives and buyers distinguish between sustainable and non-sustainable business practices. The combination of these factors is driving investigations into alternative fuel development.

**Ethanol as a Potential Solution**

Having established the necessity for the development of alternative fuels we will turn our attention to a particular alternative fuel: Ethanol. Ethanol has been vying for a share of the fuels market as a renewable alternative to light distillates such as gasoline and some middle distillates such as kerosene. Ethanol works well with existing infrastructure and can be used in both internal combustion and turbine engines without significant modifications to the engine. Ethanol tends to burn cleaner than traditional fossil fuels because the oxygen contained in the fuel itself helps reduce soot formation. Ethanol is also appealing because it is a renewable fuel and can be derived from a wide range of feed stocks, including corn, sugar, or even cellulose. This allows producers to devise a local feedstock which not only boosts local economies but allows for a more regionally secure fuel source. These characteristics enable fuel consumption to be a part of holistic community development, and, while this may not have a measurable value, it leads to increased quality of life.

The potential of ethanol as a leading alternative fuel is evident when looking at the increases in ethanol production over the past 13 years. Figure 3 shows data collected by the BP Statistical Review of World Energy. This plot demonstrates the drastic increase in ethanol production over the past 13 years. It also shows that South and Central America have been producing a significant amount of ethanol for quite some time. This is largely representative of nations such as Brazil that have a transportation system that is based on ethanol. North America, however, can be seen to have the most drastic increase in ethanol production and is currently the global leader. With such a large potential for ethanol production here in the U.S. it is imperative that we use this resource in the most effective way.

![World Ethanol Production](image)

**Figure 3: World Ethanol Production Over the Last 13 Years [BP, 2011]**
Despite its many advantages ethanol does have some significant disadvantages. The most well-known among them is its low energy density. Pure ethanol contains 27 MJ/kg compared to 44 MJ/kg for gasoline. Ethanol is commonly associated with poor fuel economy because the heating value of ethanol is approximately 2/3 that of gasoline. Another drawback of pure ethanol use is that ethanol is hygroscopic. This means that dehydrated ethanol will pull water vapor from its environment and dilute itself. As a result long distance pipelines and extended storage times are detrimental to the performance of this fuel.

The cost per unit energy delivered of ethanol must be improved in order to make it competitive with conventional fuels. This problem can be addressed in two different ways. The first method is to increase the energy density of ethanol fuel for marginal cost increase. The other method is to reduce the cost of ethanol production until the low energy density of the fuel is offset by the low cost. This concept is portrayed graphically in Figure 4.

![Cost Per Energy Delivered](image)

- Increase the Energy Density of Ethanol without drastically increasing cost
- Drastically decrease the Cost of Ethanol while maintaining its practicality

Figure 4: Strategies for Making Ethanol Economically Competitive

Present Study

In this work we strive to reduce the cost of ethanol while maintaining its practicality. This will be done by using hydrous ethanol in lieu of pure ethanol. Hydrous ethanol is less expensive to produce than pure ethanol and may still offer itself as a practical fuel. Fuel volume consumption rates will increase in order to release the same amount of energy but dollar consumption rates will be reduced.

Fuels of various water content mixtures are considered and combustion properties and flame health was evaluated. This was performed by monitoring flame stability, heat release, and emissions. This study includes a detailed literature review of hydrous ethanol combustion research; detailed description of the test apparatus, diagnostic equipment and test procedure; presentation and discussion of test results; fundamental conclusions; and a description of suggested future work.
LITERATURE REVIEW

Combustion Classification

Combustion can be defined as the exothermic reaction of a fuel and an oxidant [Lefebvre et al, 2010]. The fuel can be solid, liquid, or gaseous in state. It can be a fossil or renewable fuel. In traditional engines the oxidizer is air, or in some advanced facilities higher content oxy-fuel is utilized. Combustion involves the interaction of fluid dynamic, thermodynamic, chemical kinetic, and heat transfer characteristics of the system. It is a complex process that is dependent upon a wide range of parameters [Gabriel, 1998]. Combustion can occur with or without luminescence. A flame can be defined as combustion event that is accompanied by luminescence, and consists of a very thin fluid layer which undergoes rapid chemical changes as well as steep temperature and chemical concentration gradients. A flame front is often considered as the interface between burned and unburned mixtures [Lefebvre et al, 2010].

Combustion reactions fall into the two categories of deflagration and detonation, characterized by subsonic and supersonic combustion waves, respectively [Hinde, 1972]. Deflagration, despite being subsonic, still occurs very rapidly requiring less than 1ms for 80% completion and can be viewed as a wave that moves rapidly through a combustible mixture. Detonation is characterized by a shock wave that moves through the combustible mixture at speeds between 1 and 4 km/s, supported by a chemical reaction zone [Lefebvre et al, 2010]. Although detonation combustion is valuable in a number of processes and can even be harnessed by some types of engines it is not typical in either gas turbines, internal combustion engines or in industrial burners. The remainder of this work will consider only deflagration flames because the existing power generation and transportation infrastructure is dependent upon the use of deflagration reactions.

In fundamental flame studies it is typical that a flame front be established in a stationary space while fuel and oxidizer are fed into the reaction zone. While utilizing this arrangement flames can be characterized as either premixed or diffusion flames. Premixed flames depend on the injection of a combustible mixture where fuel and oxidizer are well mixed before entering the reaction zone. This type of flame is commonly used in the combustion of gaseous fuels such as natural gas or hydrogen [Giglio, 2008; Zhu et al, 2011]. Premixing can also be utilized if a liquid fuel is vaporized before mixing. This is often performed with the aid of fuel preheat. Aside from premixed a flame can be characterized as a diffusion flame. In a diffusion flame fuel and oxidizer are definitely separated at the inlet and are mixed within the flame itself. A burning candle is an example of a diffusion flame. This work considers diffusion flames of liquid fuel only. The liquid fuel is atomized to enhance mixing, but diffusion between the oxidizer (air) and the liquid fuel droplets still governs the nature of the reaction.

Flames can be further categorized as laminar or turbulent flames. In laminar flames air and fuel flow is laminar, in turbulent flames the fluid flows in the turbulent region. The transition between laminar and turbulent flames is determined by flow characteristics such as Reynolds number and length scale of the flow. In turbulent flows the value of parameters such as velocity are determined by evaluating the mean of the flow. Turbulence intensity is then classified as the ratio of the root mean squared of the fluctuating component of velocity to the mean velocity [Turns, 2000]. Figure 5 demonstrates a typical fluctuation of a velocity within a turbulent flow field. Equation 2 demonstrates the definition of turbulence intensity within the flow. \( V \) denotes the velocity, \( N \) represents the number of samples and \( \overline{V_x} \) denotes the mean velocity at location \( x \).
All air flows and vaporized fuel flows within this work are strongly turbulent and behave in the turbulent regime. However, because the flames in this study are diffusion flames the rate of large-scale mixing is the rate controlling step in the combustion reaction. That is to say that the flow mixing time is significantly larger than the chemical reaction time, or that the Damkohler Number (ratio of diffusion time to chemical reaction time) is high. This is typical in spray atomization flames [Lefebvre et al, 2010].

Having established the fluid dynamic classifications of flames it is also possible to classify a flame chemically, or in terms of the ratio of fuel to oxidizer. Not all air-fuel ratios are combustible. There is a minimum percentage of fuel that must be present in a mixture in order for combustion to occur. This minimum percentage is called the lean limit of combustion or lower flammability limit. Similarly there is a rich or high limit at the upper tolerance of fuel concentration. The rich limit can be increased by increasing the pressure or temperature of the mixture. Lean limit is marginally decreased by increasing pressure and temperature. Changes in flammability limit are much more sensitive to pressure changes than temperature changes. For ethanol at atmospheric pressure the flammability limit ranges from 3.5% to 19% fuel content by volume. In this study all combustion reactions are observed at atmospheric pressure. Stated flammability limits are determined by the thermo-chemical properties of the mixture, however, in experimental conditions flammability may vary due to factors such as local mixture composition and heat transfer characteristics of the mixture/surroundings.

The branch of chemistry that studies the relationships between products and reactants in a chemical reaction is called stoichiometry. In pure hydrocarbon combustion the only atoms involved are
hydrogen, carbon, and oxygen. In reality there are other players such as nitrogen or sulfur that can affect combustion. However, simplified models can exclude these interactions. Products of a reaction can be determined if conservation of mass is applied to each chemical element across the reaction. A sample hydrocarbon-air combustion reaction going to complete combustion is shown in Equation 3. This model assumes uniform and complete mixing of fuel and oxidizer [Heywood, 1998].

\[
C_a H_b + \left( \frac{a}{4} + \frac{b}{2} \right) (O_2 + 3.773N_2) = aCO_2 + \frac{b}{2} H_2O + 3.773(a + \frac{b}{4})N_2 \quad \text{Equation 3}
\]

From this equation it can be seen that, by knowing the molecular structure of a given hydrocarbon then the amount of air required for complete oxidation and the exhaust gas composition can be determined. Notice that the products contain fully oxidized hydrogen and carbon. No CO or H\(_2\) is found in the products. There is also no excess oxidizer in the products. This case of complete fuel oxidation is known as a stoichiometric reaction. By considering the chemical element quantity and molecular mass the air to fuel ratio can be determined on per mass or per mol basis. If excess oxygen is present the mixture would be considered fuel-lean. Excess fuel would result in a fuel-rich mixture. As the mixture is enriched with fuel the fuel-to-air ratio would increase. Fuel to air ratio is often normalized by the stoichiometric fuel to air ratio to determine the equivalence ratio, defined in Equation 4.

\[
\text{Equivalence Ratio} = \Phi = \frac{\text{Fuel}}{\text{Air}} \text{Actual} \div \frac{\text{Fuel}}{\text{Air}} \text{Stoichi}
\]

From this equation it should be evident that \( \Phi > 1 \) would denote a rich mixture while \( \Phi < 1 \) would be a fuel lean mixture. Reconsidering Equation 3 with the definition of equivalence ratio in mind it is observed that at \( \Phi = 1 \) Equation 3 is exactly as presented above. Increasing \( \Phi \) above unity would cause excess oxygen to appear in the reactants. Decreasing \( \Phi \) below unity would starve the combustion reaction of oxygen and stop the oxidation process short. As a result H\(_2\)O and CO\(_2\) concentrations in the reactants would reduce and CO and H\(_2\) would appear as products of the reaction [Heywood, 1998]. In this study fuel lean, stoichiometric, and fuel rich mixtures are all evaluated.

**Combustion Characteristics**

In addition to the characteristics that allow combustion processes to be classified there are other properties of the reaction that can be quantified and analyzed to predict or control flame behavior. This includes characteristics such as heat release, flame temperature, flame speed, and in the case of liquid fuel droplet atomization and vaporization properties. The first two of these parameters, heat release and flame temperature are closely related and must be considered in conjunction with one another.

If a combustible mixture were to be burned in a constant volume adiabatic environment the result would be an exhaust gas that has experienced a rise in temperature caused by the exothermic nature of the reaction. The amount of heat released is proportional to this temperature increase. The heat released is quantified by evaluating the enthalpy difference between the products and reactants. This change in enthalpy is referred to as the heating value of the fuel or the enthalpy of combustion. It is important to note here that one of the products of a combustion reaction is water. Water at room temperature is a liquid but water at typical combustion temperatures is a gas. Some of the enthalpy of combustion is devoted to the phase change of the product water. The heating value of the fuel without considering the heat sink of water vaporization is called the Higher Heating Value (HHV) while the heating value of the
fuel after considering the latent heat of vaporization for product water is the Low Heating Value (LHV). As a result, the LHV is a more practical indication of the amount of heat that can be gained from a combustion reaction because in reality the heat devoted to water evaporation is difficult to recover from exhaust gas (though water vapor can provide additional expansion that can be converted to mechanical power). [Turns, 2000]

The temperature of the gas in the case previously described is called the adiabatic temperature of the reaction. Adiabatic temperature can be determined by balancing the enthalpy of the reaction and the enthalpy of the products, provided that the heat potential associated with the fuel is known. In this calculation it is assumed that all liberated heat is devoted to increasing the sensible enthalpy of the product gas.

\[ H_{\text{react}}(T_i, P) = H_{\text{prod}}(T_{\text{ad}}, P) \quad \text{Equation 5} \]

This adiabatic flame temperature is dependent upon equivalence ratio of the mixture. A lean mixture will have a lower adiabatic flame temperature because, for a given volume of mixture, there are less combustion reactions that can occur. This effect is exaggerated by the fact that the excess air acts as a heat sink for the reactions that do occur. Adiabatic flame temperature will increase as a result of any changes that shift the reaction equilibrium towards products (I.E. increasing reactant temperature). In reality the adiabatic flame temperature is not obtained because heat is always lost to the environment. However, adiabatic flame temperature predictions and variations represent an idealized version of the behavior one can expect to observe in actual flame temperature. Therefore adiabatic flame temperature calculations are a valuable tool in predicting actual flame temperature.

Another metric that must be considered when evaluating a combustion reaction is the flame speed or flame propagation velocity. Flame speed is defined as the velocity of the unburned reactant mixture in a direction normal to the flame front [Kuo, 2005]. Or more practically, flame speed is the rate at which the flame front moves through a combustible mixture. In stable burner flames the flame front appears stationary because the burning rate is equal to the fuel/air feed rate. If the fuel/air feed rate is significantly higher than burning velocity the flame can lift and blow-off. Similarly in premixed combustion an insufficient fuel/air feed rate can result in the flame ‘flashing back’ into the premixing chamber. Flashback is not an issue in diffusion flames because combustion is dependent upon fuel-oxidizer mixing.

Flame speed in laminar flames can be evaluated analytically. Flame front thickness can also be evaluated analytically. These characteristics depend upon chemical composition of the fuel. The expressions for these parameters are shown as functions of temperature and pressure in Equations 6 and 7.

\[ \delta \propto T_b^{-3/2} \exp\left(\frac{+E_A}{2R_u T_b}\right) P^{-n/2} \quad \text{Equation 6} \]

\[ S_L \propto T_u^{-3/2} \exp\left(-\frac{E_A}{2R_u T_b}\right) P^{(n-2)/2} \quad \text{Equation 7} \]

From these relationships and it is evident that flame speed strongly depends upon flame temperature marginally on pressure. Low flame temperatures result in reduced flame speed and increased flame thickness. In industrial combustors and engines a low flame thickness is desired. Compact flames result in more concise heat release and can result in better engine efficiency.
Laminar flame speed can be determined analytically because it depends upon thermal and chemical properties of the mixture. Flame speed in turbulent flames, however, is dependent upon complex flow properties which cannot be accurately predicted. In turbulent flames the reaction zone becomes ‘wrinkled’ by the turbulence and surface area of the flame front increases. A comparison of a turbulent flame front and a time-averaged flame front is shown in Figure 6. A laminar flame would closely resemble the time averaged flame front.

Because the turbulent flame front has a larger reaction area than the laminar flame front the turbulent flame speed is higher than the laminar flame speed. The most common approach for relating turbulent flame speeds to flow properties is the Damköhler model which expresses turbulent flame speed as a function of laminar flame speed and turbulence intensity, shown in Equation 8.

\[ S_T = \left(1 + \frac{\alpha}{S_L^2}\right) S_L \tag{Equation 8} \]

Flame speed calculations become even more complicated once heterogenous mixtures of fuel drops, fuel vapor, and air are considered. Heterogenous mixtures include systems involving spray combustion, such as the system observed in this study. Fundamental studies are difficult to perform because of the experimental difficulties associated with monitoring consistent droplet formation, droplet sizing, droplet size distribution, and fuel vapor concentration. Measurements of flame propagation velocity are also more difficult to perform because of the magnified effects of buoyancy and gravitational force that can be observed on fuel droplets. A complex model has been developed by Ballal and Lefebvre [Ballal et al, 1980] based on the assumption that the rate of flame propagation through a fuel mist is governed by the balance between the quench time of the reaction zone and the sum of the evaporation and chemical reaction times. This complex model, however, is still heavily dependent upon the experimental evaluation of constants. Using this model it can be determined that smaller droplet size increases flame speed as a result of decreased evaporation time. Figure 7 shows
how the variation of flame speed as a function of droplet size and fuel/air ratio. Droplet size is expressed as a Sauter Mean Diameter (SMD) in microns. Sauter Mean Diameter is the diameter of a droplet having the same volume-to-surface-area ratio as the typical particle within the fuel spray.

![Figure 7: Dependence of Flame Speed on Fuel Droplet Size](image)

It can be observed from this plot that there is some maximum droplet size above which flame propagation velocity goes to zero and a flame will be quenched by the large droplets. Figure 8 shows the effect of increased mainstream air velocity on flame propagation velocity. Flame speed increases as mainstream velocity increases because of the increase in turbulence intensity and enhanced mixing that occurs. Droplet evaporation time is effectively reduced as a result of increased turbulence.

Having established that flame speed in heterogeneous mixtures is heavily dependent upon fuel evaporation time it is critical that the combustion engineer have a quality understanding of droplet and spray evaporation. Droplet evaporation involves heat transport through conduction and convection into the droplet surface and the removal of droplet mass by the ambient gas flow. Emulsion of a droplet in a hot gas environment will result in a period of droplet heat up during which mass transfer is minimal followed by a steady-state temperature period during which the majority of mass transfer occurs. The time for each of these periods is referred to as the heat up and evaporation times, respectively. During the evaporation phase droplet diameter decreases linearly with time. Figure 9 shows both variation of droplet diameter and temperature with respect to time.
Figure 8: Dependence of Flame Speed on Bulk Air Velocity [Lefebvre et al, 2010]

Figure 9: Variation of Fuel Droplet Temperature (left) and Droplet Diameter (right) as a Function of Time [Lefebvre et al, 2010]
It is important to note here that droplet lifetime depends upon fuel thermochemical properties, heat transfer properties of the environment, and diffusion gradients within the ambient environment. Fuels with a lower heat of vaporization will evaporate more readily than those with a higher heat. Sprays with a higher relative velocity between gas flow and droplet speed will result in greater convection heat transfer and reduced droplet life. Molecular diffusion will be delayed in cases where the ambient vapor pressure is high. In other words, the presence of vaporized fuel will reduce the propensity of additional fuel to vaporize. These factors are all important to consider when evaluating spray combustion performance. Combustion engineers generally favor shorter evaporation times which aids in increasing combustion efficiency and increased flame stability.

The final combustion characteristic that will be addressed here is the property of ignitability. Once a combustible mixture is established the mixture can be ignited if the ignition source provides enough energy for heat generation to exceed the rate of heat loss. In other words the ignition kernel must be adequately sized and of adequate magnitude to allow for flame propagation [Tozzi et al, 2006]. In heterogeneous mixtures the ignition kernel results in a region of high gas temperatures. These high gas temperatures enable the evaporation and combustion of the smallest liquid fuel drops. The larger fuel drops then act as heat sink as they vaporize. The ignition kernel will extinguish if the heat sink of vaporization is larger than the heat generated. This model is generally accepted since chemical reaction times are considered to be much less than evaporation times. Therefore the critical requirements of an ignition kernel are that it be of adequate size and meet the minimum ignition energy requirements. Minimum ignition energy requirements can be reduced by increasing the quality of the fuel atomization within the mixture. Figure 10 shows the effects of equivalence ratio and droplet size on minimum ignition energy. Typical ignition devices operate on the principle of an electrical discharge to produce a spark as the ignition kernel. More difficult to ignite mixtures can be ignited through the use of a pilot flame or ignition torch.

Figure 10: Effects of Equivalence Ratio and Droplet Size on Minimum Ignition Energy [Lefebvre et al, 2010]
Industrial Combustion Devices and Flame Stabilization Schemes

There is a wide variety of devices and configurations that have been used to produce and control combustion reactions. These range from campfires to race car engines to bombs. Mankind has used chemical to thermal energy conversion as a means to power cooking, electricity generation, transportation, entertainment, scientific investigation, and weaponry. In this paper all detonation combustion devices will be neglected, that includes bombs, some rockets, and certain types of experimental devices. Deflagration devices include various types of boilers, fluidized bed combustors, internal combustion engines, turbine engines, and numerous experimental devices. There are entire volumes of texts devoted to each of these categories of engines so a brief introduction will be given here.

Boilers are combustion devices that utilize combustion heat in order to boil water for use in steam powered systems. Steam turbines are typically powered by the superheated vapor and can be used to turn compressors, industrial equipment, or electricity generators. Boilers consist of a burner responsible for controlling combustion and a heat exchanger responsible for transferring the combustion heat to the water/steam flow. Burners can be designed to operate on either gas or liquid fuel, can be premixed or non-premixed, and have a great variety in geometric variability. Burner designs are often tailored to be optimized for a specific fuel and can possess any of the flame stabilization methods described later in this section [El-Wakil, 1984].

Fluidized bed combustors are combustors particularly useful for efficient combustion of solid particles. In a fluidized bed combustor solid fuel particles are in intimate contact with a fluid that passes through at a velocity adequate to suspend the particles. This fluid is typically the oxidizer. In an operating fluidized bed system the gravitational force acting on the fuel particles is equal to the buoyant force caused by the oxidizer flow, resulting in fuel particles suspended in oxidizer. A schematic is shown in Figure 11.

![Figure 11: Schematic of a Fluidized Bed Combustor](image-url)
Significant amount of research has been invested in understanding fluidized bed combustors, but since this study involves liquid fuel combustion fluidized bed combustors are not of much interest and the topic will be abandoned at this point.

Internal Combustion (IC) engines are the preferred choice for small scale mechanical drive applications. Internal combustion engines dominate the terrestrial, small aircraft, and small watercraft propulsion markets. Internal combustion engines also are widely used in the small-scale power generation applications such as personal generators or peaking facilities. The vast majority of internal combustion engines are of the reciprocating type (as opposed to rotary) and most are four-stroke (2-stroke is less reliable and produces more emissions). Figure 12 shows the four stages of the 4-stroke internal combustion engine operating cycle.

![Figure 12: Stages of the Four-Stroke Internal Combustion Engine Operating Cycle [Heywood, 1998]](image)

Internal combustion engines are generally operated on liquid fuels though they can be tuned to operate on gaseous hydrocarbons. IC engines experience confined combustion of a fuel-oxidizer charge that is then exhausted and replaced. Each engine cycle includes both an injection and an ignition event. Ignition can either be by spark or compression (auto-ignition), dividing IC engines into two distinct categories. Because the ignition process is repeated in an IC engine ignitability of the air-fuel mixture becomes very important. Ignition timing is also critical for effective engine operation. Since IC engines experience a large number of injection and ignition events it is critical that the charge be mixed effectively over a short period of time. Pressure fluctuations occur within the cylinder of an IC engine and a typical cycle can be seen in Figure 13. Notice in this figure the timing of the intake event and combustion event. It is critical to note the short amount of time during which the combustion event occurs and the change in pressure associated with that event. This is very different from the combustion process observed in a turbine engine.
Turbine engines are engines that produce mechanical power by expanding fluid to a lower pressure [Dixon, 2005]. A typical turbine engine includes an inlet air compressor that operates on scavenged mechanical power, a combustion chamber where fuel is added and the mixture is burned, and a turbine section that expands the hot gas and produces mechanical drive. A diagram is shown in Figure 14.

Turbine engines depend upon the momentum of the hot gas stream to turn turbine rotors and shafts. These engines are utilized in large aircraft and water craft applications as well as to provide power for electricity generators. Turbine engines can be liquid or gas fueled. Heat is often recovered from the exhaust gas stream and used to heat steam for powering steam turbines.

![Diagram of turbine engine cycle](image)

**Figure 13**: Pressure Fluctuations and Sequence of Events in a Four-Stroke Spark-Ignition Engine Cycle [Heywood, 1998]

![Diagram of gas-turbine cycles](image)

**Figure 14**: Schematic of a Direct Open Gas-Turbine Cycle, Single Shaft (left) and Two Shaft (right) [El-Wakil, 1984]
This process of cogeneration results in the highest system efficiency available for power generation. Natural gas powered cogeneration facilities account for the largest component of new power generation capacity in the United States. This growth is a result of the low capital cost, high efficiency, and relatively low emissions that result from gas turbine use. Land-based power generation gas turbines are stationary and typically fueled with natural gas and in some cases fuel oil. Propulsion turbines are generally fueled by liquid fuel.

Thermodynamic efficiency of the turbine engine is dependent upon the effectiveness of the compression, heat release, and expansion processes. The effectiveness of heat release from the fuel can also be referred to as the combustion efficiency and is a measure of the amount of available chemical energy that is converted to thermal energy. Incomplete conversion results in losses to overall engine efficiency. Unlike in IC engines turbine engines experience a continuous combustion process and do not rely on repeated ignition. Fuel injection is continuous and pressure fluctuations are generally avoided. As a result flame stability is more important than in IC engines. Combustion chamber design is critical because it determines combustion efficiency, emissions, and the thermodynamic properties of the gas as it enters the turbine section [Saravanamuttoo, 2011]. Turbine combustion chambers are of particular relevance to this work.

Turbine Combustion chambers seek to produce gas at the highest pressure and temperature possible. Since pressure loss due to combustion is proportional to the square of the air velocity it is typical to use a flow diffuser to reduce air flow velocity by a factor of approximately 5 [Lefebvre et al, 2010]. Typically design engineers desire the combustor to provide high combustion efficiency, reliable and smooth ignition, wide flame stability limits, low pressure loss across the combustor, outlet temperature distribution suitable for effective turbine operation, low emissions, elimination of pressure pulsations, durability, cost effectiveness, and in some cases multi-fuel flexibility.

Three main types of combustors exist. These are Tubular (Can), Tuboannular (Can-Annular), and Annular. Can-Annular is the hybrid of a Can and Annular design. Type is generally selected based upon overall engine design. Can combustors typically are more simple to develop and offer substantial reliability, however, they are bulky and heavy making them non-ideal for propulsion applications. Can design is the oldest type of combustor design and involves separating the compressed air stream into a number of radially distributed ‘cans’. Each can acts as a semi-independent combustion chamber and can be tested independently despite being linked to the other cans for ignition and pressure regulating purposes. Can-annular combustors are characterized by having radially distributed flame tubes but having a common annular air-flow. This reduces size of the combustion chamber while still giving the advantage of being able to test a single can at a time. Can-annular combustors allow for easy access for maintenance but still require the additional complication of cross-fire tubes between cans. The annular design involves a single combustion chamber with annular air flow. This eliminates the complications of flame tube interactions and allows overall combustor size to be reduced by as much as 75%. However, these combustors are still extremely large which creates structural design issues as well as greater expense in development and testing. Typically annular combustors are used in propulsion applications while can-annular designs are used for stationary applications.

It is important that a gas turbine combustion system avoid phenomenon such as flashback, blowoff, or liftoff. These events would result in loss of combustion efficiency and eventual loss of power output from the engine. Avoiding these phenomena requires the balance of the flame speed and the local velocity of the air-fuel mixture. Flashback is not a concern in this work because the fuel is
non-premixed. Flame lift however, is a relevant phenomenon. Flame lift is the relocation of the flame base from the injection and desired anchor point to some location farther downstream. This relocation results in overall lengthening of the flame and leads to decreased combustion efficiency and increased hydrocarbon emissions at the combustor exit.

This elongation also results in a decrease in power output due to decreased combustion efficiency and engine operating costs go up. In extreme cases flame lift can lead to flame blow off where the flame is actually extinguished by the discrepancy between fuel-air velocity and flame speed. A number of stabilization techniques have been employed in order to encourage a concise and stable flame that is anchored near to the burner lip.

These stabilization techniques are utilized in gas turbine, industrial burner, and experimental burner applications and include concepts such as sudden expansion, bluff bodies, burner tiles, bypass ports and swirl. Bypass ports and burner tiles are two techniques that are employed in some devices but are not utilized in this study. Bypass ports involve a fuel-air inlet port that is smaller than the complete burner. This smaller port presents air and fuel at a lower velocity than the main-stream flow and serves as a pilot flame capable of reigniting the main burner during an incident of flame extinction. Burner tiles are structures that are heated by the flame and serve as a consistent heat source near the base of the flame. These tiles act as an accumulator for thermal energy and behave like an accumulator tank does in a hydraulic system. If the flame begins to lose thermal momentum the burner tiles serve to heat the incoming fuel and air and boosts flame temperature.

Bluff Body stabilization is a stabilization technique utilized by the apparatus in this study and is employed in many gas turbine applications. In this technique a bluff body is present at the center of the air inlet region. The bluff body causes boundary layer separation and a shear layer at the edge of the bluff body. The resulting wake provides enhanced turbulence and a lower velocity region as air-fuel
recirculates back towards the bluff body. The reduced local flow velocity allows flame speed to exceed the flow velocity and provide for a stable flame. Ideally the flame would be stabilized and anchored immediately downstream of the bluff body [Turns, 2000].

Sudden expansion of the inlet airflow is another technique employed in this work. This diffusion technique causes flow divergence and enhanced separation. The expanded area also serves to further diffuse the air flow through velocity allowing for better flameholding. Confined expansions result in a corner recirculation zone which is responsible for recirculating hot gas back towards the base of the flame, serving to heat newly introduced fuel-air. Figure 16 demonstrates both the corner and central recirculation zones caused by the use of a sudden expansion and central bluff body system [Strakey et al, 2007].

![Diagram](image)

**Figure 16:** Flow Field Induced by Using Sudden Expansion and a Central Bluff Body [Strakey et al, 2007]

![Diagram](image)

**Figure 17:** Recirculation Effects Caused by Introducing Air Swirl [Turns, 2000]
Axial recirculation within the flame region can be enhanced by utilizing radial swirling of the inlet air flow. Swirling is commonly used in industrial burners and in gas turbine combustors. Swirl is even used in IC engines to enhance fuel-oxidizer mixing. Swirling in a gas turbine combustor increases residence time of the combustible mixture and allows for more complete combustion. It also increases turbulence intensity in the flow which improves mixing, reduces droplet lifetime and increases turbulent flame speed. There are many types of swirler schemes and significant amount of study has been devoted to understanding swirler aerodynamics.

Investigative Combustion Devices

Many types of experimental combustion devices have been developed in efforts to understand combustion processes and refine the design of industrial combustion systems. The purpose of these investigative devices ranges from fundamental studies about combustion or fuel behaviors to practical test engines for advanced system development. The complexity and design of the test apparatus depends heavily on the data to be collected.

Fundamental flames studies and fuels research is often performed in devices such as bomb type combustors. These combustors involve the combustion of a fixed volume of combustible mixture. These devices are often used to evaluate the effect of varying a fundamental parameter such as fuel type, air-fuel ratio, temperature, or pressure. Generally these devices seek to eliminate the effects of mixing and flameholding properties. Bomb type analysis is very useful in evaluating chemical rates and equilibrium as well as parameters such as flame speed and heat release. While very useful for fundamental research these types of combustors are not used in the present study.

At the other end of the spectrum one can find research that is performed in complete engine systems. These studies gauge the performance that can be achieved using current understanding of combustion engineering. Complete engine tests observe the realistic interaction of thermal, chemical, hydrodynamic, and mechanical behavior. Results serve as a benchmark for the progression of complete combustion control systems. This type of study is very practical but also is not included in the present work.

There are numerous combustion research devices that have been devised to ‘split the difference’ between fundamental studies and complete engine tests. These systems vary in complexity and the target is often to understand the interaction of some of the systems influencing parameters without achieving the full complexity of the complete engine. This is the type of system observed in the current study. A swirl-stabilized continuous flame combustor is observed in order to provide some practical insight into gas turbine combustor systems while avoiding the complications and costs associated with complex engine controls and diagnostic issues. The test apparatus is described in detail later.

Hydrous Ethanol as a Potential Fuel

As was previously discussed; global demand for hydrocarbon fuel continues to rise and available reserves of fossil fuels diminishes, significant attention is being given to the development of renewable hydrocarbon fuel sources. This includes the development of alcohol fuels such as ethanol. Ethanol can replace light distillates such as gasoline and some middle distillates such as kerosene without significant changes to existing infrastructure. Ethanol has also been used as a substitute for Jet A fuel in select test flights. A number of studies have been performed to evaluate the feasibility of ethanol as an alternative fuel for operating not only internal combustion (IC) engines [Heywood, 1998; Mack et al, 2009;
Brewster et al, 2007], but also in turbine engines both for power generation and aircraft propulsion [Lefebvre et al, 2010]. These studies generally conclude that the use of ethanol is effective for engine operation but that a modified engine tuning is beneficial for maximum performance. Particularly in IC engines it is beneficial to tune the engine specifically for ethanol. This includes modifying the injection size, injection timing, and ignition timing. Blends of ethanol and conventional fuels have also been tested and have shown some promise as potential fuels [Bayraktar, 2011].

Significantly more research has been done concerning anhydrous ethanol use in IC engines than has been done in turbine engines. Many advantages of utilizing ethanol fuel have been revealed through testing. Most of these advantages represent themselves as opportunities for increased power output for a given engine displacement when using ethanol or ethanol blended fuels. Power output was seen to increase as ethanol content increases in an engine of constant displacement [Hseih et al, 2002; Lynd et al, 1991]. This is initially surprising because ethanol combustion offers a lower heating value than traditional hydrocarbon fuels. However, a closer look reveals numerous causes for increased number of combustion reactions per cylinder charge when using ethanol as fuel. Ethanol has a stoichiometric mass air-to-fuel ratio of 9 compared to 14.7 for gasoline. This implies that much less air volume is required for ethanol to reach complete combustion than gasoline. Ethanol (C2H5OH) also contains some oxygen within its molecular structure further reducing the amount of air necessary for complete combustion. The need for less air results in more space available for additional fuel within the cylinder. By increasing the volume of liquid contained in a cylinder charge more heat is removed in fuel vaporization, resulting in a cooler operating temperature. Cooler operating temperatures result in cooler intake temperatures, resulting in higher air density and increased volumetric efficiency. This complex process results in ethanol fuel being capable of providing a much more powerful punch for a given engine displacement. The racing community has long-known these benefits and alcohol injection is frequently used to provide maximum power. The obvious disadvantage here is that while power is increasing so is fuel consumption. The apparent solution to this would be to reduce the size of the engine to reduce volumetric fuel consumption and maintain the same amount of power output.

These relationships are further magnified by the fact that ethanol has an octane number of around 108 which is significantly higher than pump gasoline fuels which are typically less than 100. Higher octane number indicates a resistance to autoignition. Practically this means that the engine can operate under higher compression ratios without the occurrence of damaging engine knock. Higher compression ratios result in increased efficiency and power from the engine, once again indicating adequate driveability with a smaller engine. These advantages are offset somewhat by the requirement for advanced ignition timing with ethanol fuel. Ethanol burns slower than gasoline so ignition must be started earlier in order to ensure complete combustion [Parag et al, 2009]. This results in increased losses during the portion of combustion that occurs before the piston has reached top dead center.

While the pressure and ignition effects seen in internal combustion engines are not as prevalent in gas turbine combustion, a similar phenomenon is observed. For a given air flow rate much more fuel can be injected, creating a larger heat sink in evaporation and resulting in a cooler combustion that fits into a smaller volume (or more combustion events in the same space). The increased density of the fuel-air flow rate results in more momentum in the exhaust gas as it passes through the turbine and creates more power. It should be noted here that reducing the operating temperature of the engine significantly
reduces NOx emissions since most NOx is formed by the thermal route.

As previously stated, one of the major drawbacks of ethanol as fuel is its relatively low heating value when compared to traditional hydrocarbon fuels. The Lower Heating Value (LHV) of pure ethanol is 21.3 MJ/L compared to an LHV of 33 MJ/L for gasoline and 34.9 MJ/L for Jet A fuel [Heywood, 1998; Lefebvre et al, 2010]. Therefore one liter of ethanol must be substantially cheaper than one liter of standard hydrocarbon fuel in order to become competitive in terms of price per unit of energy delivered. One approach for combating this problem is to raise the LHV of ethanol through the use of fuel additives such as energy intensive nano-particles [Karmakar et al, 2010; Wen, 2010]. The other approach would be to reduce the cost of producing ethanol. This would result in the consumption of larger volumes of fuel to produce the same amount of energy, but may be economically advantageous. This concept was represented graphically in Figure 4.

The ethanol production process includes the formation of the feedstock, mashing and cooking the wort, fermentation, and then distillation and dehydration. As was previously mentioned ethanol can be derived from a number of feedstocks including corn, sugar, switchgrass, and recently even cellulosic sources such as corn cobs. Fermentation is the process of converting sugars to ethyl alcohol. This is done by microbes, either bacteria or yeast, which convert the sugars to cellular energy and produce carbon dioxide and alcohol as byproducts. The alcohol concentration as it exits the fermentation vessel is limited by the tolerance of the microbe. In environments of high alcohol concentration the microbes die. Some researchers have claimed to produce yeast strains that can survive in up to 30% alcohol. However, conventional yeast strains die out at around 12% alcohol and some commercial strains can reach approximately 20% alcohol. The remaining volume of the mixture is composed of water, dead microbes, carbon dioxide, and other impurities. The mixture is then filtered before being distilled [Combe, 2011].

In order to produce ethanol fuel the ethanol must be extracted from the excess water. This is done through distillation. Ethanol and water are completely miscible in all proportions. The entire mixture is heated until a temperature of 78.6 degrees Celsius is reached. At this temperature ethyl alcohol boils. Since water does not boil until reaching 100 degrees it remains in the liquid state. The gaseous ethanol is then collected and condensed. The new mixture will still contain some water because of inefficiencies in the distillation process and non-uniformities in the temperature distribution, furthermore, Raoult’s law does not permit perfect distillation to occur even under ideal conditions. The distillation process is repeated until the desired alcohol concentration is achieved, each distillation process resulting in a higher concentration of the more volatile ethanol than the previous batch.

Hydrous ethanol is an azeotropic mixture at ethanol concentrations greater than 95.57% ethanol, or 192 proof. Because of the azeotropic nature of this mixture a significant additional techniques must be employed to achieve anhydrous fuel [Brewster et al, 2007]. The removal of the remaining water can be done by adding additional chemicals such as benzene and employing complex distillation schemes. However, in recent times molecular sieves have evolved as the primary means of further purifying ethanol. This sieve consists of a set of beads that serve as selective filters, absorbing water while rejecting ethanol. The beads, once saturated, can be dehydrated and reused. The use of advanced distillation schemes costs approximately 17000 BTUs per gallon of pure ethanol produced while the use of molecular sieves costs approximately 14000 BTUs per gallon produced. [Madsen et al, 2003]
From this information it is concluded that reductions to the production cost of ethanol can be had if the ethanol concentration is below the 192 proof at which the mixture becomes azeotropic. This would eliminate the dehydration step from the production process and could reduce the distillation cost [Ladisch et al, 1979]. It has been suggested that 37% of the production cost is associated with water removal and dehydration [Mack et al, 2009, Martinez-Frias et al, 2007]. Furthermore, it has been suggested that the production and efficient use of 70 proof ethanol would result in a 34% increase in net energy gain when compared to anhydrous ethanol [Mack et al, 2009]. This increase in net energy gain is a result of reducing the water separation cost from 37% of the total production cost for anhydrous ethanol down to 3% of the total production cost while producing 70 proof ethanol. This is graphically represented in Figure 18.

![Figure 18: Energy Consumed in Ethanol Production by Step [Mack et al, 2009]](image)

70 proof ethanol is quite diluted at 65% water (35% ethanol) by volume and would likely prove to be a difficult fuel to use. However, it is possible to find a more moderate proof of hydrous ethanol that will result in reasonable functionality while still substantially reducing the cost of ethanol production. For example, the use of an 80% ethanol fuel would require approximately a quarter of the distillation energy required to achieve 96% ethanol [Ladisch et al, 1979]. The most obvious disadvantage of decreasing the proof of ethanol is that the LHV of the fuel is quite clearly reduced. This relationship is calculated and shown in Figure 19.
Figure 19: Effect of Fuel Water Content on Volumetric Heating Value [Breaux et al, 2011]

Previous studies have considered the use of wet ethanol in IC engines [Mack et al, 2009; Brewster et al, 2007; Clarke et al, 2002]. These studies have been done in a variety of different IC engine types, ranging from a Homogenous Charge Compression Ignition (HCCI) engine to a Spray Guide Direct Injection engine. In the HCCI engine fuels as low as 40% ethanol were successfully burned. However, at this extremely high water content the fuel was required to be preheated to 140 degrees Celsius. This study found that increased water content caused flame quenching and resulted in increased exhaust hydrocarbon and decreased heat release from the fuel. It is important to note that the mixture in an HCCI engine are extremely lean and in many tests were below equivalence ratio of .3 [Mack et al, 2009]. Another study testing hydrous ethanol combustion in a direct injection engine has shown promise for hydrous ethanol up to 20% water as a practical fuel. This study found that as water content increased burn time increased and power output decreased as water content increased. However, advancing ignition timing as water content increased resulted in a recovery of lost power and engine performance competitive with a pure ethanol case. NOx decreased linearly as water content increased. When ignition timing was fixed it was found that exhaust temperature increased with increasing water content as a result of later combustion and less heat lost to the ambient environment. However, applying an ignition timing scheme to achieve maximum torque resulted in a decrease in exhaust temperature as water content increased. This is because of the heat lost to vaporizing additional water in the fuel. Furthermore, it was suggested that the use of hydrous ethanol may allow the use of higher compression ratio devices that would increase the power output of the engine [Brewster et al, 2007].

Only one study was found that observed the fundamental burning properties of hydrous ethanol combustion. This work considered the burning velocity of hydrous ethanol at concentrations greater than 170 proof [Parag et al, 2009]. The test involved injecting hydrous ethanol into a laminar cross flow through the use of a porous sphere. A flame was allowed to cover the surface of the sphere and a stable flame was achieved for various cross-flow velocities. The burning rate of the fuel was then observed. The results are shown in Figure 20.
Figure 20: Effect of Water Content on Mass Burning Rate [Parag et al, 2009]

This plot shows that the maximum mass burning rate decreases as water content increases. The burning rate increases as air velocity increases because the velocity is low so there is no issue with flame blow-off. The increase in air flow then allows the fuel mass flow to increase while maintaining the same equivalence ratio. Parag et al also determined the ‘transition velocity’ of the fuel. This transition velocity is defined as the cross-flow velocity that causes the flame to transition from fully enveloping the sphere to a wake flame. This transition velocity, though not directly related, gives insight into the effects of water content on laminar flame speed. The results are shown in Table 1.

Table 1: Transition Velocities for Ethanol-Water Mixtures [Parag et al, 2009]

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Transition velocity (m/s)</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>$d = 8$ mm</td>
</tr>
<tr>
<td>Pure ethanol</td>
<td>0.94</td>
</tr>
<tr>
<td>Ethanol 95%, water 5%</td>
<td>0.74</td>
</tr>
<tr>
<td>Ethanol 90%, water 10%</td>
<td>0.71</td>
</tr>
<tr>
<td>Ethanol 85%, water 15%</td>
<td>0.63</td>
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This indicates that laminar flame speed is reduced 20-21% when water content increases from 0 to 5%. Flame speed is reduced 24-26% when water content increases from 0 to 10%. Flame speed is reduced 33% when water content increases from 0 to 15%. This result is likely caused by the increased amount of heat and time needed to vaporize hydrous fuel.

No studies could be found that considered hydrous ethanol combustion in full-scale turbine engine tests. It has been suggested that some work was done by the United States Navy in this area. However, all work was classified and no publications could be located on the topic. It is important to note here that water injection is frequently employed in industrial applications to reduce emissions from the
turbine while adding momentum to the working fluid and boosting power output. The use of hydrous fuel would eliminate this step. This would be economically beneficial since industrial water injection skids can cost upwards of $2 million for some turbines.

Similarly no work has been done concerning the use of wet ethanol in a swirl-stabilized continuous flame combustor. Information provided from such a study will be particularly relevant to the use of wet ethanol in turbine applications. It will also allow for the elimination of factors such as ignition properties and pressure fluctuations that are inherently critical in IC engine operation. By reducing the influence of these variables during testing it is possible to glean more fundamental information concerning the combustion of wet ethanol.

Some of the changes in flame properties can be predicted from existing literature. It is known that increasing water content of the fuel will decrease the adiabatic flame temperature of the combustion reaction. Calculations of the adiabatic flame temperature reveal a theoretical reduction in flame temperature from 2200 K down to 1650 K as the fuel proof reduces from 200 to 100 proof [Bormann et al, 1998]. This reduction in temperature will undoubtedly result in a reduction in NOx formation by reducing thermal NOx. At elevated water contents a lower flame temperature may have adverse effects on fuel vaporization and combustion efficiency resulting in more hydrocarbons in the exhaust gas. This is in agreement with the results found in the internal combustion engine studies. The operational limits of the combustor, in terms of Equivalence Ratio (ER), are expected to be affected adversely by low alcohol proof.

This study seeks to provide a detailed view of how increasing water content affects flame structure, temperature, heat release, NOx formation, and exhaust gas composition. It is also pertinent to understand how elevated water content affects the operational limits of the swirl-stabilized combustor. This information is particularly relevant in evaluating hydrous fuel as a candidate in fuel flexible gas turbine operation.

**Theoretical Considerations and Predictions for Hydrous Ethanol**

The first step in determining the feasibility of hydrous ethanol as a fuel is to evaluate some theoretical consequences of its use. This includes a look into the heating value, adiabatic flame temperature, global reaction for combustion of the fuel, equilibrium modeling, and chemical kinetics effects. This portion of the work aims to give a basic view of the consequences of water addition.

If we consider the global reaction rate for ethanol we would assume that for complete combustion at stoichiometric conditions the products would be only H$_2$O and CO$_2$ with no dissociation of the excess nitrogen in the air. It is important to determine the stoichiometric air-fuel ratio for ethanol as water content varies. This is done by balancing Equation 9.

$$C_2H_5OH + aH_2O + b(O_2 + 3.773N_2) = cCO_2 + dH_2O + 3.773bN_2$$

Equation 9

The coefficient $a$ is determined by the volume percent of water in ethanol. This volume percent is converted to a mass percent which is used, along with molecular weight, to determine the moles of reactant H$_2$O per each mol of Et-OH. Coefficients $c$ and $d$ are found by balancing carbon and hydrogen across the reaction. Oxygen is then totaled and coefficient $b$ is determined. By considering coefficient
we can determine the molecular air-fuel ratio and using molecular weights we can evaluate the mass air-fuel ratio. Figure 21 shows the variation of stochiometric air-fuel ratio as water content varies.

![Mass Air-Fuel Ratio](image)

Figure 21: Stochiometric Mass Air-Fuel Ratio as a Function of Water Content

This demonstrates that as water content increases the mass air-fuel ratio goes down. This is expected because elevated water content indicates that Et-OH molecules constitute a smaller mass percentage of the fuel and therefore less air is needed for complete oxidation.

The heating value of hydrous ethanol can be determined by first determining, through stoichiometry and equation 1, the number of moles of Et-OH and H2O per liter of fuel. By utilizing the information that pure ethanol combustion releases 1367 kJ/mol it is possible to determine the total heat released per liter of fuel. This resolves the HHV of the fuel. To resolve the LHV of the fuel it is necessary to subtract from the HHV the energy required to fully vaporize the water in the products. This is done using the knowledge that the latent heat of vaporization for water is 40.66 kJ/mol. It is also possible, using density of the fuel, to convert HHV and LHV from being volume specific into density specific units. The results of these calculations are shown in Figure 19.

This plot demonstrates, as is expected, that the heating value of the fuel decreases as water content increases. This is because the addition of water replaces ethanol molecules that serve as heat suppliers. Therefore, as water content increases volumetric consumption would have to increase in order to release the same amount of energy. Keep in mind that dollar consumption would still be decreasing despite the increase in volumetric consumption.

Another important combustion property to be considered is the adiabatic flame temperature of the mixture. Once again equivalence ratio of 1 is assumed for all calculations. Traditionally adiabatic temperature is taken by thermodynamically balancing the enthalpies of the products and the reactants of a combustion reaction. Since enthalpy is thermodynamically related to temperature it is possible to solve for the uniform product temperature. Another more simplified method for calculating adiabatic temperature was proposed in ‘Combustion Engineering’ by Ragland and Bormann. Adiabatic flame temperature can be determined by Equation 10.
Equation 10

\[ T_p = T_0 + \frac{LHV}{(1 + AF_{\text{grav}})C_p} \]

Where \(T_p\) is the temperature of the products, \(T_0\) is the initial temperature of the reactants, \(LHV\) is the Lower Heating Value, \(AF_{\text{grav}}\) is the Air-Fuel ratio by mass, and \(C_p\) is the mass-averaged specific heat of the products. Employing this equation, using 298 K as \(T_0\) and the LHV and A-F as determined previously Figure 22 is obtained.

Figure 22: Adiabatic Flame Temperature of Ethanol (ER=1)

Here it is important to note that the mass-averaged specific heat of the products is dependent upon the temperature. In the ideal world a regression equation would be developed for the tabulated values of \(C_p\) and this equation would be integrated across the temperature range to find the true adiabatic flame temperature. However, taking a \(C_p\) value near the exhaust gas temperature serves as a reasonable approximation. The variation of the Adiabatic Flame Temperature result is shown for two different \(C_p\) temperatures.

Adding water to ethanol fuel will affect the thermal properties of the fuel, the fluid dynamic properties, and the chemical properties. As was discussed previously, fuel vaporization is important when considering combustion of liquid fuel sprays because the ability of the fuel to vaporize great contributes to combustion efficiency and flame health. One important characteristic to consider is the amount of time it will take for a hydrous ethanol droplet to evaporate when compared to an anhydrous ethanol droplet. A simple inquiry reveals that hydrous fuel takes more heat to vaporize than anhydrous fuel. This is evident when the latent heat of vaporization of ethanol is observed to be 846 kJ/kg compared to 2257 kJ/kg for water. Stoichiometric calculations shown in Figure 23 show the variation in latent heat of vaporization of hydrous ethanol when determined by mass fractions.
This shows that much more heat is needed to vaporize a fixed volume of hydrous ethanol. However, a more detailed look into droplet evaporation times is helpful. It is relevant to compare the lifetime of an ethanol droplet and a water droplet to determine the effects of elevated water content on vaporization time. It is also helpful to consider these lifetimes as a function of the water content in the ambient air. The droplets will be considered to be 25 microns in diameter. This diameter is selected based upon the fuel nozzle manufacturer’s data [Parker Hannifin Corp, 2009] and hopes to reasonably represent the conditions of the accompanying experimental study.

The pressure will be taken as 1 atm since the experimental apparatus is an atmospheric combustor and the ambient temperature will be taken as 1100 K which is typical of the low flame region inside the combustor. The droplet will be injected at a temperature of 298 K. Ambient water concentration will range from mass fractions of .02 to .041 which accurately represents the ambient water concentration for a 20% water-in-ethanol mixture over a range of .6<ER<1.1. Ambient ethanol concentration will range from .07 to .12 which accurately represents all fuels over a range of .6<ER<1.1. The solution assumes quasi-steady, constant properties, spherical droplets, ideal gas behavior, and uniform droplet temperature.

An interesting result that can be seen is that for E80/W20 water will not diffuse if the droplet is assumed to be at room temperature. This is because the saturation concentration of the droplet at 273 K is less than the ambient concentration of the environment. It is then necessary to assume that the droplet will receive some heat from the ambient environment before vaporization occurs. The new assumed uniform temperature of the water droplet was 348 K. Figure 24 shows the droplet lifetime as a function of equivalence ratio. Ethanol droplet lifetime shown in blue represents the life of an ethanol droplet for all fuels. Water droplet lifetime shown in red represents the life of a water droplet for E80/W20.

![Latent Heat of Vaporization](image)

Figure 23: Variation in Latent Heat of Vaporization of Hydrous Ethanol
Figure 24: Droplet Lifetime of an Ethanol Droplet and Water Droplet as a Function of ER

Keep in mind that increasing the equivalence ratio increases both the ambient water and ambient ethanol vapor concentration. While these trends appear linear they are actually exponential if viewed over a wider range of ambient concentrations. However, this wide range of ambient mass fractions does not occur in this system. Figure 24 shows that the time required for a water droplet to vaporize is significantly greater than the time required for ethanol vaporization. This indicates that the excess water will be the limiting constituent in fuel vaporization. It is also seen that droplet lifetime increases as equivalence ratio, and consequently ambient vapor concentration, increases. Overall it can be concluded that changing equivalence ratio does not dramatically affect vaporization but water will exhibit a much longer lifetime than ethanol and inhibit fuel vaporization. Lifetimes are generally low because droplet size is very small and ambient temperature is very high.

In addition to thermal-fluid considerations it is important to consider the effects of elevated water content on the chemical processes associated with ethanol combustion. This requires a detailed look into the literature to see what role water plays in the chemical kinetics of ethanol oxidation. The current portion of this paper seeks to analyze established mechanisms as well as model the combustion reaction using computational methods.

The most well-known model of ethanol combustion is a mechanism presented by Marinov (1999). This model has been validated against a number of experiments and is widely accepted. Marinov’s mechanism considers 56 chemical species and 351 reversible reactions. After a thorough review of the reaction mechanism we find that water plays a role in 59 of these reactions, is a reactant in 0 and is a product in 57 reactions. Water acts as a mandatory third body in 2 reactions and acts as an enhancing third body in 24 additional reactions. A look into the process of reviewing the role of water is found in Figure 25.

These statistics allow us to conclude that increased water concentration will speed up the reactions for which it is a third-body, and it may slow down the reactions for which it is a product by
shifting equilibrium towards reactants. The significance of this can be evaluated by evaluating the equilibrium constant for each reaction, and then evaluating the relative magnitude of the forward and reverse rate coefficients. This becomes a cumbersome job when considering 57 reactions. As a result a reduced ethanol combustion mechanism was sought out. Literature review revealed that there had been some critique of Marinov’s mechanism claiming that it did not accurately model pyrolysis reactions. As a result some reaction rate constants were changed by Dauster (2010). A reduced mechanism was developed by Vas et al (2010) which identifies the key steps of ethanol combustion and provides a reasonable accurate solution with a simplified model. The resulting mechanism is shown in Figure 26.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>A</th>
<th>b</th>
<th>Ea</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. CH(_4) + O(_2) = CO + H(_2) + H</td>
<td>3.00E-12</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>2. CH(_4) + OH = CH(_3) + H</td>
<td>3.00E-12</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>3. CH(_3) + H = CH(_2) + H</td>
<td>3.00E-12</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>4. CH(_2) + CO = CH(_3) + CO</td>
<td>3.00E-12</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>5. CH(_3) + CH(_3) = C(_2)H(_5)</td>
<td>2.00E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>6. CH(_3) + OH + CO = C(_2)H(_5) + CO</td>
<td>1.60E-14</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>7. CH(_3) + O(_2) = CO + O</td>
<td>3.50E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>8. CH(_3) + CO + H = C(_2)H(_5) + O</td>
<td>5.00E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>9. CH(_3) + CO + H(_2) = C(_2)H(_5) + O</td>
<td>3.00E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>10. CH(_3) + CO + CO = C(_2)H(_5) + O</td>
<td>3.40E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>11. CH(_3) + CO + H(_2) = C(_2)H(_5) + O</td>
<td>1.37E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>12. CH(_3) + CO + CO = C(_2)H(_5) + O</td>
<td>1.56E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>13. CH(_3) + CO + H(_2) = C(_2)H(_5) + O</td>
<td>9.46E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>14. CH(_3) + CO = CH(_2) + CO</td>
<td>1.00E-14</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>15. CH(_3) + CO = CH(_2) + CO</td>
<td>4.00E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>16. CH(_3) + CO = CH(_2) + CO</td>
<td>3.00E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>17. CH(_3) + CO = CH(_2) + CO</td>
<td>6.00E-13</td>
<td>0.0</td>
<td>0.0</td>
<td>[28]</td>
</tr>
<tr>
<td>18. CH(_3) + CO = CH(_2) + CO</td>
<td>3.43E-09</td>
<td>1.18</td>
<td>-447.0</td>
<td>[28]</td>
</tr>
<tr>
<td>19. CH(_3) + CO = CH(_2) + CO</td>
<td>2.39E-08</td>
<td>1.77</td>
<td>300000</td>
<td>[28]</td>
</tr>
<tr>
<td>20. CH(_3) + CO = CH(_2) + CO</td>
<td>3.31E-16</td>
<td>0.0</td>
<td>810000</td>
<td>[28]</td>
</tr>
<tr>
<td>21. CH(_3) + CO = CH(_2) + CO</td>
<td>1.80E-13</td>
<td>0.0</td>
<td>300000</td>
<td>[28]</td>
</tr>
<tr>
<td>22. CH(_3) + CO = CH(_2) + CO</td>
<td>7.58E-12</td>
<td>0.0</td>
<td>410000</td>
<td>[28]</td>
</tr>
<tr>
<td>23. CH(_3) + CO = CH(_2) + CO</td>
<td>1.86E-17</td>
<td>-1.0</td>
<td>1700000</td>
<td>[28]</td>
</tr>
</tbody>
</table>

We find in the simplified mechanism that water is found as a product in 4 out of 18 reactions. We can assume that the increase in water content does not appreciably affect the chemistry if the reverse reaction rate is significantly less than the forward reaction rate for these reactions. Using these criteria we find that the progress of reactions VII, XI, and XII will not be affected by the addition of more water. Each of these reactions was evaluated at combustion temperatures. Reaction I, however, could only be evaluated at room temperature because the Gibb’s Function of Formation for constituents was not available at other temperatures. The calculations showed that at room temperature water addition will drastically affect the progress of this reaction. This may change once the products and reactants are at
combustion temperatures, unfortunately not enough information is available to make this conclusion. As a result more detailed modeling of the combustion process is necessary.

As a result more detailed modeling of the combustion process is necessary.

Figure 26: Simplified Ethanol Reaction Mechanism [Vas, 2010]

It is pertinent to evaluate the full chemical equilibrium composition of hydrous ethanol fuel for various equivalence ratios and water contents. Modern computing capabilities have made it possible to perform this analysis in many different ways. Codes have been developed that are capable of predicting the equilibrium concentrations of combustion reactions for a wide range of species. One such code is the NASA developed CEA code, or ‘Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications’. This code has the ability to consider over 2000 different chemical species and executes a FORTRAN code that has been developed by NASA over the past 45 years. This code is capable of determining adiabatic flame temperature and final gas composition for ‘bomb’ type combustion events. The model assumes some user defined pressure and an initial guess for reaction temperature and then uses thermodynamic tables to affectively calculate equilibrium conditions. This software is available for free from NASA and is reasonably user friendly.

Since the CEA code is not a commercial package it was necessary to prove the results were reliable. A literature review finds that the CEA code has been used in many technical publications. To further verify the results the adiabatic flame temperature was calculated for a methane-air flame at various equivalence ratios. The result was compared to an established result from CHEMKIN software and is shown in Figure 27.

This result shows very good agreement with the CHEMKIN solution and the CEA program was deemed to be reliable. The code was then run to evaluate the equilibrium conditions of ethanol combustion at various equivalence ratios. Pressure was assumed to be 1 atm, initial guess for thermodynamic properties was 2000k, fuel/air composition was specified on a molar basis and was assumed to be at an initial temperature of 298 K. 171 chemical species were considered in this
simulation. The water composition of the fuel was also varied. Adiabatic flame temperature is shown in Figure 28.

![Verification of NASA CEA Code](image)

**Figure 27:** Verification of NASA CEA Code for Adiabatic Flame Temperature Calculations

![Adiabatic Flame Temperature as Function of ER and Water Content](image)

**Figure 28:** Adiabatic Flame Temperature as Function of ER and Water Content

This plot demonstrates that the adiabatic flame temperature increases as ER approaches 1.0 and then decreases as the fuel becomes rich. This is expected and can be found in literature. Furthermore it is seen that the flame temperature plot shifts downward as water content increases. This is because the excess water scavenges heat from the reaction as it vaporizes. Varying water concentration while holding ER=1 we find that this data agrees well with the data presented in Figure 22.
NASA CEA also enables the evaluation of equilibrium gas composition. This was evaluated for fuels ranging from 0-20% water and ER ranging from .5 to 1.1. The results for pure ethanol are shown in Figure 29. This plot shows the mol fraction of various exhaust gases at different equivalence ratios. This shows that water content increases as ER increases, and is caused by the increasing number of combustion reactions occurring and going to stable products. O₂ concentration is seen to drop to zero at ER=1. This is because there is no longer any excess air as it is all consumed by excess fuel at high ER>1. N₂ is found to be greater in concentration than any other exhaust gas regardless of equivalence ratio. This is expected because of its high concentration in ambient air and its resistance to reaction. CO₂ increases as ER approaches 1 because more reactions are occurring and going to completion, but it is found to decrease above ER=1. This decrease is a result of oxygen starvation and is complemented by CO increase in this region. H₂ concentration is also seen to increase slightly at rich ERs due to oxygen starvation. OH, NO, H, and O do not have any significant share in the mol fraction over the entire range of equivalence ratios.

![100% Ethanol Equilibrium Gas Composition (CEA)](image)

Figure 29: Exhaust Gas Composition for Pure Ethanol as a Function of ER

Having established a reliable means of determining equilibrium concentrations for hydrous ethanol combustion it is important to consider the effects that elevated water content has on the equilibrium composition. To evaluate this H₂O, CO₂, CO, and H₂ is plotted as a function of equivalence ratio for different fuels. Figure 30 shows the effect that water content has on H₂O equilibrium concentration. Final water concentration goes up as fuel water content increases. This is obviously going to be true but does not offer any insight into the amount of water produced in the combustion reaction because the combustion water may be graphically masked by the large increase in non-reacting water.
Figures 31 and 32 shows the effects of elevated water content on equilibrium CO$_2$ and CO, respectively. Both CO$_2$ and CO concentrations are found to decrease as fuel water content increases. This does not simply suggest that the percent of carbon atoms that fully oxidize is decreasing with elevating water content. The actually number of CO$_2$ and CO moles may not be affected but the mol fraction decreases because of the increase in total number of moles caused by water addition. This is the likely explanation for the small decrease in equilibrium mol fraction. It is therefore concluded that the addition of water to the fuel does not affect the oxidation of carbon in any appreciable way.
Figure 32: Exhaust CO Composition Predictions of CEA Code

Figure 33 shows the increase in equilibrium H\(_2\) mol fraction that occurs from water addition. This small increase is because of the additional H\(_2\) that is formed by H\(_2\)O dissociation. In conclusion we find that the addition of 20% water does not affect the equilibrium in any dramatic way.

Figure 33: Exhaust H\(_2\) Composition Predictions of CEA Code

While the NASA CEA code is capable of providing good information concerning combustion equilibrium compositions it does have short-comings. This code offers no insight into the time-scales associated with the chemical reaction. It also does not consider any particular chemical reaction rates or reaction mechanism, but rather determines a global equilibrium. Furthermore, the code presents results in terms of mol fraction. This is not as useful as the actual mol concentration because all data is normalized to the total number of moles. As a result it is difficult to determine if the actual concentration of a particular species has changed as a result of water addition, or if the total number of moles has changed due to the addition of a semi-inert component.
All of these difficulties can be resolved using CHEMKIN. CHEMKIN is a code developed by SANDIA Laboratories that is capable of resolving time dependent combustion events. The program allows the user to encode the desired mechanism and have complete control over the participatory reactions and species. The ideal model of hydrous ethanol combustion would be to develop a CHEMKIN code for Marinov’s reaction mechanism. This code should be executed for various initial concentrations of ethanol, air, and water. Flame speed, exhaust gas concentrations, and combustion efficiency can all be determined by this process. Unfortunately time and licensing resources did not allow the use of CHEMKIN in this work.
TEST APPARATUS

Combustor Design

As was previously described there are many types of devices and engines used to evaluate fuel performance and flame health. This study utilizes a vertically oriented, swirl-stabilized, axisymmetric shell combustor, shown in Figure 34. The axisymmetric design of the combustor allows for a uniform flame and simplifies measurements. The flame was oriented vertically in order to eliminate the radial effects of gravity and buoyancy forces and ensure axisymmetric flame structure. The combustor was designed specifically for the LSU Turbine Innovation and Energy Research Laboratory by Mr. Srinibas Karmakar and Mr. Shengrong Zhu. The combustor is a fuel flexible modular design, offering configurations for both liquid and gas fuel, as well as both premixed and non-premixed combustion modes. For this study the combustor was always operated in non-premixed mode with ethanol-water blended liquid fuel.

The combustor inlet consists of a single fuel injection point located at the center of the combustor with an annular air inlet. Air is introduced to the combustor though the use of four air inlets positioned symmetrically about the combustor center line. Air flow is then passed through a flow straightener to ensure uniform velocity flow field as air enters into the combustor. Air is swirled utilizing a swirler with eight 45 degree turning vanes. Swirling flows are often characterized by a non-dimensional swirl number to indicate the strength of the swirl. Evaluating equation 11 [Beer et al, 1972] for a swirler with constant swirl angle θ reveals an air swirl number of .755 at the exit of the swirlers used in this study. As flow exits the swirler the swirling momentum will gradually reduce as swirling component is dissipated through fluid drag and shear. The swirl number will obviously decrease as the flow moves farther downstream away from the swirler exit. The modular design of the combustor enables axial variation of swirler location (Figure 35).

In order to achieve strong recirculation within the combustion chamber it is necessary to have a swirl number greater than about 0.6 within the combustor [Lefebvre, 2010]. In order to achieve maximum swirl within the chamber the swirler was placed as close to the dump plane as possible. Preliminary tests found difficulty in achieving a stable flame, the flame tended to lift significantly above the injection point. In order to combat this problem swirl within the combustion chamber was strengthened by installing a second identical swirler at a location 1” upstream of the dump plane. This greatly improved recirculation within the combustor and resulted in a more desirable flame structure.

After passing through the flow straightener and both swirlers the air is dumped into the expansion chamber. This can also be referred to as the combustion chamber and is the place where the flame is maintained and observed. The area ratio across the expansion, or dump, is 35.37. At an air flow rate of 40 SCFM the bulk Reynolds number is calculated as being approximately 40,000 in the annulus and approximately 10,000 after the dump. Air velocity at the swirler exit is 22.3 m/s, with both axial and tangential components equally 18.6 m/s. Swirler and flow straightener design can be found in Figures 36 and 37.
Figure 34: Test Apparatus

\[ S_N = \frac{2\left(1 - \left(\frac{D_{hub}}{D_{sw}}\right)^2\right)^\frac{1}{3} \tan \theta}{3} \]  

Equation 11
Figure 35: Air Inlet System and Swirler Locations
The downstream portion of the combustor, also referred to as the combustor shell, is shown in Figure 38. This portion of the combustor includes 33 inches of straight chamber followed by a conical exhaust nozzle. This exhaust nozzle (exit cone) resulted in reduced flame stability and increased acoustic behavior within the combustor. Consequently it was removed after initial testing and was not utilized throughout the course of the study.
The downstream portion of the combustor is fitted with a variety of UV grade fused silica windows. This includes three 2.5 x 8 inch camera windows, two 0.5 x 8 inch laser windows, and two 1.5 inch diameter view port windows. These windows are arranged in a configuration that enables Particle Image Velocimetry (PIV) and Planar Laser Induced Fluorescence (PLIF) measurements. The combustor shell is also fitted with a number of 0.5 inch NPT instrumentation ports. In order to improve opportunities for instrumentation in the low flame region one of the camera windows was replaced with an instrumentation plate consisting of six instrumentation ports. This in particular allows for detailed temperature mapping of the flame close to the dump plane. Furthermore, at the combustor shell exit mounts were devised to acquire exhaust NOx and exhaust temperature measurements.

Throughout the course of this study the combustor is operated at atmospheric pressure without fuel or air preheat. However, this combustor is designed to ultimately operate at pressures as high as 10
Bar (147 PSI) and produce as much as 500 kW. As a result the combustor walls were designed to be extremely robust and are composed of 1 inch thick stainless steel. This provides a large factor of safety for high pressure operation but results in some difficulties. The combustor is very difficult to modify because of its thickness, it also has a significant thermal mass that had to be accounted for when developing testing procedures.

The combustor setup is also equipped with an inlet air heater. This industrial heater, manufactured by Chromalox, is capable of heating as much as 1 kg/s of air flow. However, it was not used in this study.

Fuel Injection System

The liquid fuel injection system is dependent upon four main components. These include the pressurizing tank, flow controller, fuel flowmeter, and the fuel injection nozzle. Each component will be addressed separately in the order that they are experienced by the fuel. An overall system diagram is shown in Figure 39.

![Overall System Schematic for the Fuel Supply System](image)

Figure 39: Overall System Schematic for the Fuel Supply System

The first component in the fuel supply system is the fuel holding and pressurizing tank. This is a 10 gallon 316 stainless steel tank dispensing tank. 10 gallons is a good volume of fuel, providing adequate fuel supply for prolonged testing but also enabling ease in batch management when considering a variety of fuel compositions. The stainless steel construction results in a tank that is chemically neutral and provides strength adequate for the 190 PSI pressure rating of the tank. The tank possesses a wide mouth for easy filling. Fuel is pressurized by nitrogen at the top of the tank and is removed through a fuel pickup tube that extends near the bottom of the tank. Tank nitrogen is necessary for pressurization to ensure an inert environment that will not present any risk of explosion within the fuel tank. The fuel tank is also equipped with a bleed valve to depressurize the system. A picture of the fuel supply tank and accompanying nitrogen tank is found in Figure 40.
It is also pertinent to note here that a fuel pumping system was devised and installed to provide a higher pressure fuel supply. This was done using a pump that was purchased prior to the arrival of the current investigators. Despite questions concerning the appropriateness of the pump for this application it was requested that use of the pump be attempted. The results were as anticipated and the pumping system did not perform well, despite requiring a significant amount of design effort and instillation/testing time.

Fuel flow rate was regulated using electronic proportional valves supplied by Hass Manufacturing. These proportional needle valves are controlled by applying a 1-5 V DC control signal which was provided by the Data Acquisition System (DAQ). These stainless steel valves have no gearing between a step motor and the valve stem resulting in zero-backlash. Resolution and range of the valve control system can be selected by the user-defined electronic arrangement within the valve controls. Initial tests utilized a Hass EPV-250-SS which has a Cv of 0.6 and is designed for higher flow rates. This proportional valve was utilized because it was already available in the laboratory. However, after time the model was changed to the smaller EPV-SS-4MG which has a Cv of 0.03 and offers a much higher resolution in flow control than the EPV-250-SS. Both valves have ½ percent resolution over their operating range. Both valves and controls are depicted below in Figure 41.
Flow was monitored through the use of low-flow turbine flowmeters. Initial tests utilized an EQUFLOW PVDF 0045 flow meter. This flow meter utilizes a turbine wheel that is turned by passing fluid. The turbine wheel is monitored by observing the infrared reflection that is returned by the rotating turbine. This pulsing Infra Red signal is then translated into a square wave output which can be monitored by a DAQ system. This meter was initially designed for pharmaceutical and bio-medical applications but is also deemed suitable for continuous use in a laboratory. The flowmeter is capable of operating at 25 bar and allegedly offers accuracy and repeatability within one percent. This meter was selected primarily for its ability to withstand the 200 PSI fuel pressure required and still offer accurate readings of flows between .03 and 2 L/min. The meter is designed to produce 100,000 electrical pulses per liter of water that passes through the turbine. Initial calibrations found that hydrous ethanol produced 104,000 electrical pulses per liter of fluid. This calibration did not change appreciably as water content changed between E100/W0 and E65/W35. An image of the flowmeter is found in figure 42.
The testing of multiple fuel compositions requires the fuel system to be purged with air between tests of different fuel types. The EQUFLOW PVDF was found to be sensitive to this purging process and the flow-tube was easily damaged. Fortunately the modular design of the flow meter allows for the simple replacement of the flow-tube in the incidence of failure. However, as time progressed the repeatability and performance of the EQUFLOW meter was found to deteriorate. This is possibly attributed to the pickup being damaged from exchanging flow-tubes so many times. Faced with the challenge of developing a complex calibration curve to accommodate an unreliable flow meter and confronted by poor support from the EQUFLOW supplier it was decided that a new type of flow meter be installed for the latter portion of this work.

The new flow meter that was selected was provided by Omega Engineering. This turbine flowmeter offered stainless steel construction and produced a 0 to 5 V DC signal that is linearly proportional to the flow through the flow meter. The FLR1009-ST-D provides an accuracy within 1% and a repeatability with 0.2% for flows between 50 and 500 mL/min. This flow rate range is much narrower than the EQUFLOW meter previously used, however, experience has suggested that the entire flow range provided by the Equflow meter is not necessary to achieve quality results. The FLR1009-ST-D is capable of operating up to 500 PSI and comes equipped with a digital display for quick reference of the flow rate without being hooked up to the DAQ system. The 0-5 V signal is more simple to calibrate and interpret in the DAQ system than the pulsed signal employed by the Equflow meter. The FLR1009-ST-D also comes standard with ¼” compression tube fittings making installation and removal easy and eliminating the flow meter from the fuel system during purging procedures. An image of the FLR flowmeter with digital display is shown in figure 43.

![FLR 1009-ST-D Turbine Flowmeter](image)

Figure 43: FLR 1009-ST-D Turbine Flowmeter

Factory calibration of this flow meter considers the use of water as a working fluid. It was necessary to develop custom calibration curves for each fuel to be monitored by this flowmeter because fuel density and viscosity vary with fuel composition and affect the rotation of the flowmeter turbine. Calibration curves were developed for fuel compositions of 0%, 5%, 10%, 15% and 20% water in ethanol by volume. The calibration curves were determined by monitoring both fuel flow rate and meter voltage under different flow conditions and evaluating the linear relationship between all test points. A sample calibration curve is shown in Figure 44. This calibration curve shows initial
calibration points shown in blue and curve verification points shown in red. A linear regression was evaluated to predict flow rate from meter voltage. From this plot it is evident that the relationship developed is a good predictor of actual flow rate.

Figure 44: Sample Calibration Curve for FLR-1009 Flowmeter

The flowmeter generates a voltage that is proportionate to the amount of rotation experienced by the turbine paddle wheel. This amount of rotation the wheel experiences is dependent upon fluid density and viscosity. Both of these properties change as fuel composition changes. While the density and viscosity of ethanol and water are similar there are still differences that can effect flow-meter performance. This was validated by developing calibration curves for E100/W0, E95/W5, E90/W10, E85/W15 and E80/W20. A comparison of the calibration curves is shown in Figure 45. From this plot it is evident that the changes caused by elevated water content are subtle, but consistent. Particularly at higher fuel flow rates it can be seen that the voltage increases as water content increases. This is primarily because the higher density of the water results in more voltage output for a given flow rate when compared to the lighter density pure ethanol. The trend of shifting calibration curve is consistent across fuel compositions and leads to the conclusion that these curves are accurate and relevant. As a result the LabVIEW code is manipulated to reference the appropriate calibration curve as fuel composition varies.
The final component in the fuel supply system is the fuel atomization nozzles responsible for injecting fuel into the combustor. In order to achieve a wide range of equivalence ratios with a variety of fuel compositions it was necessary to achieve fuel flow rates varying from 1.8 to 5.5 GPH. Fuel pressure, as previously described, ranged between 0 and 190 PSI. The objective of the fuel atomizer is to provide rapid atomization and vaporization of the liquid fuel stream in order to produce a stable flame. A variety of fuel injection nozzles were tested in order to ensure that the highest quality of flame structure was achieved. All nozzles tested were pressure-orifice atomization nozzles. This style of atomizer employs the injection of higher pressure fuel into the ambient environment through a single small circular hole. This style of atomizer works particularly well for low viscosity liquids such as water or ethanol. Pressure-orifice atomizers rely on the pressure and velocity difference between the fuel and ambient environment to produce liquid break up and droplet formation.

The three nozzle types considered in initial testing were Parker Hannifin Singlepoint Injection Spraymakers, Delavan Fuel Oil Atomizers, and custom AMFOG Three-Point Foggers. The Parker Nozzles employ the use of a hollow cone spray and come in 11 sizes ranging from .5 to 8 GPH of water at 100 PSI. The droplet size and spray cone angle can be predicted from manufacturer supplied data and is found in Figure 46(parker brochure). This plot predicts that if fuel supply pressure is greater than 100 PSI then the droplet size should be consistently smaller than 25 microns, regardless of which nozzle is being used. It is pertinent to note here that the spray angle for the Parker Nozzles offers some variability between the different sized nozzles.

Figure 45: Calibration Fuels for Different Water Compositions
Figure 46: Manufacturer’s Data for Parker Spray Nozzles; Nominal Flow Rates (top left) Droplet Size as a Function of Pressure (center), Spray Cone Angle (bottom) [Parker Hannifin, 2010]
The second style of nozzle considered, produced by Delavan, focused primarily on controlling the cone angle of the spray. Three nozzles were selected to have a solid cone spray pattern and a constant spray angle of 60 degrees. This spray cone is significantly narrower than the Parker nozzles. These nozzles have nominal flow rates determined with #2 Fuel Oil which is significantly more viscous than the ethanol and water that would be used in this study. As a result of the variation in fluid viscosity no droplet size estimations were available for this nozzle.

The final nozzle that was evaluated was a custom nozzle that was fabricated using three AmFog Misters to produce a single fuel nozzle. The AmFog Misters were selected because of their success in another ethanol fueled combustor operated by the Turbine Innovation and Energy Research Laboratory. These atomizers have a hollow cone spray pattern and deliver a droplet size between 50 and 100 microns. These misters are rated for low volume flows. In order to accommodate the flow requirements of this combustor three atomizers were mounted to the injection stick. This can be seen in Figure 48.

- Assembly of Three Single Point AmFog Atomizers
- SMD is about 50+ Microns
- Solid Cone
- Spray angle 65-75 deg

Figure 47: Delavan Nozzle Specifications

Figure 48: Custom Amfog Atomization Nozzle Specifications
After running ethanol through each of these configurations and observing flame structure it was determined that the Parker solution provided the highest quality in flame structure over a wide range of fuel and air flow rates. The three point injection scheme employed with the Amfog Nozzles proved to be difficult to manufacture, resulted in a high incidence of leaks and failures due to the thin wall thicknesses that were restricted by space requirements, and resulted in a streaking spray caused by the interaction of the three spray cones. The Delavan nozzles provided a beautiful flame structure with an air flow rate of 35 SCFM. However, this flame structure was not stable over a wide range of air or fuel flow rates. The solid cone and narrow cone angle resulted in poor mixing outside of the ideal fuel and air flow rates. In conclusion, the Parker Nozzles were selected because of the abundance of data provided by the manufacturer and the stability that could be achieved over a wider range of fuel and air flow rates. A near complete set of parker nozzles was purchased and size was varied as necessary.

Having established all of the components of the fuel supply system it is important here to describe the details of the fuel system purge process. Since the fuel supply system covers a significant distance it is necessary to purge the system when fuel composition is changed. A complete purge ensures that the behavior being observed is indeed caused by the fuel composition predicted. First the fuel tank is emptied using the fuel bypass system and any nitrogen pressure that remains in the fuel tank. Once the tank is emptied the pressure is relieved and the tank is opened and dried. The fuel flow meter is removed from the fuel line in order to avoid any damage and the fuel flow controller is completely opened. In addition the drain valve located at the base of the combustor is opened. Air is used to purge and dry the fuel lines between the flow meter and combustor as well as between the flow meter and tank. The fuel flowmeter is then reinstalled and the flow regulator is closed. The new fuel is then introduced to the fuel tank and pressurized to not more than 50 psi. The flow regulator is opened slightly, allowing fuel to slowly fill the fuel line. It is important here that the flow regulator is not opened dramatically because a sudden shock of fuel pressure could damage the flow meter. The fuel is allowed to flow until it is seen to bleed from the drain valve at the bottom of the combustor. The drain valve is then closed and the fuel is allowed to fill the fuel stick until spray is injected through the fuel atomizer. At this point the flow regulator can be closed and the fuel tank brought up to operating pressure. The system is now completely purged and fully hydraulic.

Air Supply System

The air supply system for this combustor is designed to deliver as much as 1 kg/s of air at a pressure of 160 PSI. The air is supplied by two continuous duty Atlas Copco Compressors with industrial air driers and an accumulator tank. Air inlet flow is equipped with an electrically controlled regulator produced by Fisher Controls. This regulator is rated for 300 PSI and operates on an adjustable scale, translating a 4-20 mA input signal into the correlating valve position. This regulator was installed during the development of this work but is nonessential to controlling the airflow in this study. The air flow is also equipped with a turbine flowmeter produced by Flowmetrics (FM-32NT1ALD-1030). This flowmeter is equipped with a digital display and can also be wired into a DAQ system. During installation entry length requirements were considered as a function of Reynolds number. This flowmeter also is not utilized in the present study. Throughout the course of this study failure of the industrial air driers resulted in the need for additional conditioning of inlet air. To meet this demand for dry air a Beach F600C air filter and dryer was installed in the air line. This filter is capable of drying 200 SCFM of air at a pressure of 250 PSI. Air flow rate is monitored visually using a Dwyer Rotameter. Flow is controlled through manual adjustment of a Wilkerson pressure regulator and temperature is measured utilizing a Type-K thermocouple probe with digital display, purchased from
It was determined through initial testing and observation of flame structure that all tests would be performed at an air flow rate of 40 SCFM. This air flow rate resulted in the highest achievable quality in flame structure over the range of equivalence ratios and fuel compositions. Evaluating both air and fuel supply systems and performing an uncertainty analysis for the equivalence ratio (ER) calculation reveals that the uncertainty of the ER is less than 5.25% for all equivalence ratios. This equates to a maximum ER error of .0315 at ER=0.6 and error of .0577 at ER=1.1.

Figure 49: Air Supply System Components

**Ignition System**

Throughout much of this study the combustor was ignited by directing a propane torch through one of the instrumentation ports near the dump plane prior to fuel injection. While this method is completely safe for atmospheric tests with liquid fuel it is desirable to have a more advanced method of ignition that can be controlled remotely for use with high pressure, high temperature, or high flow rate tests. In order to meet these demands an advanced ignition system was developed in conjunction with Woodward Governor Company. Woodward Governor was the ideal partner in developing this custom ignition system because of their experience with industrial turbine ignition and controls systems. Initial design requirements required the igniter to ignite an ethanol spray, methane premixed gas, hydrogen premixed gas, and ideally other liquid fuel sprays such as gasoline, jet fuel, diesel, and possibly other oils. The igniter had to tolerate 150 PSI high temperature environments, fit through the 0.7 inch
After meeting with Woodward engineers the 601P742 was selected as the igniter of choice for this application. This igniter, originally designed for use in Siemens gas turbines, met the dimensional requirements for the igniter. The igniter was paired with a 10' ignition lead and 15 kV exciter box in order to provide a 1.5 J spark energy. This spark energy was deemed sufficient to light all of the required fuels (provided that a combustible mixture was present at the igniter tip) and is frequently used in industry for ignition of difficult to ignite fuels such as fuel oil sprays. Woodward agreed to donate the igniter and sell the exciter box and lead at the OEM discounted price. As a result the Woodward igniter is to be mentioned in any publications that utilize the device. Ignition at elevated pressures was considered as a potential procedure for the high pressure combustor. However, the industry experience of the Woodward engineers suggested heavily against such a procedure. As a result low pressure ignition was accepted as standard in combustion test rigs and elevated pressures would not be reached until after ignition was achieved. This decision greatly simplified the design of the retraction mechanism eliminating the need for pneumatic/hydraulic control to actuate the retraction mechanism against combustor pressures. An overview of the retraction mechanism can be seen in Figure 51.

The igniter retraction mechanism isolates the combustion chamber from the ambient environment using a piston that mates to the housing cylinder through a pair of O-ring seals. The piston has chamfered seats for additional sealing at both the fully engaged and fully retracted positions. The igniter is manually placed in the fully engaged position with the combustor at atmospheric pressure. Fuel is injected while the igniter is sparked remotely. Upon ignition the combustor pressure is gradually increased to the operating pressure. The differential between the elevated pressure of the combustor chamber and the lower ambient pressure result in the automatic retraction and seating of the igniter on the second chamfer.

When designing the seal between the piston and cylinder it is critical to consider O-ring design theory to provide a quality seal at the elevated temperatures and pressures. Literature suggests that to
seal a pressure of 150 PSI at exhaust gas temperatures clearance between the piston and cylinder should be between .002 and .005 inches. With this narrow gap it is critical that thermal expansion be considered in design and material selection. After performing the thermal expansion calculations it was concluded that the piston be composed of 430 stainless while the cylinder be composed of 4130 stainless. Stainless ensures corrosion resistance, the variation of alloy avoids galling between the two materials, and since 4130 expands more under temperature than 430 the gap will increase as temperature increases thereby avoiding binding. Two O-rings were employed to provide redundancy to the seal and prevent pressure leaks in the event of any pressure spike caused by sudden combustion events within the combustor. The retraction mechanism components are shown in Figure 52.
Having designed and constructed the ignition system to deliver adequate spark energy and the retraction mechanism to enable safe operation it became critical to determine the optimum location for the ignition point. The design of the high pressure combustor, particularly the 1” thick stainless steel walls, greatly limits the potential locations of the ignition point. The thickness of the combustor wall results in an inability to create a new port specifically for the igniter installation and limits potential ignition points to the existing instrumentation ports. Some flexibility was gained when one combustor window was converted to an instrumentation port. Potential igniter installation locations are shown in Figure 53.

![Figure 53: Potential Igniter Installation Locations](image)

The low ignition location would be ideal for igniting a premixed fuel supply close to the dump plane, but may pose a problem with liquid fuel because of time required for atomization of the fuel. The highest ignition location is the ignition location intended by the combustor designers but is very far downstream from the ignition point. This may result in the combustion chamber filling with fuel before a combustible mixture reaches the ignition point, effectively creating a bomb at the time of ignition. Window mounting the igniter would surely result in effective and safe ignition but would result in the inability to utilize two windows and perform flame temperature measurements at the same time.

To determine the ideal ignition location the igniter was installed at each location and tested with fuels ranging from 0-30% water by volume. It was determined that a window-mounted adapter plate was necessary. The igniter performed excellently when mounted to the window adapter plate. A number of locations on this adapter were tested but the best ignition performance was achieved at an ignition location 1.5” in. above the dump plane for fuels of 20% water or less. Ignition from this location was successful for fuels greater than 20% water but ignition was not ideal. More details are
Thermocouple Probe

In order to evaluate the temperature of the flame and exhaust gas custom Type B thermocouples were employed. Type B thermocouples consist of a 70% platinum 30% rhodium positive lead and a 94% platinum 6% rhodium negative lead. These devices have an operating range of 0-1700 degrees Celsius and offer an accuracy of +/- 0.5% of the reading for temperatures greater than 800 degrees Celsius. Custom thermocouple rakes were fabricated by Gulf Sensors specifically for use with the combustor in this study. A six-thermocouple probe and a four-thermocouple probe were both developed to provide measurements at a range of radial locations within the combustor. Diagrams of the two thermocouple rakes can be found in Figure 54. Both probes feature 1/8” alumina ceramic tubes to give support to the wires, a ½” stainless steel tube for use with compression fittings, and a ¾” expansion tube where the fine thermocouple wires are linked to hafnia insulated lead wires. The four-thermocouple probe is utilized at the exhaust of the combustor to monitor exhaust gas temperature. The six-thermocouple probe mounts within the various diagnostic ports on the combustor shell and is capable of being installed in a variety of axial positions in order to provide for flame mapping opportunities. The location of the thermocouples on the six-thermocouple probe were selected in order to provide a detailed radial profile of temperature within the combustor, extending from the combustor centerline towards the combustor wall. Both probes are linked to NI-USB-9211A data acquisition modules which will be discussed in further detail in the description of the DAQ system.

Figure 54: Custom Thermocouple Rake Specifications
Exhaust NOx Analyzer

NOx concentration in the combustor exhaust was monitored utilizing an fNOx400 system produced by Cambustion Ltd. As previously discussed, NOx is a major pollutant that is controlled and often considered in engine design. It is desirable to reduce NOx formation by lowering local flame temperatures and there is reason to anticipate that such reductions may be had by utilizing hydrous ethanol. This gas analyzer extracts combustion gasses through a ¼” compression tube fitting that is coupled to the sampling head. The sampling head utilizes a Constant Pressure (CP) chamber as an intermediate chamber responsible for eliminating any pressure effects from the measurement process. The fNOx400 system generates ozone which is also piped to the sampling head. As a sample of exhaust gas leaves the CP chamber it enters a reaction chamber where the ozone and sample gas are mixed. When NO is exposed to ozone it the resulting reaction emits light that is directly proportional in intensity to the original concentration of NO in the mixture. A fiber optic cable captures this light and transmits the light to the main control unit where it is measured and NO concentration is calculated. This chemiluminescence method is capable of resolving the NO concentration in a gas sample within 4 ms.

The NOx analyzer was calibrated each time before use. The calibration process involves first zeroing the fNOx400 system by ‘analyzing’ pure nitrogen gas. This gas is NO-free therefore no signal should be detected. The fNOx400 is then utilized to analyze 100 ppm NO gas. By determining the voltage output of the analyzer for 100 ppm of NO it is possible to determine the linear relationship between NO concentration and output voltage. Establishing this relationship allows direct assessment of the sample gas NO concentration when output voltage is known. The analyzer does experience a small amount of drift when it is run for a long period of time so the calibration is periodically checked throughout testing to ensure that the calibration voltage is correct. The analyzer also has the ability to scale the output signal by adjusting the signal gain. This parameter generally does not have to be reset throughout the course of testing. Pictures of the fNOx400 system and the sample head are shown in Figure 55. This system, when operating properly, provides a sensitivity ranging from .1 mV/ppm to 50 mV/ppm in 9 ranges. Linearity should be within +/- 1% over a range of 0-5000 ppm and the noise level should be represented by an RMS value of less than 1% of the mean signal at 1000 ppm. These high levels of sensitivity and repeatability are somewhat difficult to reproduce when the sample gas concentrations are generally less than 30 ppm. Furthermore, this system was 11 years old at the time of testing and some components were not operating within their ideal parameters. The output of this system is monitored and recorded by the DAQ system.

High Speed Camera

This study employs the use of a high speed, high resolution camera to help in optical observations of the flame. The Photron Fastcam SA3 camera is situated to monitor the low-flame region through the 2.5 x 8 inch windows. This camera is capable of resolving 2000 frames per second at a resolution of 1024 x 1024 pixels. Sampling rate can be increased at the cost of resolution reduction. The camera alone is suitable for developing high speed and high resolution images of the flame within the visible light spectrum.
In addition to observing the flame structure through the visible light spectrum it is also beneficial to consider the spatially resolved light emission within a narrow bandwidth. By monitoring the light intensity at a specific wavelength it is possible to detect the presence of specific chemical species within the flame. This concept of chemiluminescence imaging is a common tool in combustion diagnostics. By resolving the spatial distribution of specific intermediate chemical species it is possible to determine the spatial distribution of combustion reactions and consequently heat release. This work utilizes chemiluminescence imaging to monitor the presence of CH* and OH* within the flame. CH* can be taken as an indicator of the onset of combustion [Han et al, 2003] while OH* is primarily formed through CH* oxidation and indicates a later phase of combustion [Najm et al, 1998]. CH* has a strong band at 430 nm and OH* has a strong band at 307 nm. These wavelengths are isolated using Melles Griot narrow band interference filters. These optical filters have a diameter of 50 mm, allow light within +/- 2 nm of the nominal wavelength to pass through the filter. All filters have a FWHM (Full Width at Half Maximum) of 10 nm. In this study water content within the flame will be very high. Therefore it is important to verify that the absorbance of water vapor is not significant at the wavelength of interest. Water absorbance at this wavelength is low and not likely to affect CH* intensity. The absorption coefficient is less than .01 M^-1 where .01 cm^-1 is ‘significant’[Pope et al, 1997].

Once the CH* or OH* filter is installed the amount of light entering the camera is greatly reduced. As a result, light sensitivity becomes critical for generating quality images. In order to amplify the light entering the camera and achieve useful results an optical intensifier was installed. A UVi Invisible Vision intensifier, model 1850-10, was employed to meet these demands. In addition to amplifying light this device also expands the range of the camera system into the near-IR and UV range. The intensifier is capable of achieving greater than 100,000 frames per second. With this complete set up the operator is able to remotely monitor the imaging as a live-feed, adjust the amplification of the signal, and trigger the camera to record data.

By comparing the intensity, or brightness, of the images it is possible to qualitatively compare the light intensity between test points. This qualitative comparison offers insight into the number of
combustion reactions and amount of heat released by the flame, but also gives valuable information concerning the spatial distribution of that heat release. In order to compare one test condition to the next it is critical that the camera settings be identical between cases. F number, intensifier gain, gate time, and focus location are all critical factors in obtaining valid results. All of these settings can be easily duplicated except the focus location. Because the camera must have its focus on the exact same position for each image it is critical that the camera is not moved or adjusted between tests. To focus the camera and coordinate the pixels to a real location a target is used. The target is placed perpendicular to the camera line of site in plane with a flame center plane. The center of the flame passes through the center of the target. By focusing the camera on this target and taking images of the grid it is possible to evaluate the scale and relative location of the features in the flame images. Throughout the course of this study the camera was kept at a focal length 4.5 ft from the flame centerplane. An image of the camera setup can be seen in Figure 56. A wide range of image post-processing tools were also developed in Matlab. These will be discussed in greater detail later in the paper.

Figure 56: High Speed Camera System Components

Photodiode

It is sometimes relevant to measure the intensity of light being emitted from the combustor without consideration for the spatial distribution of light. This can be particularly relevant when performing measurements such as global chemiluminescence intensity comparisons. This study utilizes
a silicon pin Melles Griot photodiode to monitor low-intensity light coming off of the flame. This photodiode is capable of monitoring light intensity over a wide bandwidth (350-1100 nm) with a response time as low as .35 nsec. Photodiode output at 830 nm is approximately .35-.40 A/W. This current signal is converted to a voltage using a Melles Griot Dynamic Range Amplifier. This amplifier is capable of +/- 1% accuracy in all ranges. It receives currents ranging from 1pA to 100 mA and produces a voltage between -2 and 2 V. Signals are all transmitted through BNC cable. Images of the photodiode and amplifier are found in Figure 57. The amplifier has nine different amplification settings that can be adjusted by the turn of a knob. Amplifier output is monitored by the DAQ system. The photodiode is used in conjunction with a CH* filter similar to the lens used with the camera. This filter was rated for 430 nm +/- 2 nm and a FWHM of 10 nm.

![Melles-Griot Photodiode (left) and Intensifier (right)](image)

Figure 57: Melles-Griot Photodiode (left) and Intensifier (right)

**Gas Chromatograph**

Gas chromatography (GC) is a science by which a gaseous mixture is separated and then evaluated for concentration and quality using spectral analysis. During this study the laboratory purchased a 490 Micro GC. This GC is produced by Agilent and is traditionally used for process management and quality control. This GC separates gases on the basis of thermal conductivity and enables the sampling and analysis of a gas stream all in one unit. The Agilent device can be ordered with a variety of different separation columns and heating options, the desired configuration is specified before ordering and the device is configured at the factory. This particular device includes a molecular sieve 5A unheated column and a PPU unheated column. Both columns feature 10 meter entry tube length. The MS column was used for the detection of Oxygen, Nitrogen, Methane and Carbon Monoxide. The PPU column was used to detect Carbon Dioxide. The GC was configured to operate with ultra-high purity helium as the sample carrier gas.

The micro GC is controlled using Agilent EZ-Chrome Single Instrument software. This software is a minimized version of the EZ-Chrome program that has been simplified for the operation of a single instrument. Through this program it is possible to trigger sampling, specify sampling time, control column temperature, monitor gas flow in the columns, and even store calibration curves for various gas species. In order to fully calibrate the micro GC a sample gas from Sigma-Aldrich was used. The gas (mixture no: 501743) contained 15% CO₂, 4.02% O₂, 69.48% N₂, 7.02% CO, and 4.49% CH₄ by volume/mol fraction. The calibration gas was analyzed five times and the results were averaged in order to ensure that the calibration curves were accurate. The calibration curve for each gas was assumed linear and passing through the origin. A sample of the calibration gas analysis is shown in Figure 59. The EZ-Chrome software equates the area under the peaks to the concentration of that gas. This calibration process provided reasonable accuracy to the results and was suggested by the Agilent
representative. Calibration was thoroughly verified by repeatedly analyzing air, a second mixture of Sigma-Aldrich calibration gas, and a sample bomb mixed by the LSU Chemical Engineering Department. The composition of these gases was acceptably predicted with repeated accuracy. The GC was set up to take samples from the combustor exhaust through a 1/8” diameter tube. The small tube diameter was selected in order to reduce the time required to purge the sample line between tests. A picture of the GC set up is shown in Figure 58.

The GC is designed to handle gaseous samples only and cannot process samples that contain liquid. This is a concern when handling combustion gases because water vapor is a known product of hydrocarbon combustion. Water vapor concentrations will also be particularly high when burning hydrous ethanol because of the relatively high water content that is present in the fuel. The water will be in vapor form when the sample is collected from the combustor but it is expected that some condensate will form as the sample is cooled in the small tubing of the GC. This condensate has the potential to interfere with the GC analysis, make the calibration curves invalid, and even damage the GC. Two solutions were devised in order to combat this problem. The first solution, proposed by Chemical Engineering, entailed the use of a heating tape to keep the temperature of the sample above the saturation temperature prior to injection into the device. This method would presumably prevent condensate from forming in the tubing. The second method, proposed by Agilent representatives, required the purchase of a 170 Genie Filter which would use a selectively permeable membrane to separate any liquids from the sample prior to injection into the GC. The heating method was the required method because Chemical Engineering has joint ownership of the device. The Genie Filter was purchased and kept on hand in the laboratory as a backup. A diagram of the heating system is shown in Figure 60. The heating tape was equipped with feedback control that applied heat whenever the feedback thermocouple read a temperature less than 105 C. This type J thermocouple was mounted as

![Figure 58: Gas Chromatography System Components](image)
close to the GC injection point as possible. While operating with this setup it was observed that the
temperature of the sample at the injection point never was heated above 29°C despite installing the
heating tape as closed to the GC inlet as was deemed safe. This low temperature was a result of the
rapid temperature drop experienced by the small diameter sample tube (1/16") as it passed through an
unheated environment.

Figure 59: Sample Analysis of GC Calibration Gas

Figure 60: Diagram of GC Sample Heating System
After considering the heating setup it became apparent that the temperature of the sample would quickly drop below the saturation temperature even if the sample were successfully heated until the GC inlet. Because of the danger of condensation it was determined that the GC would be backflushed after each sample. This backflush feature results in back flow through the GC columns after the sample is analyzed and helps to remove any moisture from the column. The effect of water accumulation on the GC reading was evaluated by checking the calibration gas after each set of data. Accurate analysis of calibration gas before and after a data set ensures that the sample was analyzed accurately. Water accumulation in the column resulted in a slow and gradual drift in the reading of the calibration gas. Once the calibration gas was not accurately resolved within .5% for CO₂ the calibration was no longer deemed accurate and a system bakeout was required. Considering .5% accuracy for the CO₂ as the limit for a good calibration results in even higher accuracy for the other gas species. GC bake outs were performed by raising the temperature in all columns to greater than 100 C and allowing the columns to remain at that temperature for 3-5 hours. This removed accumulated water and restored the accuracy of the calibration. Baking out resulted in shifts of species’ peak locations and required manual manipulation of the analysis method in the EZ-Chrome software. In conclusion, frequent checks of the calibration gas ensured accuracy of the results and allowed for protection of the GC through effective use of the bakeout function.

**Hot-Wire Anemometer**

Velocity and turbulence intensity measurements in this study were performed using a constant temperature hot wire anemometer, the IFA-300, produced by TSI. This device measures fluid velocity by exposing a small heated element to the fluid and monitoring changes in heat transfer. The probe is held at constant temperature and the amount of electrical power required to match the heat loss is monitored by an accompanying PC. The probe is composed of thin-film platinum and allows for a time response as short as 3 microseconds. Sensors are also very small, resulting in minimal disruption of the natural flow structure. Figure 61 shows a diagram of the hot-wire anemometer system.

![Hot-Wire Anemometer System Diagram](TSI)

Figure 61: Diagram of Hot-Wire Anemometer System [TSI]
Once heat transfer is known it can still be difficult to determine the fluid flow velocity because of variations in temperature and heat transfer properties of fluids, as well as inconsistencies from one probe to the next. In order to overcome this obstacle a detailed calibration procedure is utilized. The probe is exposed to a standard air flow through a calibration nozzle. Temperature is measured and the heat transfer is recorded for a range of flow velocities. Once the calibration curve is determined in this position the probe is then repositioned and the procedure repeated for a variety of positions relative to the flow. TSI has developed software capable of resolving these calibration curves to determine the absolute and componential velocity of the fluid flow. This software considers changes in fluid temperature. Turbulence intensity can be evaluated from a set of velocity measurements based upon the definition of turbulence intensity found in Equation 2.

Once a particular probe is fully calibrated it is possible to evaluate the magnitude and orientation of velocity vectors within a flow field. As the probe is positioned in different locations within the flow field and the data points are recorded a complete picture of the flow-field can be constructed. To save time it is critical that the locations of velocity measurements be determined strategically. It is often possible to utilize information about the velocity field to make inferences about the thermal-fluid system and in some cases CFD models can be validated with anemometer data.

**Data Acquisition System**

A data acquisition and controls system was necessary because of the variety of instruments and controls that are needed to fully manipulate and monitor the test apparatus. The purpose of this acquisition system to is first of all to provide real-time control of the combustor performance by controlling the equivalence ratio. Controlling the equivalence ratio amounts to controlling the fuel flow rate since air flow-rate is held constant in order to ensure a consistent velocity field within the combustor. The second purpose of the DAQ system is to monitor and record measurable such as the flame temperature, exhaust temperature, NOx concentration, and photodiode output. Camera controls are controlled by the same computer but through independent software that was purchased. The hot-wire anemometer system and micro GC system are both standalone systems that operate with their own computers and data acquisition boards. Although not included in this study, long-term goals of the DAQ system include controlling air flow rate electronically, controlling the air pre-heater, and monitoring combustor chamber pressure. It was determined early on that the controls and DAQ programming would be done using LabView. LabVIEW (Laboratory Virtual Instrumentation Engineering Workbench) is a visual programming language that was developed by National Instruments. LabVIEW is the industry leader for data acquisition, industrial control, and industrial automation. National Instrument hardware was also selected because of its compatibility with LabVIEW software and the high quality of user support available. The DAQ and control boards that were selected were two USB-9211A Thermocouple Input Modules and one USB-6343 X-Series Multifunction Board. The USB-9211A modules were selected specifically for use with the Type-B thermocouples. These devices each were capable of monitoring four thermocouples with high resolution of 24 bits. Two boards provided the capability of monitoring eight thermocouples in high resolution. This covered the need to monitor two exhaust temperatures and all six thermocouples on the low-flame temperature probe. While the high resolution limited the sampling rate to 12 samples per second these devices are ideal for temperature measurements which are not expected to change rapidly but will cover a wide range of temperatures. The 9211A devices communicated to the computer through USB connections resulting in
a system that could be easily switched from one computer to the next if need be. These devices were also particularly appealing because they have a legacy within the TIER laboratory.

The USB-6343 device was selected to monitor all other instruments and provide output controls. This device is capable of receiving sixteen analog inputs at a resolution of 16 bits and sampling rate of 500,000 samples per second. This high sampling rate is appropriate for monitoring characteristics such as NOx concentration, light intensity, and chamber pressure. The four analog outputs allow for 16 bit control at a rate of 900,000 samples per second. Having four analog outputs makes simultaneous control of fuel flow rate, air flow rate, inlet air heater, and auxiliary fuel pump a possibility. In this study fuel flow rate is the only feature controlled electronically; air flow rate is controlled manually and the inlet air heater and auxiliary fuel pump are not used. The USB-6343 also has ability to monitor four counters with 32-bit resolution and 100 Mhz sampling. This enables the use of any pulsing meters such as the EQUFLOW turbine flow meter. In addition the DAQ has the ability to monitor 24 digital I/O signals. This enables the control of several on-off functions that include heaters or safety switches. As the name suggests the device communicates via USB making it a versatile device should the PC need to be changed or modified. Both types of DAQ boards are depicted in Figure 62.

Once the controls hardware was selected it was necessary to develop a system network that links the instrumentation to the computer by connecting them to the appropriate terminals on the board. A network map is critical for referencing the right terminals when programming in LabVIEW. A diagram showing all of the active components of the instrumentation process and their links is shown in Figure 63. The correlation between the physical DAQ channels and the corresponding software label is catalogued in Table 2.
Figure 63: Diagram of Instrumentation System Components

Table 2: DAQ System Instrumentation and Corresponding Physical Channels

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Having established the physical configuration of the DAQ system the next step in becoming operational is to develop the LabVIEW program and the virtual control panel. For the ease of programming two separate LabVIEW codes were developed. One code was designed to monitor and record the high-sampling rate measurements within the combustor and the second was to monitor the low-sampling rate measurements. Each of these codes allows the continuous monitor and adjustment to equivalence ratio. The codes cannot be run at the same time allowing for more focus on each specific measurement. The control panels allow for real-time monitoring of the measurables. The low-frequency program samples data at a frequency of 2.4 Hz. This sampling rate is limited by the larger amount of data being collected through the USB-9211A. This program, whose virtual panel is shown in Figure 64, monitors all eight temperature measurements and exhaust NOx concentration. It exhibits real-time control of the fuel flow rate and allows for online adjustments to the NOx calibration curve. This code also allows for data logging to a specified directory at the touch of a button.

![Figure 64: Low Sampling Rate Data Acquisition LabVIEW Panel](image)

The second program that was developed samples data at 5 kHz and monitors chamber pressure and photodiode response. This program is also equipped with real-time online control of the fuel flow rate and monitoring of the equivalence ratio. Similarly, data can be logged to a specified directory. It is relevant to note here that the equivalence ratio calculation considers air flow rate, air inlet pressure, and air inlet temperature. Percent of water in the fuel is also considered when calculating the equivalence ratio. Monitoring the EQUFLOW flowmeter proved to be particularly difficult feature to implement. The pulsed output signal required some complex programming mechanisms and advanced use of the DAQ counter feature. The analog output of the FLR1009 flowmeter was much more straightforward to include in the LabVIEW code.
Figure 65: High Sampling Rate Data Acquisition LabVIEW Panel
TESTING AND MEASUREMENT PROCEDURES

Test Conditions

As was previously discussed, the main variable of this work is the water content present in ethanol fuel. Alcohol proof ranged from 200 to 120 proof ethanol in water. Fuel composition is denoted in the form EXX/WYY where XX and YY are the relative volume percentages of ethanol and water in the fuel. For example, E100/W0 represents 100% ethanol and 0% water or 200 proof ethanol, while E75/W25 represents 75% ethanol and 25% water or 150 proof ethanol. The fuels tested in this study were E100/W0, E95/W5, E90/W10, E85/W15, E80/W20, E75/W25, E70/W30, E65/W35, and E60/W40. When testing with E60/W40 a stable flame could not be achieved within the test apparatus. Therefore an alcohol proof of 120 was taken to be the minimum alcohol proof for effective combustion in the test apparatus. The first portion of the study, presented in the 2011 ASME Power Conference [Breaux et al, 2011], considered exhaust temperature and exhaust NOx measurements for all fuels with ethanol content greater than 130 proof. Flame temperature measurements were performed and temperature maps were developed for E100/W0, E95/W5, E90/W10, E80/W20, and E70/W30. This type of measurement was not performed for all fuel compositions because of the time consuming nature of the technique.

Following the completion of the first study a second study was published concerning the chemiluminesence properties of the flame, 2011 ASME IMECE Conference [Breaux et al. 2011]. Based upon the findings of the first study, the second study observed a narrower range of fuel compositions. Fuel alcohol proof was limited to fuel mixtures greater than 160 proof ethanol. This saved time in testing by restricting the test matrix to the critical fuel compositions. This limited range of water contents was also used when developing GC results.

For each fuel composition a range of equivalence ratios were tested. Target equivalence ratios included 0.6, 0.8, 1.0, and 1.1. These air to fuel ratios were selected to represent extremely lean, lean, stoichiometric, and rich test conditions. By selecting ERs over a wide range it is possible to draw detailed conclusions concerning the affects of elevated water content over the entire operating range of the combustor. The equivalence ratio was limited on the rich end by increases in flame length. Regardless of water content, increasing the equivalence ratio greater than 1.15 resulted in re-ignition of the exhaust gas as it is exposed to excess oxygen. This decreased the ability to perform affective exhaust gas measurements. In some cases of elevated water content a stable flame could not be achieved at lean equivalence ratios. The reasons for this are discussed in detail later, but for now it will suffice to say that elevated water content lead to lower quality fuel vaporization and consequently lean test conditions could not be stabilized. Table 3 shows all test points that were evaluated. Recall that air flow rate is held constant at 40 SCFM for all tests, therefore a change equivalence ratio implies a proportionate change in fuel flow rate.

Table 3 also specifies a particular nozzle for each test condition. Nozzles A, B, C, and D specify nozzles with nominal flow rates of 2.0, 2.5, 3.0, and 3.5 GPH at 100 psi, respectively. Nozzle variability is a necessity because of the large variation in fuel flow rates across the test matrix. A flow rate of 1.8 GPH is required to achieve an equivalence ratio of 0.6 with E100/W0 while a flow rate of 5.5 GPH is required to achieve an equivalence ratio of 1.1 with E65/W35. If nozzle A were to be used for all test conditions the maximum fuel supply pressure of 190 psi would not be adequate to meet the 5.5
GPH requirement. If nozzle D were to be used for all test conditions the fuel pressure would be extremely low at a flow rate of 1.8 GPH. This would result in poor atomization and spray quality and consequently a very poor spray structure. Nozzle selection is determined upon visual analysis of the flame structure, fuel pressure restrictions between 75 and 180 psi, and an estimated droplet size that is consistently between 17.5 and 27.5 microns (Sauter Mean Diameter). Visual analysis of the flame structure involved testing multiple nozzles at each test condition and evaluating which nozzle provided the most stable structure. Fuel pressure was monitored using a fuel pressure gauge mounted at the base of the combustor. Droplet size estimates were determined from manufacturers’ performance curves, seen previously in Figure 46.

Table 3: Test Points and Nozzle Selection for Each Test Condition [Breaux et al, 2011]

<table>
<thead>
<tr>
<th>Fuel Composition</th>
<th>Equivalence Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.6</td>
</tr>
<tr>
<td>E100/W0</td>
<td>A A A C</td>
</tr>
<tr>
<td>E95/W5</td>
<td>A A A C</td>
</tr>
<tr>
<td>E90/W10</td>
<td>A A A C</td>
</tr>
<tr>
<td>E85/W15</td>
<td>A A A C</td>
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<tr>
<td>E80/W20</td>
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<td>E75/W25</td>
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<tr>
<td>E70/W30</td>
<td></td>
</tr>
<tr>
<td>E65/W35</td>
<td></td>
</tr>
</tbody>
</table>

Fuel Mixing

The hygroscopic nature of ethanol was previously discussed as a concern when considering the shelf life of the fuel. During experimental investigations testing was sporadic. Long gaps were often required between tests in order to develop infrastructure and analyze results. These long periods of inoperation inherently put the fuel at risk for obtaining moisture from the air. Several measures were taken to combat the hygroscopic nature of the fuel. Fuel was purchased in five gallon sealed carboys at a concentration of 190 proof (E95/W5) and was kept sealed until the time of use. Fuel would be opened and then directly relocated to the fuel tank. In the fuel tank distilled water was added in the correct proportion to achieve higher water content fuels. Ethanol and water are miscible in all proportions so the addition of water to 190 proof fuel does not require any complex mixing process. The fuel system was purged as discussed previously and the fuel tank was sealed in an inert environment to prevent additional water absorption. Pure 200 proof ethanol was also purchased in sealed 1 gallon bottles for the E100/W0 test. In order to facilitate effective fuel mixing a calculation template and standard mixing procedures were devised.

Combustor Operation and Data Collection Procedures

Typical combustor startup and shutdown procedure involves set-up, ignition, data collection, and
shut-down. Set-up includes fuel mixing and fuel system purging as previously discussed. The air-flow is adjusted to the 40 SCFM standard flow rate. This rate is monitored manually throughout combustor operation. Some fluctuations and drift are often observed in the air flow rate as a result of different users tapping into the compressed air supply. Test preparation also includes starting up any instrumentation required for the test at hand. This includes loading the virtual control panel for the DAQ system and entering the general parameters for the test. These parameters include the air flow rate, fuel composition, air inlet temperature, and air inlet pressure. The exhaust hood is also powered up to ensure a safe working environment.

Combustor ignition is accomplished by lighting a propane torch, placing it near the fuel injection point, and then opening the fuel regulator to allow enough fuel to reach equivalence ratio of .8. The propane torch is then removed from the combustor and the port is plugged to prevent air leakage. Fuel flow rate is then adjusted via the DAQ system to achieve the desired equivalence ratio. Instrumentation is monitored and the data is recorded as is necessary. The combustor is shut down by closing the fuel flow regulator and thereby stopping the fuel flow. Starved of fuel the combustion ceases.

Shutting down the combustor involves increasing the air flow and allowing to run until the combustor shell becomes cool to the touch. The fuel safety valve is manually closed to prevent any fuel flow in the case of electrical malfunction. While the combustor cools all instrumentation and electronics are shut down. Pressure in the fuel tank is released by opening the pressure relief valve which bleeds pressure from the top of the tank, leaving all fuel in the bottom of the tank. Once the fuel tank is bled the exhaust hood can be shut off. Once the combustor shell is cool to the touch, air supply is closed.

Reaching Steady State and Ensuring Repeatability

Initial tests revealed poor repeatability between tests under presumably identical test conditions. A detailed look at the non-repeatable data revealed that tests that were performed later in the test series exhibited higher flame temperatures, exhaust temperatures, and exhaust NOx concentrations. This increase from one test to the next was attributed to the increased temperature of the combustor shell. As a large mass of stainless steel (recall wall thickness of one inch) the combustor shell has a large capacity to store thermal energy. As the combustor walls heat up the heat rate being absorbed by the walls decreases. This decrease in heat lost to the combustor walls causes changes to the measurables. Under some conditions it is even possible for the combustor walls to add heat to the flame as the walls cool. The obvious solution to obtaining repeatable data would be to allow the combustor shell to reach a steady state condition where the heat being gained from the flame is equal to the heat being absorbed by the ambient environment. However, with the large thermal mass of the combustor this technique is not practical. The combustor would take longer than 30 minutes to reach full steady-state condition, this long duration of testing places a large amount of thermal strain on the instrumentation and controls. Furthermore, fuel consumption costs would be tremendous and testing time would make extensive testing extremely time consuming and difficult. The characteristics of the steady state condition would have to be evaluated for each test condition.

An alternative solution to achieving fully steady-state heat transfer to and from the combustor shell is to consistently collect data at the same state within the heat-up procedure. Observation of the flame and exhaust temperature with respect to time revealed that, for a given test condition, the instrumentation observed a rapid increase in temperature. The rate of increase gradually was seen to decrease or ‘level off’ as changes in heat flux to the combustor shell became much less
rapid. This region of relatively gradual change in heat transfer rates was deemed a ‘quasi-steady’ period of combustor operation and was found to appear consistently after about 2-3 minutes of combustor operation at steady test conditions. It was also determined that multiple ‘quasi-steady’ test conditions could be achieved if tests were performed in order of increasing equivalence ratios. Allowing approximately two minutes between data collection points and never decreasing equivalence ratio results in a step-ladder of increasing temperature within the combustor. By monitoring temperature and NOx data over the entire test it is then possible to select the data that represents these ‘quasi-steady’ conditions and use that to develop trends and draw conclusions. Utilizing this method the data collection procedure became highly repeatable. Sample data is seen in Figure 66. This plot also exhibits a significant number of fluctuations before the ‘quasi-steady’ state is reached. These are largely caused by adjustments to the fuel flow rate required to achieve the desired ER.

**Achieving ‘Quasi-Steady’ State and Selecting Repeatable Data**

![Achieving ‘Quasi-Steady’ State and Selecting Repeatable Data](image)

**Figure 66:** Example of Combustor Heat Up and Data Collection Procedure

Because obtaining repeatable results is dependent upon evaluating test points in order of increasing equivalence ratio the combustor must be allowed to cool before a low equivalence ratio test is repeated. The combustor is allowed to cool until re-ignition can be performed without danger of being scalded by the hot combustor shell. This cooling process typically takes 45 minutes when the outside of the combustor is subjected to natural convection. In order to reduce cooling time and improve testing efficiency a forced cooling system was fabricated and installed. This system uses compressed air and serpentine tubing to cover the entire combustor shell. Heat transfer away from the combustor is improved by directing impinging jets at the combustor surface. The cooling system is shown in Figure
67. The addition of the cooling system allowed the cooling time to be reduced to 30 minutes. This procedure of achieving ‘quasi-steady’ state conditions followed by periods of combustor cooling was followed for all measurements, including optical and GC measurements.

Figure 67: Combustor Cooling System
RESULTS AND DISCUSSION

Throughout the course of this study a very wide variety of measurements were performed. As a result, the study was broken into several smaller studies, or stages. The results will be presented and discussed in the order that they were obtained in order to build the knowledge base and gradually paint a complete picture. The four stages of this study are Pre-study, Sub-Study 1, Sub-Study 2, Sub-Study 3, and Sub-Study 4. The pre-study presents results that provide insight relevant to understanding the combustion processes within the combustor but do not entail monitoring the actual combustion process. Sub-study 1 considers flame and exhaust temperature measurements, Lean Blow Out (LBO) measurements and exhaust NOx analysis. Sub-study 1 was presented at the ASME Power 2011 conference. Sub-study 2 considers optical diagnostics of the combustion process. This includes CH* and OH* imaging, processed camera data, and photodiode data. The more relevant portions of sub-study 2 were presented at the ASME IMECE 2011 conference. Sub-study 3 includes gas chromatography measurements. Sub-Study 4 considers temperature and CH* measurements taken near the flame tip. Life-Cycle analysis for hydrous fuel is also included.

Pre-Study: Hot-Wire Anemometry and Ignition Study

Hot-Wire Anemometry

Velocity measurements were performed in order to gain an understanding of the flow field within the combustor. This understanding of the fluid flow and turbulence characteristics will give insight into the affects fluid dynamics may have on air-fuel mixing and flame structure. This information can also be used in the future to validate any computational models of the combustor that are developed. By comparing the CFD results for non-reacting flows to the experimental results it is possible to gain confidence in the CFD model without activating the full complexity of the model. In order to characterize the flow field it was determined that radial velocity profiles would be developed at three different axial locations within the combustor. A diagram of the measurement locations is seen in Figure 68.

The first method used to evaluate the velocity profiles was by using a 5-hole Pitot Tube. This instrument, produced by United Sensor, is a pitot tube capable of resolving three-dimensional velocity components in a cross flow. After taking and evaluating the raw data it was found that the velocity magnitude in the flow was too low for this instrument to be effective. Pressure readings from the pitot tube were extremely small and the large error associated with the readings resulted in an inability to accurately calculate the flow field velocity. After experiencing a failure with the multi-dimensional pitot tube, hot wire anemometry was considered.

The hot wire system was described in detail previously. Because of the complexity of calibration with multi-dimensional probes, a one dimensional probe was selected. In order to ensure accurate results from the 1-D probe, the swirler was removed from the combustor inlet. The resulting flow field around the probe would consist of an axial and radial component, but due to symmetry would not contain a tangential velocity component. The 1-D probe was oriented to monitor the resultant of these two velocity components. A diagram is shown in Figure 69. After carefully calibrating the probe velocity measurements were taken three times at each measurement location. Results are shown in Figure 70. Error bars indicate the repeatability of the measurement and suggest that repeatability is very high near the dump plane but variability in the measurement gradually increases as the measurement
moves farther downstream. This is because viscous dissipation leads to increased turbulence intensity in the flow as it moves towards the combustor exit.

Figure 68: Hot-Wire Measurement Locations

Figure 69: Hot Wire Anemometer Velocity Triangle
From these plots it is evident that velocity gradients are very steep around the air inlet. Considering the axial location closest to the dump plane, plotted in blue, it is found that velocity is highest near the center of the annular air inlet. The annular air inlet covers the radial space between 0.4375 inches and 1 inch. The low flow that is found along the combustor centerline is caused by the bluff body and recirculation about the fuel injection point. At radial locations outside of the annular air inlet the velocity is found to decrease rapidly to near zero. As the axial distance from the dump plane is increased (marching downstream) the velocity profile was found to flatten. This is due to viscous forces and the dissipation of the higher velocity region into other radial regions.

Considering the turbulence intensity at the same measurement locations we find the result shown in Figure 71. Turbulence intensity was defined previously in this work. This plot reveals that, without swirl, the turbulence intensity is between 7.5% and 15% at the center of the combustor. Turbulence intensity increases as radial position increases. Turbulence increases within the shear layer between the annular air inlet and the stagnant dead space in the corner of combustor. At radial positions greater than 1” the turbulence intensity is greater than 35%. This extremely high turbulence intensity is calculated because the velocity magnitude is very low in this region, small fluctuations represent a very large percentage of the total velocity magnitude. Considering that the minimum turbulence intensity within the combustor is greater than 5% it is reasonable to assume that mixing quality in the combustor will be good.

With the addition of swirl it is found that the velocity gradients near the dump plane are increased. This is because of the increased recirculation caused by the swirling flow. Far from the dump plane the velocity gradients are reduced because the enhanced swirl results in more viscous dissipation and more thorough mixing by the time the flow has moved far from the dump. With the
swirler installed the turbulence intensity is greater than 25% at all locations. This high turbulence intensity will result in effective mixing of fuel and oxidizer and result in flame stabilization.

**Turbulence Intensity**

![Turbulence Intensity Chart]

**Figure 71: Turbulence Intensity near the Combustor Centerline, Swirler Removed**

Ignition Study

The addition of water to ethanol increases the energy required for ignition. A study was performed to evaluate the ignitability of hydrous ethanol. Advanced ignition controls were not available and the test apparatus was not designed to test ignition, but simple tests could still be performed. In addition to possessing practical flame stability and heat release characteristics hydrous ethanol must also offer practical ignitability. The fuel should be ignitable with standard industrial igniters if changes to ignition infrastructure are to be avoided. Ignition of hydrous ethanol was easily achieved at all water concentrations through the use of a propane torch. However, ignition with a spark igniter is more difficult because the region of ignition and energy delivered are much less than with a torch. Ignition of all fuel compositions was attempted using the Woodward Governor ignition system. Fuel was injected at 5% intervals of water content and the spark plug was activated continuously until ignition was achieved. The number of sparks before ignition was counted and recorded. This process was repeated for a range of ignition equivalence ratios at three different ignition locations. Locations, labeled 1, 3 and 5, are located 1.25”, 4” and 6.75”, respectively, above the combustor dump plane.

The igniter was tested at ignition equivalence ratios ranged from 0.5 to 1.1 for fuels ranging from E100/W0 to E70/W30. The ignition probability was calculated by dividing the number of sparks that led to ignition events by the number of total sparks. Results for location 1 and 5 are shown in Figures 72 and 73. These contours show a clear relationship between fuel equivalence ratio and ignition probability. Richer mixtures are more likely to ignite than lean mixtures for all fuel compositions and locations. This is true because a rich mixture will have a larger fuel vapor pressure at the igniter tip. Vapor pressure is boosted by the higher concentration of fuel in the mixture and also by the higher fuel pressure required to inject a larger volume of fuel. Ignition is found to be adversely affected as a result of water addition. This is expected because additional water acts a heat parasite and leads to undesired quenching of the ignition kernel.
To some extent it is possible to overcome the negative consequences of elevated water content by increasing the ignition equivalence ratio. It is also pertinent to note that, while ignition probability is greatly reduced by adding water, it is still relatively high when compared to industrial ignition applications. An ignition probability of .25 means that 25% of sparks will result in an ignition event. On average this means that four sparks are required per ignition event. This is not an unreasonable number of sparks especially when it is considered that industrial burners and turbines do not experience particularly frequent ignition. From these plots it can also be seen that location 1 enables higher ignition probabilities than location 5. This is because fuel atomization is excellent at the edge of the fuel spray near the injection point. Lighting the mixture near the fuel-oxidizer transition period leads to increased probability of success. In conclusion, it is seen that water content reduces the probability that a spark will lead to combustor ignition. This reduction can be offset by increasing ignition equivalence ratio. Despite reductions in ignition probability the fuel is still reasonably easy to ignite and offers practical
Sub-Study 1: Flame Structure, Lean Blow Out Limit, Flame Temperature, Exhaust Temperature and Exhaust NOx

Flame Structure

Photographs were taken of the low flame region using a digital camera. This camera was neither high resolution nor high speed and pictures are only included to give a visual representation of the flame structure. Images of the flame structure at a number of test conditions are included in Figure 75. Images were taken through the low flame window and provide a limited view of the flame. However, from these images it is plain to see that flame structure is relatively consistent between test conditions. The color variability between test conditions is of no particular significance and is more a result of poor camera quality than of actual changes in flame color. From this figure it is evident that the flame becomes longer and more robust as equivalence ratio increases. The flame also becomes more ‘wispy’ and longer as water content increases. These changes will be analyzed in greater detail throughout the study, while the current figure is presented to offer a frame of reference for the reader. It is important to note that for water contents less than 35% by volume it was possible to obtain a stable flame with a conical base that is not lifted appreciably above the point of fuel injection.

Taking pictures of the flame from obscure angles it is possible to view two competing flame structures. The flame consists of a well stabilized, tulip-shaped structure located near the point of fuel injection as well as a less stable donut shaped structure that hovers around the tulip shaped structure. These structures can be seen clearly in Figure 74 and are reinforced later with CH\* images. Both structures are present at each test condition but their relative strength changes indicating some competing effects between the two structures.

![Competing Flame Structures E95/W5 ER=0.6](image)

Figure 74: Competing Flame Structures E95/W5 ER=0.6
Figure 75: Images of Flame Structure for Various ER and Water Contents
Lean Blow Out Limit

It has been previously hypothesized that increasing the water content of ethanol fuel would decrease the stability of the flame. This hypothesis is based on the presumption that increased water content at a constant equivalence ratio will result in lower flame temperatures and an increased volume of fuel to be vaporized by the flame. In many cases it is pertinent to know the lowest equivalence ratio that is capable of producing a stable flame. This is particularly relevant in power generation applications such as boiler or industrial gas turbine applications where engines may be run near their lean limit in efforts to conserve fuel and reduce pollutant formation. The lower limit of equivalence ratio is referred to as the Lean Blow Out (LBO) limit because at mixtures more lean than the LBO the flame will extinguish or ‘blow out’. A large amount of work and a large number of studies have invested in understanding and predicting LBO in flames because in industrial applications flame extinction events can be costly. When evaluating the practicality of a new fuel it is important to consider the lean limit of that fuel. A lower lean limit is desirable because it implies a wider range of combustible equivalence ratios and greater flexibility in engine operating range. It is important to establish the combustible range for a given fuel in order to predict the range engine operability.

The LBO of the flame was evaluated as fuel water content varied, resulting in a relationship between the water content and the minimum ER that is achievable before flashback or flame lift occurs. LBO limit was determined through a specific and highly repeatable procedure. First a stable flame was achieved with equivalence ratio significantly greater than the LBO. Fuel flow rate was gradually reduced until flame structure was lost. Two modes of flame structure failure were observed. Flame lift describes a case where the low-flame region was extinguished, this is the first stage of flame blow off. The second mode of failure was a form of flashback that occurred when the recirculation of fuel allowed the flame to stabilize below the fuel injection point. Both of these cases were viewed as a failure to achieve a stable flame structure and are thus considered outside of the operating range of the fuel. Pictures of a stable flame, a lifted flame structure, and a flash-back flame structure are shown in Figure 76. The equivalence ratio at which the flame loses structure was recorded as the LBO. This procedure was repeated several times with each nozzle for each fuel composition.

It was observed that, for a given fuel composition, the lower limit of flame stability varied depending upon what nozzle was selected. Larger nozzles generally result in a higher LBO limit because at low fuel flow rates the fuel pressure is very low, resulting in breakdown of the spray and poor atomization. Smaller nozzles cannot be used for all fuels because the required flow rate could not be achieved within the window of practical fuel pressures. Because of these restrictions nozzle variability was a necessity in this study. Figure 77 presents the results of the LBO study. This plot demonstrates not only the effect of water content on LBO but also the effects of nozzle selection. The most meaningful plot in this figure is the ‘Minimum Nozzle’ trend. The nozzle selection criteria for obtaining this relationship was the utilization of the smallest nozzle capable of achieving a stable flame at one of the established test conditions of ER=0.6, 0.8, 1.0, or 1.1. It should be noted that this plot shows that for some fuel compositions, such as 0%, 5% and 10% water content, the lower limit of stability is below the theoretical flammability limit of 0.5 [Breaux et al, 2011]. This is because, while global equivalence ratio will theoretically not allow for a stable flame, local mixing effects result in a local equivalence ratio that is within the acceptable range for achieving a flame.
Figure 76: Depiction of Typical Stable Flame (left) Lifted Flame (center) and Flashback (right) Flame Structures

Figure 77: Lean Blow Out Limit as a Function of Water Content
From this plot it is evident that the LBO limit predictions are very repeatable. The range of repeatability is shown by the error bars. From the ‘Minimum Nozzle’ data it is clear that in general the LBO limit increases as water content increases. This verifies what intuition suggests. The water acts as a heat sink and effects fuel vaporization. As water content is elevated the volume flow rate of the fuel must increase to maintain the same equivalence ratio. Due to the increased flow of water molecules the heat required to vaporize the fuel increases. Therefore more combustion reactions are required to meet the demand of vaporizing heat. This means that a higher molecular flow rate of ethanol is required to sustain a combustion reaction and the minimum requirement for equivalence ratio increases.

It is interesting to note that LBO limit is found to decrease when fuel composition changes from E100/W0 to E95/W5. This is contradictory to the general trend and indicates that the addition of water to the fuel in low levels may actually decrease the lower limit of operation and stabilize the flame. While not quantified, it was noticed during testing that E90/W10 and E95/W5 flames were more stable than E100/W0 flames during events of changing air flow (during adjustments to the air flow rate). It is known that the addition of water in reduces the flame propagation velocity within the mixture. It is hypothesized that this reduced burning rate leads to increased flame stabilization because the delayed burning rate prevents local extinction caused by fuel starvation in fuel lean regions. It also may be possible that the addition of water vapor simply leads to increasing the amount of hot vapor in the reaction zones, resulting in a more uniform temperature distribution and increased stability. Information from additional diagnostics are required to draw definitive conclusions.

Flame Temperature

As water content was varied temperature maps were generated within the base of the flame. Using the six thermocouple temperature probe flame temperature was recorded at 24 different locations in a plane through the flame centerline. The resulting 5” by 6” image was then mirrored across the flame centerline to give an accurate temperature map of the flame base. This allows for visualization of flame ‘hot zones’ as they vary with not only fuel composition, but also with equivalence ratio. Each measurement location was monitored in two different tests. The average temperature is depicted in the flame temperature maps. These tests were very time consuming due to the large number of temperature locations to be observed. A sample flame map representing the temperature contours observed when burning E95/W5 at ER=0.6 is shown in Figure 78. This contour plot is depicted with all dimensions to geometric scale. The flame centerline is represented on the R-axis at radial location R=0 inches. The color-bar indicates a temperature scale ranging from 400 to 1500 Kelvin. Radial measurement locations are spaced at one inch intervals starting at the combustor centerline. Axial measurement locations are spaced at two inch increments starting at a height 0.5 inches above the dump plane. All contour plots depicted in this paper will be consistent with the geometric and color scaling shown in Figure 78. Figure 79 depicts a flame temperature map under the same test conditions with a resolution of 96 measurement locations. The resulting temperature map exhibits the same features but more detail and smoother contours.

Considering Figure 78 and Figure 79 it possible to observe some of the typical features seen in temperature contour plots. The extremely cold regions that are found near the dump plane at a radial location of 1 inch are caused by the heat sink of fuel vaporization. Recall that fuel is injected in a hollow cone at radial location r/D=0 at an axial location x/D=0.047 below the bottom of this plot. The regions of high fuel concentration near the injection point remain cold because it is difficult for heat to penetrate the higher density fuel stream. A particularly hot region can be found near the dump plane.
along the flame centerline. This hot zone represents the central recirculation zone caused by swirl stabilization where hot gas is recirculated and fuel penetration is low. Similarly, slightly colder areas are found near the dump plane at the combustor wall. These regions represent the dead space that occurs near the corner of the combustor. Hot gas circulation is restricted in these areas. The two hot regions located at r/D=0.23 and r/D=-0.23 between axial locations of x/D =0.326 and x/D=0.512 represents the hot zone that is expected within and immediately downstream of the primary reaction zone. The large amount of heat released in this primary reaction zone shows up in these hot spots and dissipates as the hot gas moves farther downstream.

![Flame Temperature Map](image)

**Figure 78:** Sample Flame Temperature Map of Low-Flame Region-Moderate Resolution

![Flame Temperature Map](image)

**Figure 79:** Sample Flame Temperature Map of Low Flame Region- High Resolution
In addition to plotting the full temperature contours, a diagnostic was devised for representing the flame temperature by a single value. This metric, called the Average Low-Flame Temperature or ALFT, represents the spatially averaged temperature of the low-flame region. This value is determined by averaging the value of the 24 measurement locations presented in low-flame temperature contours. The ALFT is taken as the best approximation available for an average flame temperature. Figure 80 shows the results of calculating the ALFT. This plot also indicates the nozzle used to determine each data point. This is relevant for comparing data points with consideration for nozzle variability.

![Average Low-Flame Temperature](image)

**Figure 80: Average Low Flame Temperature Dependence on ER and Fuel Composition**

From the ALFT data, it is clear that low-flame temperature increases as equivalence ratio increases. This is expected because a higher equivalence ratio implies the presence of more ethanol molecules and results in more chemical reactions. This is also predicted by the adiabatic flame temperature calculations shown previously. From this data, it is clear that the addition of 5% water by volume results in reductions in ALFT regardless of equivalence ratio. Increasing the water content to 10% results in further reductions of the ALFT at high equivalence ratios, but does not adversely affect the ALFT at ER<0.85. This is pertinent because turbines and burners are generally operated at lean equivalence ratios. It shows that with proper nozzle design, E90/W10 can be utilized without any negative consequences in the low flame region when compared to E95/W5. The data also shows further reductions in ALFT as water content increases to 20%. Reductions are particularly dramatic at ER=0.8. It is important to note here that reductions in low flame temperature only address the temperature in the low flame region and do not reflect total heat release from the combustion event. Flame lengthening with increased water content may lead to increased flame temperatures in the mid and late flame region.
After considering the general consequences of elevated water content by observing the ALFT it is relevant to consider the entire temperature contour plot through a flame centerplane. Figure 81 shows flame temperature maps for a number of test conditions. Recall that spatial and intensity scaling is consistent between figures. The figures represent variability of both equivalent ratio and water content. It is possible to draw conclusions by considering the effect of changing equivalence ratio at a constant fuel composition. A look at E100/W0 as ER increases reveals three primary changes. First, the temperature generally increases. This is due to the higher number of combustion reactions that can occur as more fuel is introduced to the combustor. Second, the reaction ‘hot zones’ move farther downstream. This is a result of the increase in time taken to fully atomize and vaporize the larger volume of fuel. Third, the reaction hot zones are seen to combine with the hot central recirculation zone. This is once again attributed to the increased availability of fuel within the flame. Heat release occurs more abundantly and isolated region of heat release are less defined at higher equivalence ratios. Similar trends are observed with E95/W5 and E90/W10. When fuel composition is changed to E80/W20 it is found that the combination of the reaction hot zones and the central recirculation zone does not occur until ER=1.0 instead of the previously observed transition at ER=0.8. This is expected because the increased water content scavenges heat from the low flame region and delays the complete heat release.

![Flame Temperature Maps for Various Test Conditions](image)

**Figure 81: Flame Temperature Maps for Various Test Conditions**

Considering a fixed equivalence ratio of 0.8 and observing the changes caused by increasing water content it is found that generally temperature reduces as water content increases. It is also seen that the higher temperatures are found farther from the dump plane at elevated water content. Again, this is due to the delayed evaporation of the hydrous fuel. Similar trends are observed for all equivalence ratios. It is pertinent to point out here that as water content changes from E95/W5 to E90/W10 the flame structure does not change appreciably and in some instances actually becomes more concise with hot zones moving slightly closer to the dump plane. This may be attributed to the
stabilizing affects of the moderate water addition that was previously discussed in the discussion of LBO. This may also be attributed to improved atomization with a given nozzle at a given equivalence ratio caused by the increase in fuel volume flow rate and consequently increased fuel pressure.

Exhaust Temperature

Exhaust gas temperature was taken at radial locations 2.25 and 3.5 inches from the combustor centerline. These measurements were performed at an axial location 33 inches downstream of the dump plane. These temperatures were averaged to evaluate the average temperature of the exhaust gas flow. This data was collected at least three times for each test condition. The results are shown in Figure 82. Repeatability error bars are displayed and indicate a reasonable level of repeatability. For comparison purposes red boxes are used to indicate the nozzle used to collect each data point. This data shows a clear trend between exhaust temperature and equivalence ratio. As equivalence ratio increases the average exhaust temperature is seen to increase. This is predicted by adiabatic flame temperature calculations and is consistent regardless of fuel composition.

![Figure 82: Exhaust Temperature as a Function of ER and Fuel Composition](image)

From this figure a relationship between water content and average exhaust gas temperature is not clear. However, statistical analysis of the data reveals a Pearson’s Correlation Coefficient (PCC) of -.12 between exhaust temperature and fuel water content. This suggests that there is a weak correlation between the two parameters but that increasing water content leads to slight decreases in exhaust temperature. (A PCC with absolute value of 1.0 indicates perfect correlation between two parameters while a PCC of 0 indicates no correlation.) This makes sense because, for a particular ER, an increase in
water content results in more heat loss to fuel vaporization. Since more heat is devoted to phase change less heat should remain for increasing exhaust gas temperature. However, since the correlation between the two parameters is relatively weak it is relevant to note that there is an observable amount of variability that does not appear to depend on fuel composition. This variation is attributed to changes in fuel pressure and consequently spray characteristics that results from changing the volumetric flow rate as water content changes.

Exhaust NOx

The importance of low NOx levels in the combustor exhaust was discussed previously. To evaluate the effects of fuel water content on exhaust NOx concentration the exhaust gas was sampled from the combustor centerline at a location 33 inches downstream of the dump plane. The exhaust gas was analyzed for each test condition using the Cambustion NOx analyzer. Each test condition was evaluated during three separate runs and the results averaged. The results are shown in Figure 83. Repeatability error bars are shown and demonstrate reasonable repeatability for the data. For comparison purposes red boxes are used to indicate the nozzle used to collect each data point.

![Figure 83: Exhaust NOx Variation as a Function of ER](image)

This data demonstrates that exhaust NOx concentration is generally reduced as water content increases, regardless of equivalence ratio. NOx also generally increases as equivalence ratio increases. There is no nitrogen in the fuel so all NOx that is formed is either thermal NOx or prompt NOx. It should also be noted that under no test conditions did the exhaust NOx concentration exceed 15 parts per million (PPM). This is low enough concentration to meet current exhaust standards for power generation and transportation applications.

At ER=0.6 it is found that the addition of 5% water to the fuel leads to a 33% reduction of exhaust NOx. Additional increases in water content continued to lower the concentration of exhaust NOx. 15% water was the most hydrous fuel that could be burned at ER=0.6 and resulted in a 49%
reduction in exhaust NOx when compared to pure ethanol. At ER=0.8 exhaust NOx is seen to be reduced by 12%, 29% and 40% for fuels containing 5%, 10%, and 15% water respectively. When using a fuel with a water content of 20% or 25% by volume it is possible to achieve exhaust NOx reductions of greater than 69%. However, the flow condition at these higher water test points utilized a different atomizing nozzle and therefore cannot be directly compared.

At higher equivalence ratios it is seen that, with enough water addition, it is possible to keep exhaust NOx concentration below 5 ppm even for ER=1.1. However, the use of E90/W10 results in the most dramatic reductions in exhaust NOx PPM. With this fuel reductions of 49% and 36% were achieved at equivalence ratios of 1.0 and 1.1, respectively.

Recalling that the maximum observed temperature within the combustor for any test condition was 1390 K it is known that thermal NOx formation will be low. Thermal NOx is often considered to be negligible at temperatures less than 1800 K. However, since the concentration of NOx in the exhaust gas stream is low, a large percentage of the NOx may be still thermal NOx despite the low temperatures of the flame. Having eliminated fuel NOx from the contributing sources of exhaust NOx, it can be concluded that prompt NOx makes up the remaining contribution to NOx in the exhaust stream. Prompt NOx can be expected to be a contributor in rich flames of low temperature. The temperature within this combustor has been shown to be low and it is expected that locally rich regions exist in the early stages of fuel atomization and evaporation. By plotting exhaust NOx concentration as a function of exhaust gas temperature instead of equivalence ratio we find that exhaust temperature plays a significant role in predicting NOx concentration. However, considering the influence of exhaust gas temperature does not eliminate the dependence of exhaust NOx concentration on fuel composition. Figure 84 shows this dependence and verifies the effects of water content on exhaust NOx.

![Figure 84: Exhaust NOx Variation as a Function of Exhaust Temperature](image-url)
It is interesting to point out that both thermal and prompt NOx formation are endothermic reactions and result in scavenging heat from the hot gas stream. Therefore it seems reasonable to conclude that exhaust temperature for anhydrous fuel is reduced in the formation of NOx. This was hypothesized as a potential contributor to the lack of exhaust temperature variation between fuels of varying water content. To consider the validity of this claim it was relevant to calculate the energy saved by reducing exhaust NOx from 13 ppm to 9 ppm. This energy savings will represent the gains in exhaust heat that result from increasing water content from 5% to 10% at an ER of 1.1. This energy savings will be compared to the energy cost of vaporizing the additional 5% of water that was added. These particular data points were considered because they demonstrate a particularly large change in exhaust NOx for a relatively small change in water content. This will present a best case in hopes of proving the hypothesis as valid.

A number of assumptions must be made in order to make this comparison. All assumptions are made to assume the most energy possible is saved, because if results are not significant under these assumptions then the hypothesis can be deemed invalid. The calculation assumes that all exhaust NOx is produced by the Zeldovich mechanism. This mechanism for thermal NOx production consumes more energy than the alternative prompt formation mechanism. Reaction steps and rates for the Zeldovich mechanism are found in ‘Introduction to Combustion’ by Stephen Turns. These are shown in Figure 85.

The thermal or Zeldovich mechanism consists of two chain reactions:

\[
\begin{align*}
O + N_2 & \leftrightarrow NO + N \quad (N.1) \\
N + O_2 & \leftrightarrow NO + O \quad (N.2)
\end{align*}
\]

which can be extended by adding the reaction

\[
N + OH \leftrightarrow NO + H. \quad (N.3)
\]

The rate coefficients for N.1–N.3 are [22]

\[
\begin{align*}
k_{N.1} &= 1.8 \cdot 10^{11} \exp[-38,370/T(K)] \quad [\text{m}^3/\text{kmol-s}], \\
k_{N.2} &= 3.8 \cdot 10^{10} \exp[-425/T(K)] \quad [\text{m}^3/\text{kmol-s}], \\
k_{N.3} &= 1.8 \cdot 10^7 \exp[-4680/T(K)] \quad [\text{m}^3/\text{kmol-s}], \\
k_{N.4} &= 3.8 \cdot 10^6 T \exp[-20,820/T(K)] \quad [\text{m}^3/\text{kmol-s}], \\
k_{N.5} &= 7.1 \cdot 10^6 \exp[-450/T(K)] \quad [\text{m}^3/\text{kmol-s}], \\
k_{N.6} &= 1.7 \cdot 10^{11} \exp[-24,560/T(K)] \quad [\text{m}^3/\text{kmol-s}].
\end{align*}
\]

Figure 85: Zeldovich Mechanism of Thermal NOx Formation [Turns, 2000]

For the sake of this calculation it is assumed that all NO is formed by reaction N.1. N.3 is neglected because it is not always a participant, and produces NO at a much lower energy cost than N.1. N.2 is neglected because it may not occur under fuel rich conditions, and consumes less energy per mol of NO than N.1. Calculations reveal that NO is formed at a cost of 319,008 kJ/kmol. Considering the ‘savings’ in NOx PPM to be 4 ppm it is found that the energy consumption rate to produce this NO is 1.11 J/s. By evaluating the additional mass flow of water concludes that 529 J/s must be consumed to fully vaporize the additional water. This shows that the energy saved by reducing NOx formation does not offset the energy consumed by vaporizing the additional water. Less than 1% of the expended energy is recovered even in this best case scenario. This demonstrates that thermal gains achieved through exhaust NOx reduction are a minor contributor to changes in exhaust gas temperature.
Sub-Study 2: Flame Imaging, Spatial Distribution of Heat Release, Time Dependence of Heat Release

The second sub-study used optical methods to gain additional insight into the effects of water content on flame performance. This included CH* and OH* imaging of the flame for indication of heat release and photo-diode measurements. A wide range of post-processing techniques were utilized to analyze this data, with a particular emphasis being placed on CH* and OH* measurements. Data was analyzed for both spatial distribution and time dependence and qualitatively compared between various fuels. As was previously mentioned, due to the time consuming nature of this type of measurement the entire range of fuel compositions was not tested. Fuels ranging from 0% to 20% water were observed in the combustor. This range of fuel compositions represents the fuels of interest based upon sub-study 1.

Time-Averaged CH* Images

CH* images were taken at 2000 frames per second for each test condition using the Photron Camera and the 430 nm filter. A total of 500 images were collected to cover a total time of .25 s, resulting in .5 ms between images. The UVi intensifier gate time was set to 200μs, F number on the focusing lens was set to 8, and the UVi gain was set to 76. This resulted in sensitive capture of CH* chemiluminescence while still offering adequate spatial and time resolution. Three image sets were taken for each test condition and the combustor was allowed to cool between runs. Recall that CH* is accepted as an indicator of the onset of combustion and therefore indicates heat release.

To evaluate global heat release distribution the CH* image set was averaged with respect to time. This consisted of evaluating the time-average of each pixel. A sample time-averaged CH* image is shown in Figure 86. From this image we can see the dimensions of the field of view, evaluated at the flame center plane. The bottom of this image is located 0.5 cm above the combustor dump plane. CH* intensity is indicated by the color bar shown. Color scaling is consistent between all CH* images, units are an arbitrary intensity unit and images offer a qualitative comparison within the CH* set. It is important to note here that the flame front extends out of the field of view and is indicated by the red dashed line. The location of the flame centerline is also evident. This image represents a line of sight measurement and does not represent the CH* distribution within a flame center plane. From this typical CH* image it is also possible to see two competing flame structures. The primary tulip structure is stabilized near the injection point and is mostly within the field of view. However, a secondary flame structure is represented by the second region of increased CH* intensity found about halfway up the field of view. Visual inspection of the flame suggests that this secondary flame structure is ring shaped, but is wider than the camera field of view. The secondary flame structure is subject to rapid fluctuations that the central, primary flame structure does not experience.

Time-averaged images were generated for each image set resulting in three images for each test condition. These images exhibited reasonable repeatability which is demonstrated later during analysis of spatially averaged data. The three runs were averaged together to obtain a time-averaged, run-averaged image. Figure 87 shows the results as fuel composition and equivalence ratio vary.

From this image set it is observed that the CH* emission is greater closer to the point of fuel injection at ER=0.6 and ER=1.0 than at ER=0.8 and ER=1.1. In other words, the flame front is stabilized closer to the injection point and the flame is better anchored. This is a result of increased velocity of the fuel droplets that results from increased fuel flow. Injection velocity increases as ER goes from 0.6 to 0.8 but is reduced again at ER=1.0 as a result of the nozzle change discussed.
previously. Under conditions of a higher fuel inlet velocity the low flame reaction zone is more likely to lift because increased fuel velocity results in increased fuel momentum. With more momentum the fuel is not as readily captured by the recirculation zones, resulting in decreased mixing in the low flame region. This phenomenon is also observed within the OH* images shown in Figure 88.

As ER increases CH* intensity in the mid-flame region is seen to increase while the low flame CH* intensity is seen to decrease. This indicates that, while more heat release occurs as a result of increased fuel flow rate, the region of high concentration tends to move from the low- to mid-flame region. This is explained by two contributing factors. First, increased fuel flow rate requires more time to vaporize than a lower fuel flow rate. Second, at a higher global equivalence ratio the mixture near the fuel injection point will be exceptionally rich and more time is required to achieve the atomization and mixing required for bulk combustion. These effects are more dominant than the changes in flame propagation velocity that result from changes in equivalence ratio.

![Figure 86: Features of a Typical Chemiluminescence Image](image)

Considering changes in fuel composition and closely considering Figure 87 we find the predictable result that CH* intensity decreases as water content increases. Taking CH* chemiluminescence to indicate the presence of combustion reactions it can be concluded that the number of complete combustion reactions within the field of view decreases as water content increases. This
would indicate a decrease in combustion efficiency in this region caused by elevated water content. Interestingly, it is observed that the CH* emission does not appear to be significantly affected as water content increases above 10%. It is important to note here that the field of view is quite limited and that reduced heat release in the low flame region does not necessarily indicate reduced heat release throughout the entire combustor.

Figure 87: Complete Set of Run-Averaged CH* Images for all Test Conditions
Time-Averaged OH* Images

OH* images were also taken at 2000 frames per second for each test condition. Once again 500 images were collected to cover a total time of 0.25 s, resulting in 0.5 s between images. OH* chemiluminescence was not as strong as CH* chemiluminescence was still resolved by making some adjustments to the intensifier unit. UVi intensifier gate time was increased to 450μs, F number was increased to 22, and UVi gain was maintained at 76. This enabled successful capture of OH* chemiluminescence while once again offering adequate time and spatial resolution. The time- and run-averaging process was identical to the process described for CH*. Once again scaling is consistent between OH* images but is not comparable to CH* scaling.

Figure 88 demonstrates the variation in OH* distribution as equivalence ratio changes. Though not as obvious as with CH* images, it can be seen that as fuel velocity increases the flame tends to lift with the combustion reactions occurring farther from the fuel injection point. Keep in mind that OH* indicates the presence of CH* oxidation and therefore should be expected to appear slightly downstream of the CH* which indicates the presence of the onset of combustion. The OH* emission increases as ER increases as a result of the increasing number of combustion events occurring. The region of high OH* chemiluminescence is seen to move slightly downstream as ER increases for the same reasons as CH*. This includes increased fuel velocity with higher flow rates as well as increased atomization and vaporization time for a larger volume of fuel.

Figure 88: Variations in OH* Imaging as ER (left) and Fuel Composition (right) are Varied
Figure 8 shows the effects of fuel composition on OH* imaging. Unlike the CH* images we see a consistent decrease in OH* chemiluminescence across the full range of fuel compositions. This indicates that OH* emission is steadily decreasing as water content increases and suggests either a reduction in combustion efficiency or enhanced transport of the CH* away from the site of the initial reaction as it continues to oxidize. Based upon OH* imaging at ER=0.6 increasing water content does not result appreciable loss of flame anchoring ability. This indicates that in the lean regime a stable hydrous ethanol flame can be established without suffering from flame lift. This is consistent with the results of the CH* images and suggests that if fuel momentum is low enough to enable effective mixing in the low flame region then a stable, well-formed flame can be achieved for elevated water content. Once again it is pertinent to point out that the field of view is limited and while these images clearly show the effects of water content in the low flame region they do not justify inferences about the heat release across the entire combustor volume. Gas analysis is once again critical to fully evaluate the total combustion efficiency across the entire combustor.

Spatially-Averaged Time-Averaged CH* Intensity

In order to qualitatively evaluate the total heat release from the flame the signal intensity was spatially averaged over the entire field of view. This spatially-averaged, time-averaged intensity is plotted as a function of water content and equivalence ratio in Figure 8. A spatial average is determined by taking the time averaged value for each pixel location and then averaging all pixels. This plot demonstrates the repeatability of the measurement between runs. Repeatability across runs is presented by the error bars and line plots are representative of the run averaged value. The plot also reveals the general trend of decreasing global heat release as water content increases. This is true for all equivalence ratios. Reductions in global heat release in the field of view caused by the addition of 20% water are 44%, 60%, 21%, and 14% at equivalence ratios of 0.6, 0.8, 1.0 and 1.1, respectively. This demonstrates a significant loss in low flame heat release at the lower equivalence ratios and it can be concluded that low-flame heat output from hydrous ethanol flames is substantially lower than anhydrous flames. Keep in mind that this reduction in heat release was not definitively reflected in the exhaust gas temperature and may simply suggest that globally a more even distribution of heat release is experienced. The field of view cannot be expanded for this combustor and this must be verified through gas composition analysis or through testing in a different apparatus.

This plot also demonstrates the change in heat release as equivalence ratio changes. Water content-intensity trends are seen to shift upward as equivalence ratio approaches stoichiometric. This is because the mixture is still lean and the addition of fuel leads to more combustion in the low flame region. However, as ER exceeds 1.0 global intensity is found to slightly decrease for all fuel compositions. This is because as the flame moves into the rich region more fuel does not equate to more combustion events due to oxygen starvation. The additional fuel instead acts as a heat sink during vaporization and does not contribute to heat release, especially in the low flame region. It is important to point out that the data here shows the spatial averaged intensity over the entire field of view. The intensity was also evaluated over several other regions, including the lower and middle portions of the field of view as well as multiple local regions near the primary reaction zone. Analysis of these other regions offered either the same trend or no trend and did not provide additional insight into the flame properties therefore they are not presented.
Spatial Distribution of Time-Averaged CH* and OH*

Because CH* and OH* measurements are line of sight measurements it is difficult to resolve the distribution of the signal in the radial direction. It would be easier to resolve radial distribution if the images represented a cross-section through the flame center plane. For this reason lasers are often employed with chemiluminescence imaging to perform Planar Laser Induced Fluorescence (PLIF) measurements. These measurements involve passing a planar laser through the flame center plane to excite radicals within this plane and allow for images to show CH* or OH* distribution within the center plane. Line of sight measurements can also be converted to flame centerplane measurements using the ABEL transformation. However, this method requires the assumption that the flame is perfectly axisymmetric. As it is seen in the previous CH* and OH* images it is difficult to obtain a perfectly symmetric flame. Due to slight asymmetries in the flame smoothing is needed before performing an ABEL transformation resulting in reduction of quality in the results. Therefore ABEL transformations were not performed and this study is limited to light of sight optical analysis.

While resolving the radial distribution of the combustion reaction may be difficult it is reasonable to consider the axial variation of the signal as an indicator where in the flame combustion reactions are occurring most abundantly. Axial distribution of CH* and OH* was determined by first considering time-averaged run-averaged images. Then each row of pixels was averaged to give a single value. The resulting mean value for each pixel row was then plotted as a function of axial location. This process was completed for CH* and OH* at various equivalence ratios and fuel compositions. The results are displayed in Figure 90.
Considering ER=0.6 we see that both CH* and OH* exhibit a high intensity region between approximately 3 cm and 5 cm above the dump plane. A second peak in intensity occurs at approximately 9-14 cm above the dump plane. The first peak builds from the dump plane and indicates a region in which fuel is being vaporized before peak combustion is reached. There is then a decrease in intensity before the second peak. This two peak shape is the result of the two competing flame structures described previously. The first peak represents the primary, tulip-shaped, structure that is stabilized by the central recirculation zone. This structure fits within the field of view. The second peak indicates the presence of the secondary reaction zone which is ring shaped and much wider than the field of view. The separation between the peaks is less defined in the OH* images which is expected since OH* represents CH* oxidation and we can expect more uniform spatial distribution of OH* emission compared to the spatial distribution of CH*. At ER=0.6 it is evident that as water content increases heat release in the field of view decreases without substantially affecting flame structure.

Figure 90: Axial Distribution of CH* and OH* Emission Within the Low-Flame Region

When equivalence ratio is increased to 0.8 some changes in flame structure are observed. The trend of decreasing heat release with increasing water content is still observed and is consistent for all
fuel compositions. At this equivalence ratio for water contents greater than 5% a flame structure similar to ER=0.6 is found. At ER=0.8 both peaks occur farther downstream than ER=0.6 because the larger momentum of the fuel allows it to progress farther downstream before vaporization and combustion is complete. An alternative profile is found at ER=0.8 for E100/W0 and E95/W5. A single large heat release peak is observed instead of the two smaller peaks previously described. This may be caused because the increased fuel velocity leads to increased fuel momentum and the spray cone remains tighter around the centerline, preventing the separation of the fuel injection into the two distinct flame regions. As water content increases the heat release is adequately inhibited to cause a return to the original flame structure.

Observing that heat release in the low flame region is significantly reduced by elevated water content it seems inconsistent with results showing that exhaust gas temperature is not drastically affected by water addition. However, Figure 90 has shown that while CH* emission rapidly drops to near zero for cases of low or no water content, it declines more steadily in cases of high water content. This suggests that heat release from hydrous fuels continues outside the field of view and that redistributed heat release may be a contributor to the exhaust gas temperatures previously observed.

Time-Dependent Chemiluminescence Data

Because CH* and OH* images were taken at intervals of 0.5 ms it was possible to analyze the spatial distribution of the radicals as a function of time. Considering CH* images for E95/W5 at equivalence ratios of 0.6 and 1.0 it is found that the time variation in CH intensity is significant. Sample frames are shown in Figure 91. The time variation of CH intensity suggests that the flame may be periodically surging. Combustion reactions often surge periodically with the surge frequency having significant affects on combustion performance. The surges in combustion are often caused by inequalities between the fuel mixing rate and the combustion reaction rate. Since the combustion reaction time is significantly less than the mixing time, especially with liquid fuel injection, typical surges in combustion consist of the flame rapidly propagating to consume the available combustible mixture followed by a period of fuel and air replenishment. The images seen in Figure 91 suggest that surges of combustion reactions occur both in the mid-flame region as well as near the fuel injection point. It is better for the combustor to have low periodicity because high periodicity within the flame results in flame instabilities and can lead to extinction events as well as events of high pollutant formation. If the periodicity of the combustion process can be determined it may be possible to evaluate the fundamental causes behind the effects of elevated water content on flame stability and operability limits.

In order to evaluate the amount of fluctuation and periodicity that characterizes the CH* or OH* signal it is first necessary to determine the region over which to consider the signal. A spatial average over the region of interest must be developed for each time frame. These spatially averaged values can then be plotted as a function of time to represent the variation in CH* or OH* intensity in that region. The time series of signal intensity can then be evaluated to determine standard deviation of the signal, the intensity of the fluctuation, and through the use of a Fourier Transform it is possible to determine any resonant frequency or periodicity in the signal. In order to fully evaluate the time dependent nature of the combustion process both CH* and OH* were evaluated over a variety of different regions. These regions of spatial averaging include the entire field of view, a low-flame region, a low-flame plane, and multiple localized regions of interest. Each of these regions is depicted in Figure 92.
Figure 91: CH* Variation with Time (E95/W5)

Figure 92: Definitions of Flame Regions for Spatial Averaging
By evaluating the standard deviation over a 500 sample set of images at each region it was possible to plot standard deviation within the signal as a function of equivalence ratio and water content. These plots did not show any consistent correlation between fuel equivalence ratio and flame stability. However, it was generally shown for each region that the standard deviation of the signal decreased as water content increased. Having already established that the mean signal throughout the low-flame region decreased as water content increased it can be concluded that the flame was significantly more stable at higher water contents. This validates previous claims and is attributed to the reduction in flame propagation velocity caused by higher water content. Reduced flame propagation velocity diminishes the ability of the flame to experience events of local extinction.

The spectral density was evaluated in order to determine the periodicity of the flame behavior. CH* images over the full flame window and both local regions were evaluated. Evaluation of the spectral density involves performing a Fourier Transform on the time series and results in a plot that shows the intensity of the signal that is behaving within a each frequency. This procedure is performed using MATLAB software. The procedure was performed not only on the 500 sample sets of data previously discussed but also on 2000 sample sets of data. This represents one second of data being sampled at 2 kHz. Nyquist frequency dictates that at this sampling rate any periodicity that occurs at less than 1000 Hz should be resolved. When analyzed over the local field of view the data did not exhibit any strong resonance. The spectral density exhibited a number of peaks increasing in intensity as frequency decreased, but did not show any standout frequencies. This leads to the conclusion that there is no strong periodicity in the low flame region and that the fluctuations are either extremely complex or somewhat random in nature. Evaluating the spectral density over the entire flame region yielded reasonably repeatable results but no standout trends were observed. The only resonance that was identified was an acoustic resonance at 160 Hz that can also be recognized audibly. This resonance is attributed to the vibration of the exhaust gas on the fume hood and does not appear to consistently affect flame behavior.

Photodiode Data

The photodiode described previously was used in an effort to perform a spatially independent measurement of CH* and OH* intensity being emitted from the flame. The photodiode was used in conjunction with an intensifier. Even on the highest amplification setting the photodiode could not resolve a signal for OH* emission. This is because the wavelength of OH* emission is near the lower limit of the photodiode sensitivity and the signal is very low anyway. CH* intensity could be resolved when utilizing the highest magnification settings on the amplifier. However, the noise of the signal was on the order of the measurement itself. This noise level could not be reduced and was actually quite low. The low level of the signal allowed the standard deviation to, in most cases, be greater than the mean value. This made the measurement unreliable and trends could not be trusted to make practical conclusions. Photodiode measurements were abandoned because of the low signal strength and the relative sensitivity of the device.

Sub-Study 3: Gas Composition Analysis

The third sub-study included a detailed gas composition analysis of the combustor exhaust using the 490 Micro-GC. This study seeks to provide insight into the efficiency of the combustion reaction by analyzing the exhaust gas composition at the combustor exit. By considering the oxygen, carbon dioxide, methane, and carbon monoxide compositions at various equivalence ratios it is possible to make inferences concerning the relative completeness of the combustion reaction. Equivalence ratios tested
included ER=0.6, ER=0.8, ER=1.0 and ER=1.1. Fuels ranging from 0% to 20% water in ethanol were tested. This data validates some of the hypothesis presented in sub-study 1 and 2.

Data Collection Method

Exhaust gas samples were taken through a 1/8” stainless steel sample probe. The probe was required to be 6” long in order to prevent heat damage to the GC. The small diameter of the probe was selected in order to minimize the volume inside of the sample line. This volume was kept small to reduce the amount of time required to purge the sample line between measurements. Even with the small diameter tubing it was necessary to sample for two minutes per measurement in order to fully purge the sample line and achieve accurate readings. Measurements were taken in sets of two for each measurement. This repetitive measurement technique validated the repeatability of the gas analysis and sampling process for each test condition. Repeatability of the test condition was verified by taking three sets of measurements separated by a combustor shut down. Repeatability was excellent and is shown in all plots with error bars.

The sample probe was positioned at the combustor exit plane exactly in the center of the combustion cross section. This is the same location of the NOx sampling location and in plane with the exhaust temperature measurements. The sample time in the GC was set to 120 seconds with a 5 second stabilizing time. Both columns (MS 5a and PPU) were set to analyze the sample for 70 seconds with a sampling frequency of 100 Hz and no acquisition delay. The MS 5a column was operated at a temperature of 80 C, an injection time of 40 mSec and a backflush time of 12 seconds. The PPU column was operated at a temperature of 60 C, an injection time of 40 mSec, and a backflush time of 18 seconds. These settings were recommended by the Agilent representative and provided repeatable and accurate results. Recall that the backflush and bakeout functions were utilized to protect the GC from condensate. The bakeout function elevated the temperature of the MS5a and PPU columns to 140 and 120 C, respectively. These temperatures were held for 3-5 hours to allow for evacuation of the columns.

Exhaust Oxygen Concentration

Considering the exhaust oxygen concentration as a function of equivalence ratio it is found that the mol fraction of oxygen in the exhaust generally decreases as fuel to air ratio increases. This is expected because for lean mixtures the addition of more fuel results in more combustion reactions and the consumption of more oxygen. All of the oxygen present in the exhaust gas is either excess oxygen that could not be used in the combustion reaction or is oxygen that was not effectively mixed with unburned hydrocarbons. As the ER approaches unity the amount of excess oxygen decreases toward zero. This trend was observed for all fuel compositions regardless of water content. At ER>1.0 the concentration of oxygen in the exhaust was found to be consistently less than 2%. This suggests that some oxygen appears in the exhaust because of mixing and combustion inefficiencies. However, a small amount of unreacted oxidizer is expected and it is not found to be dependent upon water content. A slight increase in O₂ concentration is seen when ER increases from 1.0 to 1.1. This is caused by localized flame quenching that can occur as the mixture becomes rich. All results are shown as a function of equivalence ratio in Figure 93.
Figure 93: Exhaust Oxygen Concentration as a Function of ER

Figure 94: Exhaust Oxygen Concentration as a Function of Water Content
Figure 94 shows the exhaust oxygen concentration presented as a function of water content. This plot again reinforces the dependence on equivalence ratio that was previously discussed but also enables a more clear visualization of the lack of dependence on fuel water content. While some fluctuations in exhaust oxygen concentration are observed with different fuels there is no consistent trend between water content and the presence of oxygen in the exhaust. This leads to the conclusion that combustion efficiency over the entire length of the combustor is not changed as a result of water addition. The fluctuations that are seen between test points with different fuels can be attributed to changes in spray structure that result from changing fuel pressure and droplet size. These changes to the spray characteristics cause variation in the fuel-oxidizer mixing process and affect combustor efficiency. Repeatability for each test condition is shown by the error bars and indicates the variation between three tests. Results are reasonably repeatable.

Exhaust Carbon Dioxide Concentration

Considering the concentration of carbon dioxide in the exhaust gas we find trends that behave as expected. Results are presented as a function of fuel equivalence ratio in Figure 95. As equivalence ratio increases towards unity the concentration of carbon dioxide in the exhaust is found to increase. This is predictable because increasing fuel flow rate in a lean combustion reaction will result in more complete combustion events because excess oxygen is present and the formation of the stable CO\(_2\) product will be encouraged by the presence of more C\(_2\)H\(_5\)OH. As equivalence ratio increases greater than one the concentration of CO\(_2\) in the exhaust is found to decrease. This is because a rich combustion reaction will be starved of oxygen and will inhibit the formation of fully oxidized carbon. The reduction in CO\(_2\) should be coupled with an increase of unburned hydrocarbons as well as an increase in incomplete combustion products such as CO or CH\(_4\). These trends were consistent for fuels of all compositions.

![Exhaust Carbon Dioxide Concentration](image)

Figure 95: Exhaust Carbon Dioxide Concentration as a Function of ER
Figure 96 shows the same exhaust CO$_2$ data but is presented with water content on the x-axis. This plot shows that there is no strong correlation or trend between exhaust CO$_2$ concentration and fuel water content. This plot reinforces the conclusions made previously that water content does not affect combustion efficiency over the combustor volume. Once again any variations between tests with different fuels can be attributed to changes in fuel pressure and spray characteristics. Repeatability is again excellent.

Exhaust Methane and Carbon Monoxide Concentration

Exhaust methane and carbon monoxide concentrations were tracked in addition to oxygen and carbon dioxide. These species were not found at equivalence ratios less than 1.0 and were generally found to increase in concentration as the mixture became richer. This is because oxygen deprivation in rich mixtures inhibits the complete oxidation of the carbon and hydrogen. H$_2$O and CO$_2$ concentrations are reduced and incomplete combustion products such as CH$_4$ and CO form.

For ER<1.0 the measurement was generally deemed below the detection limit (‘BDL’) by the GC. The actual detection limits were approximated to make sure this was not a result of poor calibration or user error. The manufacturer does not give an actual detection limit because it varies with individual device. Regardless, the limit was estimated by the supplier to be between .01 and .02 volume percent. This detection limit equates to a minimum concentration on the order of 100-200 ppm. Theoretical CO calculations for a perfectly mixed reaction are shown in Table 4 and indicate that for stoichiometric or lean mixtures the CO concentration will be BDL. This validates previous results and assessment that the current GC set-up is not sensitive enough to resolve CO in this combustor. These concentrations in CO are consistent with literature and are typical in swirl-stabilized combustors.
Table 4: Detectable Levels of CO Within the Combustor

<table>
<thead>
<tr>
<th>CEA Theoretical CO Concentration</th>
<th>Vol %</th>
<th>PPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 % Water</td>
<td>0.6</td>
<td>0.00001</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>0.00975</td>
</tr>
<tr>
<td></td>
<td>1.1</td>
<td>0.028</td>
</tr>
<tr>
<td>5% Water</td>
<td>0.6</td>
<td>0.00001</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>0.0086</td>
</tr>
<tr>
<td></td>
<td>1.1</td>
<td>0.027</td>
</tr>
<tr>
<td>20% Water</td>
<td>0.6</td>
<td>0.0056</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>0.023</td>
</tr>
</tbody>
</table>

**Sub-Study 4: Flame Tip Temperature and CH* Intensity**

Having established that elevated water content leads to reduced heat release and temperature in the low-flame region, it became relevant to evaluate temperature and CH* emission in the latter regions of the flame. This was done by reconfiguring the combustor shell to provide access to a region of the flame farther from the dump plane. This would give information concerning the flame length and behavior of heat release near the flame tip.

**Flame Tip Temperature**

Radial temperature profiles were taken at a number of axial locations. Flame temperature contours were generated near the flame tip for a range of water contents at ER=1.0. The contour plots included 24 measurements at axial locations 18 to 24 inches downstream of the dump plane. These measurements were run-averaged to produce repeatable contour plots. The resulting contour plots were spatially averaged and the result is plotted in Figure 98a. This metric reveals that the addition of water reduces temperature not only at the base of the flame but also at the tip. Figure 98b also shows the temperature distribution along the combustor centerline for both E95/W5 and E80/W20 fuels. It can be seen that along the centerline elevated water content universally reduces flame temperature, though the decrease is much larger in some regions than others. From these plots it can be concluded that increasing water content generally reduces flame temperature as expected.

Figure 99 displays both upstream and downstream temperature contours for various fuel compositions at ER=1.0. All dimensions and spacing between the two contours are to geometric scale. The grey block represents the gap between the two measurement planes where access ports to measure temperatures were not available. From these contours it is clear that increasing water content does not drastically change the structure of the temperature contour within the flame, it does however lead to lower temperatures within the combustor.
Figure 98: Flame Temperature Measurements at ER=1.0 a) Over a Centerplane Near the Flame tip  
b) Along the Combustor Centerline
Figure 99: Upstream and Downstream Temperature Maps for Various Fuel Compositions, ER=1.0

Figure 100 presents a detailed comparison of radial temperature distribution at different axial locations for E95/W5 and E80/W20 at ER=1.0. At x/D=0.05, the low temperature region near r/D=0.1 corresponds to the unevaporated spray core, but it can be seen that along the centerline the recirculating hot gases lead to elevated temperatures (>1200 K) while along the outer edges of the spray temperatures are in the 1000 K range. By x/D=0.23, the spray has moved radially outwards (r/D>0.2) as represented by the lower temperature region, and has mostly evaporated. Significant combustion of the vaporized fuel occurs in the x/D=0.23-0.60 region as evidenced by the increasing temperatures, with the E95/W5 fuel experiencing earlier combustion (temperatures elevate by d/D=0.42) due to the lower water content, and the E80/W20 showing rapid temperature increases later from x/D=0.42-0.60. In general temperature reduction as well as a more uniform distribution of heat within the combustor is observed with the higher water content, and leads to the reduced concentration of exhaust NOx presented in this study.
Figure 100: Radial Temperature Distribution at Various Axial Locations, ER=1.0
Flame Tip CH* Intensity

After considering temperature near the flame-tip it was beneficial to consider CH* emission in this region. By observing the intensity of heat release near the flame tip it was possible to evaluate the effects of water content on flame length. Line of sight CH* images were taken over a 5 x 3 inch region located 18-23 inches downstream of the dump plane. The CH* intensity in this region was extremely low and a high gain of 200 had to be used to intensify the signal. Images were taken at ER=1.0 for fuels ranging from E100/W0 to E80/W20. Three time-averaged images were combined to obtain a run-averaged time-averaged representation of CH* release in this region. These images were then spatially averaged to a single value which is presented in Figure 101. This data reveals that CH* intensity in this region is generally reduced as water content increases. This suggests that the flame is not appreciably lengthened as a result of water addition and that heat release near the flame tip is indeed reduced in the presence of excess water. From this plot it is also apparent that CH* release at the flame tip is not solely dependent upon water content which suggests that flame length is appreciably affected by the inevitable changes in fuel spray velocity and atomization quality that result from increased volumetric fuel flow rate. Repeatability error bars are shown for reference.

![Figure 101: Flame Tip CH* Emission at ER=1.0](image)

System Performance and Life-Cycle Savings

It has been established that elevated water content generally leads to temperature reductions, both within the flame and in the exhaust, but exhaust gas concentration suggests that elevated water does not lead to reductions in combustion efficiency. At the same equivalence ratio and operating at the same combustion efficiency a hydrous fuel flame and an anhydrous fuel flame will release the same amount of heat over the entire combustor volume. However, at a given equivalence ratio hydrous fuels require

108
more heat to vaporize. The presence of water provides a parasitic heat load on the flame. When heat is released it is devoted to water vaporization before temperature increase. Furthermore, increased mass flow rate of the fuel means more heat must be supplied to achieve the same temperature. At first glance it is expected that reduced exhaust temperature corresponds to decreased available heat in the exhaust gas stream and poor combustor performance. A holistic analysis of heat flux into and out of the combustor leads to a different conclusion.

The rate of heat coming from the combustor exhaust is dependent upon the temperature of the exhaust, the mass flow rate through the combustor, and the average specific heat of the exhaust gas \( \dot{Q} = \dot{m}C_pT \). Exhaust heat rate was calculated for each fuel composition and equivalence ratio. The mass-weighted specific heat of the exhaust gas was calculated based on exhaust gas composition. Exhaust temperature was a measured value presented previously, and mass flow rate was calculated based upon fuel and air flow-rates. The results, shown in Figure 102, show that heat rate out of the combustor is not negatively affected by the addition of water. Pearson’s Correlation Coefficient of 0.07 suggested a negligible correlation between fuel water content and exhaust heat rate. Reduced exhaust temperatures were off-set by the increase in mass flow rate required when burning hydrous fuel. This reinforces GC measurements suggesting that heat release over the entire combustor is not appreciably affected by the use of hydrous fuel.

![Figure 102: Exhaust Heat Rate as a Function of Equivalence Ratio and Fuel Composition](image)

Calculations also revealed that the thermal efficiency of the combustor \( (Eff = \frac{\text{Exhaust Heat Rate}}{\text{Fuel Heat Potential}}) \) was not reduced as a result of water addition and actually improved slightly as water content increased. Thermal efficiency across the combustor was highest at ER=0.6 and lowest at ER=1.1. A leaner mixture leads to more complete combustion because of excess air and more complete mixing. Peak efficiency values of 57% were achieved. This number is reasonable for a combustor that was not tuned specifically for maximum thermal efficiency.
Utilizing previously published data concerning the energy cost associated with hydrous ethanol production as well as the data from this study it was possible to determine the life-cycle energy savings associated with burning elevated water content ethanol. Figure 103 demonstrates that life-cycle energy savings increases as water content increases, but with a diminishing return. This diminishing return is experienced because further increases in water content leads to minimal savings during production and simultaneously has a greater affect on combustor performance. From this data it can be estimated that the use of E85/W15 or E80/W20 could result in greater than a 25% energy gain when compared to anhydrous fuel over the entire life-cycle of the fuel.

Figure 103: Life Cycle Energy Savings at ER=0.8
SUMMARY AND CONCLUSIONS

General Conclusions

A study was performed to evaluate the feasibility of hydrous ethanol as a suitable fuel. Theoretical evaluation of the fuel was performed and fundamental relationships between water content and flame temperature, exhaust NOx, LBO, flame structure, exhaust gas composition, and chemiluminescence properties were observed. Fuels ranging from E100/W0 to E60/W40 were evaluated in a swirl-stabilized combustor. Stable combustion was achieved for fuels with water contents between 0% and 35%. LBO, exhaust temperature and exhaust NOx measurements were performed on fuels in this range of water concentration. Chemiluminescence techniques were employed to gain information concerning heat release and flame structure in the low flame region. Gas Chromatography was used to analyze exhaust gas composition and make conclusions about combustion efficiency. Fuels ranging from E100/W0 to E80/W20 were evaluated using Chemiluminescence and GC methods. The following conclusions were made:

- A stable flame could be achieved for fuels of up to 35% water by volume.
- Lean blow out limit is reduced by the addition of 5% water but is adversely affected as water content increases beyond 5%.
- Flame stability is not noticeably affected by the addition of up to 20% water.
- Increasing water content reduces the probability that a spark will lead to combustor ignition. This reduction can be offset by increasing ignition equivalence ratio. Despite reductions in ignition probability the fuel is still reasonably easy to ignite and offers practical ignition characteristics.
- Average temperature of the low flame region is seen to be reduced as water content increases. The change of water concentration from 5% to 10% does not adversely affect average flame temperature for ER<0.9.
- Exhaust gas temperature is found to increase as ER increases and is slightly decreased as water content increases. However, exhaust heat rate is not adversely affected by the addition of up to 20% water to the fuel.
- The concentration of oxides of nitrogen in the exhaust gas stream, despite being less than 20 ppm at all times, were found to be reduced significantly as water content increases. This reduction is not solely dependent upon changes in exhaust gas temperature. The use of E90/W10 was found to reduce NOx concentration by greater than 30% at all equivalence ratios.
- CH* and OH* chemiluminescence data reveals that global heat release from the low, central region of ethanol flames is reduced by as much as 60% by the addition of 20% water to the fuel.
- Ethanol flame heat release increases as ER approaches unity and decreases as the flame becomes rich, regardless of water content.
- Carbon dioxide concentration in the exhaust gas is found to increase as equivalence ratio approaches unity. Exhaust oxygen concentration is found to decrease as equivalence ratio increased.
- At ER=1.0 exhaust oxygen concentration is less than 2% and suggests that mixing and combustion is near complete.
- Exhaust gas composition, and therefore combustion efficiency, are not affected by the addition of water.
Flame structure and combustion efficiency are dependent upon fuel equivalence ratio and fuel spray velocity.

- The temperature distribution is more uniform throughout the combustor when burning hydrous ethanol.
- The flame is not lengthened as a result of water addition.
- The use of E85/W15 would result in as much as 25% life cycle energy savings when compared to anhydrous ethanol use.

In conclusion, this study has validated up to 20% water in ethanol as a practical fuel for continuous flame applications. This fuel can be produced at a lower capital cost than anhydrous ethanol and will provide an economic benefit despite increased volumetric consumption. The use of up to E80/W20 offers a reduction in exhaust NO\textsubscript{x} concentration and a reduction in peak flame temperatures without reducing combustion efficiency or exhaust gas temperature. Negative effects on flame stability are minimal and are restricted to extremely lean equivalence ratios. Despite the many advantages that can be had by using E80/W20, or any lesser water content fuel, the engine designer should be prepared to re-tune fuel injection specifically for hydrous fuel since increased fuel flow rate will result in changes to the fuel spray characteristics and have significant implications on combustor performance.

**Future Work Recommendations**

While this work is fairly comprehensive there are a number of improvements and additional diagnostics that can be performed to progress. Many obstacles were faced throughout the course of this study that resulted from performing research in a previously untested combustor. In hindsight it would have been beneficial to select a combustor that has previously been characterized in terms of flow field and mixing characteristics. If this study were to be continued it would be beneficial to perform some PIV or CFD analysis of the flow field within the combustor. Another extremely beneficial study would be to perform a detailed analysis concerning the spray characteristics of hydrous ethanol. This study uses fuel pressure and manufacturer’s data to predict droplet size. Nozzle variability was a necessity to accommodate for the wide range of fuel flow rates. It would be beneficial to spend some time monitoring spray velocity, spray angle, and droplet size for various fuels and test conditions. It also may be a worthy endeavor to consider another type of nozzle that would be capable of providing more consistent spray characteristics over the range of fuel flow rates required. Chemiluminescence measurements in this study were particularly limited by the restricted field of view. It may be beneficial to modify the combustor to extend the field of view. Planar Laser Induced Fluorescence (PLIF) measurements may be beneficial to provide additional insight into combustion stability or the mechanisms that lead to LBO.

Progress can also be had by performing research that is unrelated to the experimental apparatus used in this study. Detailed modeling of hydrous ethanol combustion using CHEMKIN software to fully understand any affects on chemical kinetics (though there appear to be none). It also would be beneficial to test hydrous ethanol in an actual turbine and monitor the performance of that engine. Finally, it would be extremely beneficial to perform a detailed economic analysis for hydrous ethanol. Considering the life-cycle costs associated with both hydrous and anhydrous fuel would enable plant managers to make a decision concerning which fuel is most beneficial for their application.
REFERENCES


VITA

Baine Breaux was born in Lafayette, Louisiana, to Rodney and Belinda Breaux in May 1987. He spent his formative years in St. Tammany Parish, Louisiana. After obtaining a bachelor of science degree in mechanical engineering at Louisiana State University, Baine decided to continue his studies by obtaining an master of science degree specializing in the thermal/fluids sub-discipline. With research interests in fuel flexibility, engine controls, and efficiency he hopes to pursue a doctoral degree after taking time off to travel with his wife. In the future he hopes to raise more of his own food and become faster than a deer in a long distance footrace.