Understanding the Effects of Nozzle Design and Spray Characteristics for Optimizing Pyrolysis Liquid Biofuel Ignition and Combustion

by

Steven Albert-Green

A thesis submitted in conformity with the requirements for the degree of Master of Applied Science
Department of Mechanical and Industrial Engineering
University of Toronto

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Abstract

This thesis examines how nozzle design and spray characteristics influence the combustion and emissions of a pure pyrolysis liquid biofuel (PLB) flame in a 10kW, insulated, swirl burner using an internally mixed air-blast nozzle. PLB is a carbon-neutral fuel made from waste wood, but its properties make efficient combustion challenging. First, atomization trends were examined with distilled water to elucidate the important parameters and design aspects and to determine the nozzle's primary atomization mechanism(s). With this information, combustion experiments studied how carbon monoxide, nitric oxide, carbonaceous residue, flame stability and coking were influenced by the nozzle's mixing chamber diameter and outlet number/diameter, angle and total area in order to optimize the design of the nozzle. Ultimately, an optimized nozzle was designed that achieved a self-sustaining PLB flame with good stability, low emissions and low coking. In addition, it allowed for "cold-starting" and pilot flame extinguishment at steady-state while maintaining stability.
Acknowledgments

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Finally, I would like to give a special thank-you to all my friends and especially my family for their incredible support throughout this degree. Despite all the set-backs, countless late nights and a few unavoidable early mornings they were always there to motivate me and keep me focused on completing this thesis project. Without them this would have been much more difficult.
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# Nomenclature

## Acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASTM</td>
<td>American Society of Testing and Materials</td>
</tr>
<tr>
<td>CO</td>
<td>Carbon Monoxide</td>
</tr>
<tr>
<td>CR</td>
<td>Carbonaceous Residue</td>
</tr>
<tr>
<td>FTIR Spectrometer</td>
<td>Fourier Transform Infrared Spectrometer</td>
</tr>
<tr>
<td>HHV/LHV</td>
<td>Higher/Lower Heating Value</td>
</tr>
<tr>
<td>HMW/LMW</td>
<td>High/Low Molecular Weight</td>
</tr>
<tr>
<td>IMAB Nozzle</td>
<td>Internally Mixed Air-Blast Nozzle</td>
</tr>
<tr>
<td>IMTF Nozzle</td>
<td>Internally Mixed Twin-Fluid Nozzle</td>
</tr>
<tr>
<td>NASA</td>
<td>National Aeronautics and Space Administration</td>
</tr>
<tr>
<td>NOAA</td>
<td>National Oceanic and Atmospheric Administration</td>
</tr>
<tr>
<td>NO</td>
<td>Nitric Oxide</td>
</tr>
<tr>
<td>NOx</td>
<td>Nitrogen Oxides</td>
</tr>
<tr>
<td>PM</td>
<td>Particulate Matter</td>
</tr>
<tr>
<td>ppm</td>
<td>parts per million</td>
</tr>
<tr>
<td>PSig</td>
<td>Pounds per Square Inch (gage)</td>
</tr>
<tr>
<td>PLB</td>
<td>Pyrolysis Liquid Biofuel</td>
</tr>
<tr>
<td>SMD</td>
<td>Sauter Mean Diameter</td>
</tr>
<tr>
<td>SLPM</td>
<td>Standard Litre per Minute</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>--------</td>
<td>------------------------------------------------</td>
</tr>
<tr>
<td>SOx</td>
<td>Sulfur Oxides</td>
</tr>
<tr>
<td>TGA</td>
<td>Thermal Gravimetric Analysis</td>
</tr>
<tr>
<td>(U)HC</td>
<td>(Unburned) Hydrocarbons</td>
</tr>
<tr>
<td><strong>Math</strong></td>
<td></td>
</tr>
<tr>
<td>ALR</td>
<td>Air/Liquid Mass Ratio</td>
</tr>
<tr>
<td>C</td>
<td>Constant of Atomization/Characteristic Nozzle Dimension</td>
</tr>
<tr>
<td>cP</td>
<td>centiPoise</td>
</tr>
<tr>
<td>cSt</td>
<td>centiStokes</td>
</tr>
<tr>
<td>ρa</td>
<td>Air Density [m]</td>
</tr>
<tr>
<td>ρl</td>
<td>Liquid Density [kg/m³]</td>
</tr>
<tr>
<td>Di</td>
<td>Diameter of the i&lt;sup&gt;th&lt;/sup&gt; Droplet [m]</td>
</tr>
<tr>
<td>do</td>
<td>Diameter of Liquid Jet [m]</td>
</tr>
<tr>
<td>m&lt;sub&gt;a&lt;/sub&gt;</td>
<td>Air Mass Flow Rate [kg/s]</td>
</tr>
<tr>
<td>m&lt;sub&gt;l&lt;/sub&gt;</td>
<td>Liquid Mass Flow Rate [kg/s]</td>
</tr>
<tr>
<td>Ni</td>
<td>Number of Droplets with the i&lt;sup&gt;th&lt;/sup&gt; Droplet's Diameter</td>
</tr>
<tr>
<td>Nh</td>
<td>Number of Nozzle Outlet Holes</td>
</tr>
<tr>
<td>P&lt;sub&gt;a&lt;/sub&gt;</td>
<td>Pressure of the Atomizing Air (gage) [PSI]</td>
</tr>
<tr>
<td>P&lt;sub&gt;a,a&lt;/sub&gt;</td>
<td>Pressure of the Atomizing Air (absolute) [PSI]</td>
</tr>
<tr>
<td>r&lt;sub&gt;h&lt;/sub&gt;</td>
<td>Radius of Nozzle Outlet Holes [m]</td>
</tr>
<tr>
<td>D&lt;sub&gt;32&lt;/sub&gt;</td>
<td>Sauter Mean Diameter [μm]</td>
</tr>
</tbody>
</table>
\( \sigma \) \quad \text{Surface Tension [N/m]}

\( U_a \) \quad \text{Velocity of the Atomizing Air [m/s]}

\( U_o \) \quad \text{Velocity of the Spray at the Nozzle Outlets [m/s]}

\( \dot{V} \) \quad \text{Volumetric Flow Rate of the Atomizing Air [m}^3/\text{s]}

\( \mu \) \quad \text{Liquid Dynamic Viscosity [Ns/m}^2\text{]}
Chapter 1

1 Introduction

1.1 Motivation

Reducing greenhouse gas emissions in an effort to halt ever-increasing climate change is one of the primary issues influencing energy and environmental policy worldwide. In fact, fossil fuel combustion systems contributed to 81.4% of the world's energy supply while producing 99.4% of carbon dioxide (CO$_2$) emissions in 2013 [1]. Furthermore, statistics jointly released by NASA and NOAA suggest that 2016 was the warmest year on record and the third record-breaking year in a row [2]. The temperature defining a "tipping point" for irreversible climate change is the subject of great debate, but trends show that global warming is an accelerating process [2], illustrating that real environmental innovation is imperative in order to create a more environmentally sustainable and prosperous global economy moving forward. In the near future, global energy needs are expected to rapidly increase as developing countries and economies with large populations continue to grow [3] and currently in the United States, 70% of energy production still relies on fossil fuels [4].

Although the reliance on combustion as a worldwide energy source is unlikely to decrease significantly in the near future, fuel sources themselves can be made more environmentally friendly while minimizing the consumption of non-renewable resources. Pyrolysis liquid biofuel (PLB) is created from biomass, which already supplies more than 10% of the world's energy [1]. Direct combustion of biomass is disadvantageous as it is plagued by very high emissions, particularly with respect to particulate matter, and low efficiencies [5], but liquid biomass fuels can be combusted far more cleanly. With regards to sustainable liquid fuels, PLB (also called bio-oil or pyrolysis oil) is widely regarded as the only realistic renewable resource to facilitate the replacement of petroleum fuels [6] and is also the lowest cost liquid biofuel available [7], [8]. A detailed life cycle assessment concluded that greenhouse gas emissions from power generation could be reduced by 77-99% just by switching current facilities over to PLB rather than continuing to run on fossil fuels (natural gas, fuel oil and coal) [4].

Biomass fuels can be sourced from a number of different feedstocks. First generation biofuels, such as ethanol and biodiesel, are created from edible feedstocks and most are no longer thought
to significantly reduce greenhouse gas emissions and are also economically and environmentally unsustainable moving forward [9], [10]. On the other hand, second generation biofuels, such as PLB, made from non-edible biomass feedstocks, can be carbon-neutral and are more sustainable because they do not compete for agricultural space or with the food supply and thus have not caused food prices to rise [10]–[12]. However, PLB’s composition and properties present unique combustion challenges that need to be addressed.

PLB can be made from a wide variety of biomass feedstocks, but it is commonly a wood-derived fuel (and is such for the research conducted throughout this thesis). The quality of the wood or other biomass source will determine the quality of the fuel produced. Wood feedstocks provide the best quality second generation biomass-derived fuel because of their higher energy density and yield along with their lower ash, nitrogen and water content compared to fuels made from other feedstocks [7], [13]–[17]. PLB has the potential to provide a renewable, carbon-neutral source of energy with lower harmful emissions [12], [18]. As such, it has been the subject of a great deal of research over the past few decades and is important for the future health of the global energy economy.

PLB has the potential to be used in gas turbines, reciprocating engines, furnaces, burners and boilers [7], [19]. These combustion applications all have varying requirements and a wide range of operational standards for achieving high efficiencies. Currently, PLB is beginning to replace heavy fuel oils in large-scale industrial burners, furnaces and boilers [19]–[22] and the world’s first combined heat and power plant running on PLB was commissioned in 2013 by Fortum in Finland [23]. These are applications where hot-zone residence times are large and high combustion efficiency is simpler to achieve. The use of PLB in smaller combustion devices such as turbines and compression-ignition engines, where lighter fuel oils typically dominate, is still in the research and development stage with some successful demonstrations available [24], [25]. In these applications, combustion must take place within a short time frame and small volume, still requiring high combustion efficiency in order to maintain low emissions. PLB combustion generates oxides of nitrogen (NOx) and particulate matter (PM) emissions in varying amounts while incomplete PLB combustion also results in emissions of carbon monoxide (CO) and unburned hydrocarbons (UHC). All of these combustion emissions can be harmful to human and/or environmental health [26], [27].
Given the continually increasing need for environmentally sustainable fuel, PLB research and commercialization across the major combustion industries is progressing and an overview of current research initiatives is available [28]. Fuel specifications are also being standardized [29]–[32] to provide consistent fuel quality which is critical moving forward. In addition, novel combustion strategies for pyrolysis fuel are being developed and this thesis is part of that body of research.

Often, combustion quality is determined by spray atomization. Efficient combustion requires the fuel to vaporize and mix with the oxidizer, ignite and completely burn within the limited residence time and volume of the combustor. For these processes to occur, a sufficiently fine spray is required, which is particularly important when using PLB due to its limited volatility and therefore slow ignition. As a result of this and other fuel properties, PLB requires a longer residence time for complete oxidation compared to standard petroleum fuels [33], [34]. Enhanced combustion performance of PLB has been demonstrated when blended with ethanol [25], [35]–[39] or when co-fired with conventional fuels such as natural gas [20], [21], [40], but this research project aims to show the potential of PLB as a sustainable alternative in its own right, without any contribution from other fuels. Spray atomization is important for all combustion applications and fundamental for further turbine and engine research which require comparatively rapid rates of combustion.

Research regarding sprays has been carried out for decades, elucidating important fuel parameters and nozzle designs to enhance atomization. However, applicable spray research regarding PLB and/or internally mixed air-blast nozzles is sparse and PLB parametric combustion studies with respect to spray patterns and characteristics are virtually non-existent. Previous research [5] has been successful in forming a functional PLB flame, but has also stalled because of the difficulty in atomizing PLB and a lack of understanding as to how nozzle design and spray characteristics influence the numerous competing combustion priorities (CO, NOx, PM, flame stability and coking) that must be considered with this fuel. PLB combustion and atomization are areas with a great potential for optimization through a more thorough understanding of the important spray parameters involved, their effects and how they are influenced by controllable variables, thereby formulating a targeted approach with which to
improve flame stability and reduce emissions. Ultimately, a more stable flame can achieve greater combustion efficiencies with a lower sensitivity to its environment.

1.2 Objectives

This research will examine the effects of geometric design parameters and the resulting spray characteristics from an internally mixed air-blast atomizer, establishing the important trends and underlying critical parameters. Subsequently, this data will then be used to understand how established parameters, nozzle designs and spray characteristics influence PLB combustion dynamics and efficiency, as determined by observing pollutant emissions and flame stability. Experiments will be conducted with a 10kW, swirl-stabilized, doubly insulated and optically accessible spray combustor. Results will be directly applicable to all laboratory and industrial combustion devices that wish to incorporate PLB as an energy source and will ideally serve as an important resource for the optimization of PLB commercial applications.

The objectives of this work are:

- Understanding how geometric design parameters of an internally mixed air-blast nozzle affect droplet size, distribution and other spray characteristics in order to establish trends and determine their underlying cause
- Understanding how primary atomization occurs within the internally mixed air-blast nozzle
- Determining the accuracy of known spray correlations for use with this nozzle
- Understanding how nozzle design and the resulting spray characteristics and patterns influence PLB combustion, stability and emissions
- Designing an optimized nozzle for use with crude PLB in order to establish that this fuel is viable in an industrial setting by demonstrating:
  - The potential for combustor “cold-starts” without a preliminary heat-up using a secondary fuel
  - That such a flame can remain stable and anchored, without the use of a pilot flame, while maintaining consistent levels of pollutant emissions
  - That the flame can be desensitized to burner operating characteristics, in particular atomizing airflow rates
Chapter 2

2 Literature Review

2.1 PLB Production

PLB is produced using the fast pyrolysis method which involves the decomposition (or thermal cracking) of the biomass feedstock in the absence of oxygen at 400-500°C [41]. The pyrolysis vapours have a short residence time of up to two seconds during processing, before being quenched to form a liquid biofuel. Longer residence times will reduce the fuel's average molecular weight, but also decompose the feedstock into additional non-condensable gases which will lower the liquid fuel yield [41]. Process yields are around 60-75% [13], [41], [42] with by-products in the form of heat, char and non-condensable gases representing around 30% of the biomass energy. The char and non-condensable gases can then be used as a fuel source for maintaining the pyrolysis oil production process which requires only about half (15%) of the available by-product energy content [42], [43]. The only real energy lost during fuel production is in the form of heat amounting to approximately 5% [44]. A schematic for the fast pyrolysis production process along with an image of the product fuel are shown in Figure 1 below.

Figure 1: A schematic of the fast pyrolysis process [43] (left) and the final PLB product [45] (right)
Char removal is important as it is a vapour cracking catalyst of the pyrolysis fuel which if not removed will reduce the process yield [41], [43], age/polymerize the final PLB product [43], [46] and lead to PM emissions during combustion [47], [48]. Char is typically removed with the use of cyclones prior to vapour quenching [41].

2.2 PLB Properties

PLB provides a promising and inexpensive alternative to fossil fuels, however its composition compared to that of standard fuels necessitates special considerations with respect to combustion. Typical fuel properties of PLB and other common fuels are presented in Table 1 below. Properties vary for PLB based upon feedstock and processing so typical ranges are given. Testing procedures and standards for these various PLB properties are also available [31], [32], [49]. PLB is comprised of two phases: the first phase has a high water content and forms an aqueous solution with a large variety of volatile, low molecular weight (LMW) compounds and the second phase is composed of water insoluble, non-volatile, high molecular weight (HMW) compounds in a tar-like phase. The LMW aqueous phase represents about 60-80% of the fuel's weight (depending on the feedstock and processing) [14], [32], [33], [36], [50]–[53], but it is the high molecular weight compounds which contain the majority of the fuel's energy content [52]. A lower average molecular weight of the fuel correlates with a lower fuel viscosity, beneficial for spray atomization. PLB is considered to be a high viscosity fuel, especially compared to transport-grade fuels, such as diesel or gasoline.
Table 1: PLB and common fuel oil property values [15], [19]–[21], [29], [32], [36], [54]–[56]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Typical Range of PLB</th>
<th>ASTM D7544, PLB Grade G and D</th>
<th>No. 2 Fuel Oil (Diesel)</th>
<th>No. 6 Fuel Oil</th>
<th>Test Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water Content</td>
<td>wt%</td>
<td>15 – 30</td>
<td>30 max</td>
<td>0</td>
<td>0.1 – 7</td>
<td>ASTM E203</td>
</tr>
<tr>
<td>Kinematic Viscosity</td>
<td>cSt at 40°C</td>
<td>10 – 90</td>
<td>125 max</td>
<td>2 – 6</td>
<td>200 – 2000</td>
<td>EN ISO 3104, ASTM D445</td>
</tr>
<tr>
<td>Surface Tension</td>
<td>mN/m at 25°C</td>
<td>36</td>
<td>-</td>
<td>28</td>
<td>23</td>
<td>-</td>
</tr>
<tr>
<td>Acidity</td>
<td>pH</td>
<td>2 – 3</td>
<td>-</td>
<td>7</td>
<td>7</td>
<td>ASTM E70</td>
</tr>
<tr>
<td>Density</td>
<td>kg/m³ at 20°C</td>
<td>1100 – 1300</td>
<td>1100 – 1300</td>
<td>830 – 860</td>
<td>900 – 1000</td>
<td>EN ISO 12185, ASTM D4052</td>
</tr>
<tr>
<td>Solids Content</td>
<td>wt%</td>
<td>&lt;1</td>
<td>2.5 max (G), 0.25 max (D)</td>
<td>-</td>
<td>0.1 – 1</td>
<td>ASTM D7579</td>
</tr>
<tr>
<td>Ash Content</td>
<td>wt%</td>
<td>&lt;0.3</td>
<td>0.25 max (G), 0.15 max (D)</td>
<td>&lt;0.001</td>
<td>0.05-0.1</td>
<td>EN ISO 6245</td>
</tr>
<tr>
<td>Carbon Content</td>
<td>wt%, dry</td>
<td>50 – 60</td>
<td>-</td>
<td>87</td>
<td>85 – 88</td>
<td>ASTM D5291</td>
</tr>
<tr>
<td>Hydrogen Content</td>
<td>wt%, dry</td>
<td>6 – 9</td>
<td>-</td>
<td>13</td>
<td>10 – 11</td>
<td>ASTM D5291</td>
</tr>
<tr>
<td>Nitrogen Content</td>
<td>wt%, dry</td>
<td>&lt;0.5</td>
<td>-</td>
<td>&lt;0.01</td>
<td>0.3 – 0.5</td>
<td>ASTM D5291</td>
</tr>
<tr>
<td>Sulfur Content</td>
<td>wt%, dry</td>
<td>&lt;0.05</td>
<td>0.05 max</td>
<td>0.1</td>
<td>0.8 – 1</td>
<td>EN ISO 28846, ASTM D5453</td>
</tr>
<tr>
<td>Oxygen Content</td>
<td>wt%, dry</td>
<td>30 – 40</td>
<td>-</td>
<td>0</td>
<td>1</td>
<td>By Difference</td>
</tr>
<tr>
<td>Adiabatic Flame</td>
<td>K</td>
<td>1700 – 2000</td>
<td>-</td>
<td>2229</td>
<td>2238</td>
<td>-</td>
</tr>
<tr>
<td>Temperature</td>
<td>Flash Point</td>
<td>40 – 110</td>
<td>45 min</td>
<td>60 – 90</td>
<td>60 – 80</td>
<td>EN ISO 2719, ASTM D938</td>
</tr>
<tr>
<td></td>
<td>Pour Point</td>
<td>-36 – -9</td>
<td>-9 max</td>
<td>-15</td>
<td>15</td>
<td>EN ISO 3016, ASTM D87</td>
</tr>
</tbody>
</table>

2.2.1 Water Content

The high water content (15-30wt%) of PLB is from a combination of pyrolysis reactions and the moisture content in the original feedstock [20], [42], [57], [58]. A higher degree of vapour cracking during the pyrolysis process leads to a higher amount of water in the fuel product [15]. A high water content in the fuel leads to combustion/flame instabilities because it results in a lower energy density, delayed/poorer ignition from slow vaporization and reduced flame temperatures and combustion rates due to the high heat capacity of water [20], [32], [54], [58]. On the other hand, the elevated water content in the fuel can be beneficial by reducing the fuel's rate of aging, viscosity and NOx and soot emissions [15], [20], [57], [58].

2.2.2 Oxygen Content

Pyrolysis fuel has a high oxygen content (30-40wt% dry) because it contains most of the oxygen in the original feedstock [20], [21], [57]. This is a major distinction between PLB and petroleum...
fuels which are not oxygenated as shown in Table 1 PLB oxygen content (on a dry basis) decreases with increased thermal cracking during PLB production [59]. The high oxygen content is responsible for the fuel’s low energy density (in conjunction with the water content), corrosivity and chemical instability/aging [15], [20], [21], [57]. The organic oxygen content of PLB reduces the amount of oxidizer needed for stoichiometric combustion conditions, thereby lowering the air/fuel ratio during combustion and increasing flame temperatures [15], [20], [21].

2.2.3 Heating Value

The energy density of PLB is typically about 40% of that found in standard fossil fuels on a per mass basis. However, it is the volumetric flow rate that is most important for combustion and storage considerations and, due to PLB’s higher mass density, its energy content on a volumetric basis is closer to 55% (about 20 MJ/L versus 36 MJ/L) of conventional petroleum fuels [15], [21], [57]. The lower energy density of PLB results in a comparatively higher fuel flow rate during combustion for a fixed energy throughput, requiring combustor modifications, especially with respect to the nozzle and injection system in order to maintain adequate spray atomization [15], [21], [57], [60].

2.2.4 Acidity

One of the most common challenges with PLB is its acidity (a pH of 2-3 compared to 7 for conventional fuel oils), due to the LMW components [21] which causes corrosion that worsens at elevated temperatures and higher water contents. This fuel therefore requires all interacting components to be manufactured from corrosion resistant materials, such as stainless steel, which is usually more expensive than standard components [15], [19]–[21], [58], [61]–[64].

2.2.5 Fuel Aging and Stability

Fuel aging occurs during long-term storage as the LMW compounds react to become HMW compounds (also known as polymerization) [12], [19], [46], [54], [57], [65]. This happens because of the rapid quenching used during the fast pyrolysis production process, which prevents the product oil from reaching an equilibrium state. If given an appropriate time and temperature, the chemical species contained within the fuel will chemically react to approach equilibrium [46], [57], [66]. Fuel stability is therefore somewhat determined based on feedstock and
Temperature is the dominant parameter which determines the rate of aging (occurring rapidly above 80°C) and thus to prevent or reduce aging related reactions from taking place, PLB must be refrigerated during storage [12], [54], [57], [68]. An ideal storage temperature is between -5 and -10°C where no aging occurred [21]. Additionally, the presence of char, and specifically the alkali metals on the surface of the char, such as potassium, promotes polymerization reactions which greatly increase the rate of aging, so char removal improves fuel stability [55], [69]. Aging can also cause the fuel to separate (which can be prevented with mechanical mixing [7], [55]), decrease in volatility and heating value and increase in viscosity, non-evaporative components (including solids) and water content; all of which degrade atomization and combustion processes and increase emissions [12], [15], [21], [36], [38], [51], [53], [54], [57], [58], [68]–[70]. The rate of viscosity increase across several studies is graphically depicted below in Figure 2.

Figure 2: A comparative assessment across several studies of the effect of temperature on the rate of viscosity increase [46]

2.2.6 Solids Content

The suspended solids within PLB are composed of organic char and also contain, in part, inorganic ash that cannot be burned [35], [36], [43], [57], [71]. The fuel's solid content is typically under 1.0wt% (as shown in Table 1) and acts as a catalyst, even at room temperature,
increasing the rate of fuel aging [15], [43], [46], [57], [68]. Additionally, the solids content in PLB causes clogging, erosion and coke deposition. These are all problematic for the longevity, reliability and functionality of the nozzle/fuel injection system and combustor [15], [20], [57]. The average solid particulate is 5-10 microns in diameter, with 50% of particulates usually being smaller than 3 microns [15], [21], [32]. While large particles are removed from the fuel during the pyrolysis process using cyclones [41], they can agglomerate during storage up to a size of about 200 microns, further exacerbating the problems mentioned above [15], [21], [36], [57]. HMW compounds also form additional solid particles as the fuel ages over time, with the rate of change increasing with the initial solids concentration in the fuel [68]. Solid char within the fuel presents an additional problem if it is not fully oxidized during combustion as it can produce hazardous pollutants in the form of PM emissions [27], [47], [48], [57]. With efficient PLB combustion and good combustor design, ash should comprise nearly 100% of a device's PM emissions [20]. Furthermore, the alkali metal content within the ash was found to accelerate/increase the formation of CO and HC emissions from char particles during combustion [72].

2.2.7 Non-Volatile Residue

PLB is a mixture of over 300 components [12], [20], [21], [73] with a wide range of molecular weights and boiling temperatures (up to about 650°C [63]). The LMW components, such as water, begin to vaporize/boil at or below 100°C [54], [57]. Above 280°C, residues comprise the remaining non-volatile fraction, representing 35-50wt% of the original PLB [15], [54], [57]. Other studies with higher final distillation temperatures of 330°C showed non-volatile residues as low as 25wt% [74], 20wt% at 600°C [36] and 17wt% at 800°C. In oxidative (air) environments, all solid residue was completely oxidized around 600°C [63]. Fuel residue is typically measured using thermogravimetric analysis and is dependent upon feedstock, pyrolysis process methodology and post-production upgrading such as filtering (discussed in section 2.3). In comparison, light fuel oils like diesel are fully distillable [75] and can vaporize at about twice the speed of PLB [15]. The residual non-volatile residue from PLB is responsible for coking deposits and PM emissions if burnout within the combustion region is incomplete. Solid particle burnout is a slow, heterogeneous process requiring longer combustion residence times and PLB can therefore not be used in applications requiring the fuel to be fully evaporated (i.e. fully
distillable), such as premixed combustion [36]. As PLB is not fully distillable, distillation cannot be used for fuel upgrading as is used for petroleum fuels.

The amount of residual char should be minimized which can be accomplished by optimizing the fuel's heating rate. When small droplets of pyrolysis oil are heated very quickly (≥10⁵ °C/min) through the 100-350°C range, significantly less char (only about one quarter) is formed [37], [76]. With smaller droplets being able to heat-up more rapidly, the importance of high quality spray atomization prior to combustion is evident. With proper combustor design and atomization generating small droplets and high heating rates, spray combustion studies have found that residual char or carbonaceous residue in the exhaust can be as low as 0.1wt% or less, relative to the initial weight of the fuel [77].

2.2.8 Minor Elemental Species

Wood-derived PLB, on which this review is based, contains fuel-bound nitrogen; this tends to dominate the fuel's NOx emissions with thermal NOx accounting for the balance [15], [20], [32], [36], [78], [79]. Fuel-NOx emissions (from fuel-bound nitrogen) typically form through a similar conversion pathway to the Fenimore Mechanism and are therefore relatively insensitive to temperature [27]. Conversely, thermal NOx are very temperature dependent and are formed comparatively slowly in the post-flame region via the Zeldovich Mechanism, but are usually reduced during PLB combustion as a result of the decreased flame temperature from the fuel's high water content [15], [20], [26], [27], [32], [70], [80]. NOx emissions are difficult to control, but localized fuel rich combustion zones have been shown to preferentially convert fuel-bound nitrogen into nitrogen gas rather than into NOx emissions [62]. Other combustion or post-combustion based NOx control strategies, in particular staged combustion, can be effective, but implementation is application specific [20], [21], [26], [80], [81]. Though NOx encompasses many pollutants, NO is the major constituent, accounting for up to 95% of NOx emissions in some practical combustion applications [81].

PLB tends to have little to no sulfur content and hence there are negligible SOx emissions, unlike from coal and many petroleum-based fuels [12], [20], [32], [82], [83]. SOx emissions harm the environment through acid rain, cause corrosion and poison catalysts, such as those in emission reduction devices [26], [60], [82], [84].
Soot is elemental carbon that forms in fuel-rich flame regions as a result of gas-phase reactions, unlike coke and char. Soot gives flames high luminosity (typically a yellow-orange colour) which results in higher thermal radiation [27]. With PLB spray combustion, soot usually represents only a small fraction of the overall PM emissions [36], [79]. This is because PLB is highly oxygenated and has a high water content which acts to suppress soot formation through a lower flame temperature and accelerate its oxidation from the increased hydroxyl radical concentration [27], [57].

2.3 Upgrading PLB

PLB suffers from many adverse fuel properties, most notably: low energy density, high viscosity, solid particulates, non-volatile residue, chemical instability and an incompatibility with conventional petroleum fuels [19]. However, PLB can be upgraded for more challenging applications to improve its chemical and physical properties, making it more similar to fossil fuels and more suitable for use in standard combustion systems. Physical upgrading methods involve altering specific undesirable fuel properties without the use of chemical reactions [40]. Some methods include: filtering out solids through hot gas or liquid filtration, blending or emulsifying with more conventional fuels and removing water using fractional/sequential condensation (which drastically increases fuel viscosity). Chemical upgrading methods are still in the research phase, but use catalytic conversion to create a higher grade fuel structures [73], [83] as detailed in Appendix A.

2.3.1 Physical Upgrading

Hot gas filtration is used to remove additional char left behind after cyclonic separation and can be conducted during the fast pyrolysis process. Cyclonic separation is not very effective at removing char particles smaller than 10 microns in size and so hot gas filtration can be used as a supplementary process to upgrade the pyrolysis fuel [46], [54], [57], [71]. Studies show that the average solid particle size after typical cyclonic separation is about 5 microns in diameter or smaller, but hot gas filtration can greatly reduce char amounts further while bringing the ash content down to below 0.01 wt%, removing virtually all solids (including alkali metals) [7], [49], [69] after which the fuel displays excellent stability [69]. Hot gas filtration however, does require the PLB vapours to spend additional residence time in a high temperature environment.
(with the filter heated to around 350-400°C [71]), leading to greater thermal decomposition (or cracking) and a yield reduction of about 10-20% because additional non-condensable carbon monoxide and hydrogen gases are formed [33], [41], [54].

Fuel filtering can be useful if the solids content is high or if the solid particles have agglomerated during storage, but filters can clog rapidly [84]–[86] and even after filtration, polymerization can form new solids within the fuel and so in-line filtering is often recommended [55]. However, liquid filtration is often unsuccessful [54] because the fuel's high viscosity presents significant challenges when pumping through a filter, particularly when conducted without heating or solvent addition. Furthermore, such filtering reduces the fuel's energy content and yield by unintentionally removing HMW compounds [15], [36], [54]. Recently, a liquid filtration study was successful in removing char and ash particles greater than 1 micron while having little effect on the PLB's composition or energy content. Fouling of the filter did occur and this process is still currently relegated to the research stage, but it shows promise [87].

To improve the combustion quality of PLB, it is often blended with polar solvents such as ethanol or methanol. The oxygenated compounds in PLB give it polar properties and consequently it is insoluble with hydrocarbon fuels, requiring emulsification with the aid of surfactants to form mixtures [54], [57], [58], [88]. Blending PLB with alcohol stabilizes the fuel by reducing the aging rate by a factor of up to 18 [89]. Blending with a solvent also helps the fuel's homogeneity [90] and increases the resultant heating value of the mixture [54] and its burning rate slightly [15] which correspondingly eases combustor residence time requirements. Furthermore, mixing PLB with alcohol can reduce the fuel's surface tension and viscosity (by up to half at 40°C [89]) and increase its volatility, all of which improve the blend's atomization and ignition characteristics, helping to stabilize the combustion process, thereby reducing emissions [15], [20], [25], [36], [54], [91] and expanding its operational range within spray combustors [62]. Alcoholic solvents can however be costly [21]. PLB/diesel emulsions, which can be stable even when a large majority of the mixture is PLB [58], present similar combustion benefits (with respect to viscosity, aging/stability, ignition and atomization) and cost disadvantages [25], [92].
2.4 Single Droplet PLB Combustion

While single droplet combustion is not the dominant mode of spray combustion in practical applications, it does occur in the case of larger rogue droplets and can be useful in understanding the overall spray combustion process. The number of these droplets should be minimal with proper atomization, but sprays form a wide range of droplet sizes with some inevitably falling into this upper size range.

Pyrolysis oils undergo different combustion processes than conventional petroleum fuels due to their chemical composition [15], [93]–[97]. Understanding these combustion characteristics, and also the role of spray atomization, is critical in order to design suitable combustors. PLB requires a strong ignition source, after which the fuel will burn with a stable, self-sustaining flame [19]. As a PLB droplet enters the combustion chamber, the water and other volatile compounds (LMW components) begin to vaporize and burn with a quiescent blue flame [15], [97], mostly in accordance with the $D^2$ law [7], [15], [59], however some studies have reported some deviations from the constant $D^2$ model due to PLB's multi-component composition [98], [99]. As burning progresses, the droplet can swell and distort as the HMW compounds polymerize [21], [94], [95], [97] forming a skin along the surface of the droplet. The exterior of the droplet continuously remains near the boiling point of the external polymerizing components which increases as lighter volatiles are vaporized. Beneath the droplet skin, LMW constituents continue to vaporize as they surpass their superheat limit, increasing the internal pressure of the droplet, which can eventually cause the skin to rupture and result in a micro-explosion [15], [93], [97]. The remnants of this explosion may then coalesce and again burn briefly with a blue flame before changing to a bright yellow flame as carbonaceous residue forms and undergoes sooty burnout [15], [93]–[97].

Droplet shell rupture may also occur without fragmentation, also similarly forming char residue [93]. The carbonaceous residue comes from the non-distillable portion of the biofuel and only burns along the surface rather than on a volumetric basis so combustion is much slower (potentially only 10% of the rate of volumetric combustion [100], [101]), requiring longer combustor residence times for complete oxidation. The carbonaceous residue can contain about half of the fuel's original carbon content and its size is similar to that of the original fuel droplet,
indicating the importance of effective fuel atomization prior to combustion for rapid particle burnout and complete oxidation in order to utilize the fuel's full energy potential [20], [74]. Insufficient or incomplete burnout results in particulate matter and gaseous emissions as well as char deposits [15], [36]. Ideally, the final sooty burnout phase should encompass only very fine particulates, assuming there has been effective primary atomization so that only ash remains. For comparison purposes, diesel fuel undergoes quiescent, sooty burning throughout its entire combustion process [15], [57] with no solid residues other than soot [97]. However, heavy fuel oils can also experience micro-explosions followed by coking during subsequent burnout [59].

Micro-explosions offer a convenient secondary atomization method to improve combustion and fuel burnout. However, droplets in practical spray combustion devices have a greater tendency to undergo group combustion and vaporization, reducing heat transfer rates and reducing the likelihood of micro-explosions occurring [15], [20]. Studies have yet to visually confirm the occurrence of droplet micro-explosions in practical PLB spray combustion applications [36].

### 2.5 Spray Atomization

Atomization is one of the most critical aspects of combustion. Smaller droplets have a larger relative surface area, allowing for more rapid heat transfer and increased vaporization since vaporization is inversely related to the droplet diameter squared [39]. Enhanced vaporization greatly improves ignition and air/fuel mixing while reducing the flame length and required fuel droplet residence (burnout) time. Therefore, better atomization ultimately improves combustion processes and reduces emissions [33], [85], [100], [102]–[104]. The spray pattern and cone angle are also important aspects of a combustion atomization and injection system, strongly influencing mixing and flame characteristics and facilitating recirculation dynamics.

In general, atomization is the break-up or disintegration process of a liquid jet or sheet occurring when disruptive forces overwhelm consolidating ones. It is by nature a random and unsteady process [100], [102]. Efficient atomization relies predominantly upon three fuel properties: viscosity (μ), surface tension (σ) and density (ρ); viscosity is generally considered to be the most important property and density the least important [20], [32], [100], [103], [56]. Fuel sprays in combustion applications are often compared by their Sauter Mean Diameter (SMD) which
represents a measure of the volume to surface area ratio of an average droplet within a given spray, as calculated from the equation below [20], [33], [100], [101].

\[
D_{32} = \frac{\sum N_i d_i^3}{\sum N_i d_i^2} \text{ (\mu m)} \quad [100]
\]

The effects of atomization are even more important when working with difficult-to-burn fuels like PLB. Typically, for light fuel oils, simple pressure or pressure-swirl atomization is used, creating droplets in the range of 20-60 microns while for more viscous heavy fuel oils, steam/air or rotating cup atomization is used more frequently. For light fuel oils, minimal or no fuel preheating is required while for heavy fuel oils, fuel preheating to 85-140°C is common with far higher atomizing pressures in order to get droplets in the 50-70 micron range [85], [105].

2.5.1 Atomization Mechanisms

Fuel is injected in the form of a jet or sheet, depending on the configuration of the nozzle. The most common nozzle designs for combustion applications are pressure and twin-fluid atomization. After injection, these liquid jets and sheets experience frequent and significant instabilities (oscillations, waves and perturbations) which are amplified by a high degree of turbulence and aerodynamic shear, eventually causing the liquid to disintegrate into droplets whose characteristics depend on flow rates, physical properties and nozzle design [100], [102].

Turbulence enhances disintegration of the liquid as surface waves and roughness form while aerodynamic forces increase with increasing relative (air to liquid) velocity and air density. Increasing liquid surface tension, viscosity and sheet/jet thickness, along with decreasing turbulence and relative velocity, all result in a larger spray SMD.

For most liquid jets, aerodynamic drag tears their surface into fine ligaments from which surface tension acts to form spherical droplets where they have a minimal surface energy and resist any

\[1\] Within this Section 2.5.1, most information is from the textbooks written by Liu [102] and Lefebvre [100]. The first applicable sentence in each paragraph will be cited and all subsequent sentences will similarly apply to the initial citation unless otherwise noted.
further distortion or disintegration [100], [102]. Smaller jets break up more easily because they are susceptible to a wider range of disturbances, determined by jet circumference. There are however several different modes of break-up depicted in Figure 3 depending on the Reynolds number (influenced strongly by jet velocity) and the characteristics of the surrounding medium.

![Figure 3: Jet disintegration mechanisms with increasing Reynolds number to the right](image)

In general, break-up length is proportional to the jet diameter and increases with liquid viscosity while decreasing with increasing liquid density and surface tension [100], [102]. Viscosity continuously acts to inhibit the growth of instabilities and to maintain the liquid's current geometric configuration, thereby delaying disintegration to ligaments and droplets [100], [102], [56]. Delayed disintegration causes break-up to occur further downstream from the nozzle where the relative velocity between the air and liquid is generally lower so aerodynamic forces are correspondingly reduced, leading to larger ligaments and thereby larger droplets [100], [102], [106].

Liquid sheets have a larger surface energy and an increased susceptibility to disturbances and instabilities as compared to jets, especially if they are curved, and as such tend to result in finer sprays [100], [102]. After injection, a sheet expands and thins against the contraction force of surface tension. High liquid surface tension and viscosity make sheets more resilient to disintegration, increasing ligament size, break-up length and spray SMD, while liquid density has a negligible effect [100], [102], [103]. Ultimately, the drop size distribution formed is dependent on ligament uniformity with small ligaments stemming from thin sheets at a high relative velocity [100], [102]. The basic process of atomization when viewed as the growth of
instabilities is similar for both sheet and jet configurations, however the detailed mechanisms do differ and are described in detail within the textbooks written by Liu [102] and Lefebvre [100], referenced throughout this section. Liquid sheet atomization modes are illustrated in Figure 4.

![Figure 4: Sheet atomization from rim (left), wave (middle) and perforated sheet (right) disintegration mechanisms](image)

Figure 4: Sheet atomization from rim (left), wave (middle) and perforated sheet (right) disintegration mechanisms [102]

For both jets and sheets, droplets can break up further, forming smaller droplets, when the magnitude of aerodynamic forces (increased with higher ambient pressure and/or density) within the combustion/spray environment exceed the consolidating force of surface tension, known as secondary atomization [100], [102]. Droplets will continue to disintegrate into smaller diameters until reaching a critical size where the forces are balanced. Droplet break-up time increases as the droplets approach their final critical size as forces equalize and liquid viscosity also acts to slow down this process. Atomization is a chaotic process and during secondary atomization, in addition to droplet disintegration, droplets may also collide and/or coalesce, forming a wide final size distribution [102].

### 2.5.2 Twin-Fluid Nozzles

Twin-fluid nozzles induce large interfacial forces, particularly shear [101], [107], between high velocity air and low velocity liquid (large relative velocity) to cause the liquid to disintegrate into ligaments and ultimately droplets [100], [107], [108]. Twin-fluid nozzles can be further broken down into internally mixed or externally mixed varieties. For internally mixed twin-fluid nozzles, much of their ligament and droplet formation, also classified as primary atomization, occurs within the nozzle [109], [110]. Externally mixed twin-fluid nozzles are a less efficient atomization scheme, but their design prevents the oxidizer from entering the fuel line in combustion applications, preventing flashback and improving safety. In both cases, secondary atomization occurs exclusively outside of the nozzle. Twin fluid air-blast nozzles can be internally or externally mixed, but are classified by their use of high amounts of air at a low
pressure for atomization [111]. Sprays are commonly in solid or hollow-cone patterns. Solid-cone sprays result in more uniformly sized droplets while hollow-cone sprays provide finer atomization [108], [112].

Twin-fluid nozzles produce finer sprays at lower injection pressures than pressure atomized nozzles. Compared to pressure atomization, which forms a spray by squeezing a liquid through a small orifice into quiescent air, twin-fluid nozzles provide a more even spray dispersion, have larger internal cross-sections to resist clogging, are effective over a wider operating range and allow for independent control of air and liquid flow rates [37], [79], [100], [101], [109], [113]–[115]. Twin-fluid nozzles however, are also more complex and are therefore, generally more expensive [15], [79], [101]. For twin-fluid nozzles, the air-to-liquid mass flow ratio (ALR) is typically the most crucial spray parameter affecting SMD and is directly related to the air/liquid relative velocity. Higher ALR values reduce the spray SMD and generally display asymptotic behaviour beyond a certain point [37], [116]–[123]. Furthermore, larger ALR values indicate a greater relative velocity between the air and liquid, meaning that more energy is available to break up the liquid/fuel. In reacting sprays, a higher atomizing airflow rate also induces strong turbulence that can enhance mixing, but consequently also increases shear rates, which if too high can cause the flame to extinguish or prevent (re)ignition.

Classic atomization mechanisms, where instabilities grow and ultimately form droplets, depending on initial liquid dimensions and viscosity, no longer occur for twin-fluid nozzles above a certain value of relative velocity and/or air/liquid impingement angle. Beyond this point, atomization switches from a classical mechanism to a so-called "prompt" mechanism where the liquid disintegrates almost instantaneously before instabilities can form or grow [106], [111], [124]. With prompt atomization, drop sizes are mainly determined by the magnitude of the air velocity component normal to the liquid, along with the ALR and surface tension [111].

Twin-fluid nozzles are relatively insensitive to liquid properties or those of the surrounding gas medium [100]. In particular, twin-fluid nozzles are far less sensitive to liquid viscosity than pressure atomizers, making them good for highly viscous fuels (viscosity had a minimal effect on atomization in two studies up to 100-120cP [115], [125]), particularly if internally mixed [100], [103], [104], [115], [125]. Therefore, twin-fluid atomizers are often used with heavy fuel
oils and PLB [56]. In combustion applications, twin-fluid nozzles also enhance fuel/oxidizer mixing, compared to pressure atomization, which can increase combustion efficiency and reduce pollutants [100], [113], [114], [126].

Air-blast atomizers are often classified as either of the plain-jet or pre-filming variety. Air-blast atomization is improved with smaller nozzle jet diameter/sheet thickness, lower liquid surface tension, viscosity and mass flow rate and higher ALR [113], [127], ambient pressure, atomizing air density/pressure and air/liquid relative velocity [100], [111], [113], [127], [128]. Typically, the pre-filming atomizers produce finer sprays as compared to the jet atomizers, especially when ALR and air velocities are low [100], [113] or when fuel viscosity is high [129], but plain-jet nozzles are much simpler in design [113], [114], [116].

Internally mixed twin-fluid (IMTF) nozzles are capable of producing fine sprays very efficiently. For these nozzles, SMD is lowest at the centre of a spray jet (and increases towards the spray periphery), corresponding to the highest droplet velocity where aerodynamic forces induce break-up and where coalescence is minimal [79], [107], [117], [120], [121]. Droplet SMD decreases downstream of the nozzle until the spray becomes fully developed (estimated to be about fifty times the nozzle exit diameter [121] though this will vary with nozzle design and operating parameters). Once fully developed, the SMD begins to increase from droplets losing momentum, colliding and agglomerating as well as from smaller droplets evaporating. In fact, as the spray develops, the droplet size distribution range tends to narrows [107], [118], [120]. Smaller nozzle outlet areas tend to produce finer sprays, though the effect of the outlet area decreases with larger ALRs [130]. An additional study [123] found that an equal outlet area, dispersed between a larger number of smaller holes, led to an increase in spray SMD, believed to be caused by the collision and agglomeration of droplets, with the effect greater at lower ALRs. Furthermore, for IMTF nozzles, increasing the atomizing air density can greatly decrease the spray SMD [112] and similarly, higher atomizing airflow rates and pressures reduce the break-up length and therefore also the SMD [112], [131]. However, the diameter of the liquid ports leading to the internal mixing chamber were shown to have no effect on the spray [119].

IMTF nozzles with eccentric outlets (in this case spaced 5mm from the centre of the internal mixing chamber) produce smaller spray SMDs than their coaxial outlet counterparts. This is
because after a liquid jet hits the bottom of the internal mixing chamber, internal air recirculation deposits the liquid on the internal surfaces of the nozzle and atomization ultimately results from a thin-film mode. The difference in spray SMD between eccentric and coaxial outlet nozzles diminishes at larger ALRs and in general, the spray SMD from IMTF nozzles with eccentric outlets is less sensitive to the ALR value [123]. This study however, did not examine the effect of internal pressure on atomization.

For IMTF nozzles at low ALR values, the emerging spray can be very unsteady [118], but steadiness can increase with liquid viscosity which also results in a narrower droplet size range [121]. Viscosity's effect on the spray SMD is actually fairly minimal for IMTF nozzles, but has been shown to negatively affect primary atomization while negligibly affecting secondary atomization. Even though the viscosity's effect on the spray SMD is muted, a greater proportion of large droplets are present, reducing spray quality, so SMD alone is insufficient to fully characterize the spray and a size distribution is also useful [121]. It should be noted that all IMTF papers discussed had nozzles of differing designs so results indicate useful trends, but the direct applicability of the results would likely vary.

2.5.3 Spray Parameters

The spray half-cone angle is measured from the spray periphery with respect to a vertical axis down the centre of the nozzle (throughout this thesis the "spray cone angle" refers to the full-cone angle). Narrow cone angles form narrow flames which reduce mixing and lead to localized rich/lean zones while wider cone angles form more diffuse and shorter flames which result in more uniform combustion [81]. In general, wider cone angles result in smaller average droplet sizes [112] and cone angles tend to decrease with more viscous fluids [21], [39], [132]. For IMTF nozzles, the cone angle from a single jet increases with increasing injection pressure and ALR from an increased atomizing air velocity [118], [122], [123], [132]. For nozzles with eccentric outlets, spray cone angles were not found to be sensitive to ALR values [123].

Spray dispersion is the ratio of the spray volume to the volume of liquid contained within it. A high degree of spray dispersion allows for good air/fuel mixing which helps to promote evaporation, efficient combustion and lower emissions [21], [100]. Good spray dispersion also helps to prevent droplet coalescence downstream of the nozzle which can increase the SMD
Spray penetration is defined as the maximum distance a spray reaches when injected into stagnant air, governed by the jet's kinetic energy versus the aerodynamic drag of the gaseous medium. Compact sprays tend to have a high spray penetration while fine sprays with wide cone angles are affected more by air resistance (since smaller droplets have less momentum) and thus have a lower penetration. Over-penetration can cause fuel to contact combustor surfaces leading to quenching which greatly reduces combustion efficiency and increases emissions [100].

Droplet size distributions describe the volume percent (or frequency of occurrence if number-based) of various droplet sizes within a given spray. Non-uniform sprays will have populations of small droplets that evaporate quickly, helping to improve ignition, along with populations of large droplets which require longer residence times for complete evaporation and combustion.

### 2.5.4 PLB Spray Atomization

While PLB is a promising fossil fuel alternative, its physical properties (viscosity and surface tension) hinder atomization, further exacerbating the difficulties associated with its combustion and making it more difficult to compete with lighter fuel oils, such as diesel. PLB's viscosity can be upwards of 50 times that of diesel [133] (sitting between light and heavy fuel oils [63]) and its surface tension can be about 30% greater [21]. Therefore, the spray SMD for PLB is usually significantly larger than that of diesel sprays [7] resulting in longer flames [134] and many combustion issues discussed throughout this literature review. Furthermore, as a result of PLB's low volatility and solids content, the fuel is tougher to ignite and requires longer residence times for full burnout, meaning that PLB droplets would have to be smaller than those of conventional fuels. While significant challenges exist, pressure-swirl nozzles [25] along with internally [36], [79], [135], [136] and externally mixed [21], [133] twin-fluid nozzles have all been used to successfully atomize PLB.

A direct comparative spray assessment of PLB and diesel was conducted using a diesel engine injection system, corresponding to pressure atomization. At 50°C, the diesel spray had a 10 micron SMD and the PLB spray had a 100-110 micron SMD. At a fuel temperature of 70°C, the
PLB SMD was substantially reduced to between 35-45 microns and slightly reduced further to 30 microns at 90°C (still well above the SMD of diesel) [63]. It should however be noted that the PLB in this study was aged for one year prior to testing, so the differences in its SMD as compared to diesel are likely exaggerated. The substantial reduction in SMD as temperature increases follows a similar profile to a typical PLB viscosity curve with a rapid decline followed by an asymptotic progression and likely little improvement above 80°C. The viscosity of PLB decreases faster with temperature than the viscosity of light or heavy conventional petroleum fuels [55], [84], [137]. While different PLBs have different absolute values of viscosity, they all display the same temperature dependence and behaviour [32]. The addition of 12wt% ethanol at 50°C had a similar effect with respect to the spray SMD and the droplet size distribution as additional heating to 70°C [63].

Fuel preheating, up to about 80°C, is a simple first step for improving the atomization quality of PLB because it reduces the fuel's viscosity and surface tension, thereby lowering the energy required for atomization [63]. It should be noted that temperatures near or above 80°C can lead to rapid polymerization, nozzle clogging and severe fuel quality degradation so preheating should always be done in-line, just prior to fuel injection [15], [20], [21], [32], [39], [63], [138]. With adequate preheating, the viscosity of PLB will likely be between 5-10cSt [39] which is good for pumping, atomization, ignition, combustion and minimizing emissions (explained in detail in Section 2.6). Even with effective injection system design and preheating, consideration should be given to the PLB droplet size distribution since even with an acceptable spray SMD, some large droplets can form. Larger droplets can fail to evaporate or ignite, reduce flame stability through poorer ignition and mixing and result in incomplete combustion and/or wall quenching, forming deposits and emissions [7], [21], [25], [101], [139]. In spray experiments, PLB formed wider spray distribution size ranges than did water or number two (diesel) fuel oil [139].

When atomizing PLB, because of its higher viscosity, more atomization energy is required [79]. For twin-fluid nozzles, this corresponds to a higher atomizing air pressure, relative velocity or ALR and for pressure atomizing nozzles, a higher liquid pressure. This greater amount of energy imparted to the droplets however, can increase flame shear, causing lift-off or blow-out. This
then increases the likelihood of larger droplets blowing through the combustion zone prior to complete burnout, causing a lower combustion efficiency and higher emissions [64].

One of the great challenges with pyrolysis oil and its spray behaviour is the lack of standardization between fuel batches and suppliers, for instance with respect to fuel viscosity [15], [21], [30]–[32]. Such differences can be drastically decreased by preheating the fuel or blending with alcohols, resulting in far more consistent spray behaviour [33], [38], [91].

PLB has a surface tension of around 36mN/m at room temperature (25°C), dropping by about 5mN/m at 80°C [56], in a linear fashion, matching the findings from a separate study [101]. The surface tension is dependent on the fuel's water and char content which is why its surface tension is higher than heavy fuel oils, which measure about 23mN/m at 40°C, and diesel fuel, which measures about 28mN/m at 25°C, both of which contain no water [15], [56]. Additionally, the density of PLB varies very little with temperature, exhibiting negligible thermal expansion.

The higher mass flow rate (and therefore linear momentum) of PLB, due to its lower energy content, causes the fuel jet to penetrate deeper into the combustion chamber compared to diesel fuel [140]. The longer spray penetration is likely also due to the PLB's lower volatility, longer ignition delay and tendency to polymerization. Therefore, superior atomization and/or a larger combustor are required to ensure that the fuel does not contact the burner walls and quench.

Externally mixed twin-fluid atomizers have been successfully used in PLB combustion applications to form stable flames [21], [133], but one study tested both an internally-mixed and an externally-mixed nozzle, concluding that the internally-mixed twin-fluid configuration was much more effective with PLB [38].

### 2.6 Spray Combustion

Spray combustion generally occurs in a non-premixed or diffusion combustion mode and for these conditions, the flame sheet (i.e. the interface between the fuel and air) burns at a stoichiometric equivalence ratio of one. Under these conditions, the flame temperature is very high (flame temperatures peak at an equivalence ratio of about 1.1) imparting stability, but also reducing control of the flame parameters which can be useful for pollutant mitigation strategies.
Since there is no pre-mixing of the fuel and oxidizer, diffusion flames are inherently safer since flashback cannot occur. This type of combustion is mixing-controlled and both the mixing and chemical reaction rates increase with combustor pressure. Slow mixing, based solely on diffusion processes (or due to a low oxygen environment), results in long flames while turbulence allows for the formation of compact flames through rapid mixing, improving combustion performance. Poor mixing can result in incomplete and/or localized combustion, forming high amounts of pollutants. The bright yellow/orange colour associated with diffusion flames is typically the result of particulate matter [26], [27].

For low velocity gaseous jets, diffusion flames stabilize at the nozzle outlet, but as the jet velocity is increased, the flame will lift off because of excessive shear leading to localized extinctions, and if the jet velocity is too high, the flame will blow out [141]. Spray flames should follow the same dynamics with the added step of requiring rapid vaporization of the fuel after atomization. Spray flame stabilization therefore occurs where small droplets are able to vaporize and appropriately mix with the oxidizer. Upstream of a stabilized, lifted flame, air is entrained, helping the spray/reactants to vaporize and mix at its base. Air entrainment of a lifted spray flame increases with lift-off height and with co-flowing air streams [142].

In practical spray combustion systems, such as burners and turbines, flames usually envelop a large group of droplets simultaneously, causing them to undergo what is known as external group combustion (Figure 5) where peripheral droplets vaporize and burn more quickly than those near the centre of the group [27], [143]. Dense sprays within two-phase spray clouds decrease droplet burning rates by forming a saturated, non-flammable mixture that impedes thermal and oxidizer diffusion, preventing ignition near individual droplets. As droplet spacing increases, the flame approaches the droplet cloud and eventually penetrates its boundaries as an internal mode of combustion (Figure 5) becomes dominant. Fuel sprays with low volatility (such as PLB) and/or those that are injected at a high velocity can transition from an external to an internal combustion mode quickly, before significant fuel droplet burnout. In addition, the droplet size distribution within a spray cloud affects combustion rates. If droplet size decreases radially from the centre of the cloud, overall burning rates will be higher [143].
Figure 5: Spray combustion droplet burning modes [144]

Practical spray combustion systems that rely on diffusion flames usually operate lean (with excess air). This helps to ensure sufficient oxidation for complete combustion and minimizes the formation of localized rich zones that promote CO, HC and PM (soot) emissions [26]. In addition, higher amounts of oxygen also help to oxidize any soot that does form. UHC and CO emissions can also form in regions that extinguish (incomplete combustion) because they are too lean and/or where mixing is too rapid causing high shear rates [26]. Furthermore, for twin-fluid nozzles, if the atomizing airflow rate is too high, flame extinction or blowout can occur due to high shear rates, so proper operating conditions need to be determined for each combustion system.

2.6.1 PLB Spray Combustion

PLB undergoes the following combustion stages: (1) Evaporation and combustion of LMW volatile components, including the evaporation of water, alongside the thermal cracking and gasification of HMW components, and subsequently (2) the combustion of HMW components and the burnout of non-volatile components, such as char [36], [85], [90], [93], [145]. The
second combustion stage gives PLB its unique appearance as the non-volatile PM undergoes heterogeneous surface combustion, emerging from the flame as luminous streaks [47]. As previously discussed, the formation of non-volatile char during spray combustion can be suppressed with high heating rates and the formation of small droplets from effective atomization [37], [76], [93], [125].

Ignition issues with PLB occur because the LMW components that vaporize at low temperatures are oxygenated, so they have a low energy content and a small heat release. In addition, the water content of the fuel also evaporates, absorbing a significant portion of the available thermal energy [15], [36]. The longer ignition delays of PLB limit the amount of heat released near the nozzle, reducing flame stability [146] and flame seating/attachment. While PLB is hard to ignite, it burns steadily after ignition [30], [32], [137], [147] with high quality PLB capable of providing a greater heat release and brighter flames than conventional petroleum fuels [148]. Brighter flames can help to promote better fuel vaporization and burnout from increased radiant heat transfer [36].

Despite challenges, flames from PLB can be stabilized with the use of a flame holder (bluff body) or strong swirl, both of which can generate centralized hot-gas recirculation zone(s), turbulence and rapid mixing. The impacts of these effects are to heat and ignite incoming reactants, reduce the local flow velocity to more closely match that of the flame (reducing flame shear and increasing stability), extend the flame's lean blow-out limit, decrease the length of the flame, seat the flame on or near the nozzle, increase the fuel hot-zone residence time (by entraining droplets and residues) and reduce the CO, HC and PM emissions [20], [21], [36], [79], [90], [91], [133], [149]. With PLB combustion, central recirculation zone(s) are very beneficial and are often facilitated with the use of a hollow-cone spray nozzle.

PLB flames are usually of comparable or greater length than conventional petroleum fuels, but the flame length is dependent on a number of variables, including: atomization quality, fuel flow rate, nozzle jet velocity, jet penetration and recirculation within the combustor [19]–[21], [40], [64], [133]. The adiabatic flame temperature of PLB is 1700-2000K compared to 2200-2300 K for diesel. The low stoichiometric air-to-fuel ratio of PLB helps to offset the flame temperature reduction caused by its high water content [20], [25], [150], [151].
A study [101] looking at PLB atomization and combustion made several relevant findings. Pressure atomization with PLB produced comparatively poorer sprays than when using twin-fluid nozzles and so, during combustion, more flame stabilization strategies were required and higher emissions were produced. The greater spray dispersion from twin-fluid atomization also reduced PLB agglomeration, reducing PM emissions. Additionally, CO, HC and PM emissions all decreased with increasing atomizing air from increased spray dispersion and lower spray SMD, all near zero at high airflow rates. Comparatively, light fuel oil had consistently low emissions with little dependence on the airflow rate, likely due to its superior atomization. Compact flames gave faster combustion rates, reducing hot-zone residence times and CR burnout which increased PM emissions. Low atomizing airflow rates generated shorter and yellower flames, indicating PM from poor mixing, while increasing airflows lengthened the flame and reduced its luminosity (from reduced PM), width and emissions. Overall, PLB flame stability comes from the combustion of its LMW volatile components.

To ensure effective combustion, PLB should always be well mixed before use to ensure homogeneity and that heavier elements have not settled at the bottom of the fuel tank, affecting viscosity [90], [145], [152].

2.6.1.1 Burners, Boilers and Furnaces

Testing has been conducted in applications ranging from 10kW to beyond 10MW [148] and results have shown that PLB combusts well in conventional oil furnaces, boilers and burners (though some modifications are often required) [90] and can even provide a similar or greater heat release and efficiency as compared to light (number 2) fuel oil [153]. However, a separate study found that PLB burns slower and with a larger flame at a given power input, providing a lower heat release per unit volume and thus a lower power output if switching a conventional oil burner to PLB [90]. Emissions from stable PLB combustion were within acceptable limits when running solely on PLB with only minor modifications to the burner, though PM emissions were high from solids and ash content, polymerization and poorer atomization [15], [19], [67]. PLB’s bright, luminous, orange flame (from PM) provides substantial radiative heat transfer which is ideal for boilers and similar applications [40], [57], however carbon and ash surface deposits from the fuel can also form a shield, blocking the radiation.
PLB causes significant combustion challenges for furnaces, boilers and burners resulting from [15], [19], [105], [133]:

- poor ignition and flame stability due to poor volatility, water content and HMW components
- high viscosity causing poor atomization
- clogging, coking and PM from polymerization and/or fuel solids
- corrosion
- PM emissions and deposits

Pressure atomization is still the most common burner atomization method overall, especially with lighter fuel oils, though results with PLB have been mixed [7], [20], [21], [25], [79], [101], [139], [145]. An important concern with using pressure atomization with PLB is that solids within the fuel and/or from polymerization can clog the small internal passageways required to generate the high pressure necessary for good spray quality. Therefore, often PLB burner, furnace and boiler systems have air or steam atomizing nozzles with swirling/recirculating flows (producing compact and intense flames) to increase combustion stability and efficiency [15], [21], [38], [78], [79], [90], [91], [101], [135], [140], [152]–[154]. For twin-fluid systems, high air/steam atomization pressure improves the spray quality and reduces emissions, notably CO and PM, but only up to a certain point [79], [101]. Above this point, flame instabilities and blow-out are likely to occur from high shear rates.

Poor ignition quality, especially when starting the combustor or when using low quality PLB, can be managed through initial heating with conventional fuels, beginning PLB combustion when the system is between 500-800°C, and/or through the use of pilot fuels/flames, fuel blending or co-firing [5], [15], [21], [30], [38], [64], [85], [90], [91], [101], [105], [135], [145], [152], [153], [155]. If using a dual-fuel burner, preheating with conventional fuels is recommended and when the PLB stream is initiated, the original flame can be used as a pilot until stability is reached and the system can be operated solely on PLB [105]. Once stable combustion is achieved with a high combustor temperature, the pilot flame tends to have only a minimal effect [133], assuming heat losses are small (not usually the case with small lab-scale combustors [36], [62]). Radiative heating, for example from a combustor's refractory (insulative) lining, and hot-gas recirculation can be used to heat the incoming fuel and to increase the flame temperature, improving fuel vaporization and ignition which helps to stabilize the
flame and offset the effects of the fuel's high water content [15], [20], [21], [85], [90], [105]. Heating the primary combustion air to a temperature of 180-350°C also increases fuel vaporization and the flame temperature, promoting ignition and fuel burnout and reducing emissions [21], [38], [78], [85], [101]. Additionally, heating the atomizing air, if using a twin-fluid nozzle, can provide combustion benefits as well [21].

Co-firing PLB with a petroleum fuel or coal during start-up is another method to warm up the combustor, though with lower quality PLBs, co-firing may also be required during standard operating conditions [15], [19]–[21], [90]. Co-firing can stabilize and/or anchor PLB flames by enhancing ignition, resulting in high combustion efficiencies, minimal carbon residue, lower emissions and reduced localized extinguishment. A major advantage with co-firing is that few modifications are generally required (and hence a lower capital investment is needed) to function with PLB [7], [20], [21], [40], [44]. Tests in a 600kW boiler with 66% PLB, 17% ethanol and 17% natural gas generated stable, high efficiency combustion without fuel or air preheating, beneficial for on-demand applications. Emissions were also similar to diesel operation [79].

Within the injection system, the nozzle is particularly prone to blockages and clogging due to its narrow geometry and susceptibility is high during shut-down when the fuel is no longer flowing, but the combustion environment is still hot and radiative heat transfer from the nozzle's surroundings is high. This can easily heat the stagnant PLB sitting in the nozzle enough to cause rapid aging, polymerization and clogging [15], [67], [85], [90], [91], [145]. To prevent this, the injection system should be flushed with an appropriate solvent, such as ethanol, after every use [15], [38], [64], [67], [85], [101], [135], [145], [152]. The nozzle and injection system are also quite susceptible to corrosion, requiring the use of stainless steel components where direct contact with the fuel occurs (i.e. on all wetted parts) [15], [19], [20], [36].

With proper atomization, carbon residues and deposition can be minimized and when combined with a sufficient residence time for the non-volatile fuel components, complete fuel burnout can be achieved. For these combustion systems, proper atomization requires in-line fuel preheating between 40-90°C or 10-15% solvent addition (depending on the specific PLB's properties) to reduce the fuel viscosity to within the recommended range of 4-25cSt [15], [21], [78], [85], [90], [101], [105], [145], [152], [153]. While adequate residence times will allow for complete carbon
burnout, the inherent ash content within the fuel will still always cause particulate emissions and surface deposits since the ash will not react or burn. Furthermore, if fuel preheating is too high, above 80-90°C, in addition to polymerization, fuel boiling of the LMW components can occur, creating major instabilities from high intermittent shear rates and resulting in a pulsating flame [5], [15], [21], [68].

Table 2 illustrates typical emissions from PLB, which often fall between light and heavy fuel oils [36], [85], [105], [148]. With complete combustion from good atomization, adequate hot-zone residence time and proper mixing, low CO values (though still usually above those of light fuel oils) can be achieved with negligible HC emissions [36], [90], [101], [145], [153]. SOx are usually low or negligible since PLB has near-zero sulfur content [12], [20], [82], [83], [148], [153]. Studies indicate that NOx emissions from PLB are mainly the result of fuel-bound nitrogen, and so they are feedstock dependent [15], [36], [64], [78], [80], [85], [91], [105], [133], [140], [145], [152], with a lesser contribution from thermal NOx because the fuel's water content reduces combustion temperatures [152]. The ash and solids content of PLB can vary widely and therefore so too can the PM emissions because they are closely related [85], [152]. PM emissions can be higher than those from heavy fuel oils and are almost always greater than those from light fuel oils [90], [101], [105], [145], [153]. Consequently, the removal of solids and ash during PLB production is very important and it is recommended to keep the fuel's organic solids content below 0.1wt% and the inorganic solids (ash) content below 0.03wt% in order to minimize PM emissions as well as the potential for clogging, corrosion and erosion [20], [21], [30]. Testing has shown that PLB emissions from commercial applications can be odour free [14].

Table 2: Comparative summary of typical emissions between PLB and conventional petroleum fuels [5], [15], [19], [36], [85], [90], [105], [148], [153]
Small-scale burners are far more sensitive to the properties of PLB due to their lower residence times. In these smaller applications, proper atomization is even more critical and the viscosity should be on the low end of the recommended range (4-25cSt) [21]. Flame tests in a small-scale (10kW), uninsulated, swirl burner found that pure PLB had unstable combustion and the flame lift-off increased as the ethanol content decreased due to lower fuel volatility and a narrower flammability range. Therefore, it was concluded that blending with at least 10% ethanol was required to form a stable PLB flame with adequate emissions [72] which was confirmed by a second study in a 35kW, insulated burner [91].

Another set of experiments [36], [47], [62], [75] in a 10kW, uninsulated, swirl burner using a 80/20vol% PLB/ethanol blend came to a number of conclusions. These experiments found that the effect of swirl on PM emissions was greater than that from the atomizing air. The amounts of atomizing and primary combustion air used to increase the turbulent mixing, atomization quality and combustion efficiency were constrained by higher spray jet speeds that reduced the combustion zone residence time, by lean blow-out from flame shear and by the fuel's limited volatility. Preheating the primary air and fuel lowered the HC and CO emissions, but had a minimal effect on the PM emissions, which were mostly comprised of ash. Increasing the pilot flame energy lowered the CO emissions, reducing the effects of poor ignition, but it had no real effect on the PM or HC emissions. Preliminary testing revealed that stable combustion could not be achieved with a solid-cone spray, even with ethanol blending at 50vol%. Alternatively, hollow-cone sprays generated a stable flame with reduced HC emissions by strengthening the combustor's central recirculation zone.

2.6.1.2 Preceding Burner Research on PLB Combustion

The experiments conducted for this thesis were an extension of the research previously conducted [5] using the same combustion system (a 10kW, insulated, swirl burner) and internally mixed air-blast nozzle (mostly with the S2B6 air cap, described in Section 3.2.3). The findings of the earlier research are reported in the following paragraphs.

During initial experiments, combustion was highly unstable as a result of low primary air swirl which induced large flame instabilities. Instabilities were reduced by placing the swirl generator
closer to the combustor inlet, reducing the cross-section of the burner throat to increase air velocity and ensuring airflow was circularly symmetric.

The high temperatures from the PLB flame (thermal feedback) caused significant coking on the external surface of the nozzle due to fuel polymerization which eventually built up enough to deteriorate atomization and increase emissions. To reduce coking, the atomizing airflow was increased to reduce the spray SMD, but due to the low fuel volatility, the tolerable atomizing air range for the flame was narrow and this caused flame instabilities, lift-off and blow-out. Swirl number and nozzle position were also varied, but proved ineffective, so the nozzle outlet was instead redesigned with smaller external orifices (reduced spray outlet area) to reduce coking through better atomization. The S2B6 design, with a reduced outlet area compared to the standard nozzle, improved coking, but further reductions in outlet area worsened coking. A smaller overall nozzle design with a narrower internal mixing chamber, resulting in a higher air/fuel relative velocity, significantly reduced coking, but its small outlets quickly clogged. Therefore, the S2B6 nozzle was used to generate all following results and conclusions. It should be noted that, these experiments were run with peristaltic pumps which have discontinuous fuel flows and minor pulsations that could have contributed to the nozzle coking.

Emissions were very good for a small-scale combustion system. PM emissions were found to be about 90% ash and 10% carbonaceous residue at optimal operating conditions. NOx emissions were fairly stable since they were dominated by fuel-bound nitrogen. At the optimal operating conditions of the burner, CO and HC emissions were below their detectable thresholds of 10ppm and 3ppm respectively, but had a strong temperature dependence during transient operation (decreasing emissions with increasing furnace temperature). Primary airflow rates of 280-294SLPM (an equivalence ratio of 0.57-0.58) were found to form the lowest CO emissions. CO emissions increased when the airflow was lowered since less oxygen was available for CO oxidation and less turbulence and air/fuel mixing was induced, all reducing combustion efficiency. Increased primary airflow rates also increased CO emissions despite better mixing and a more compact flame since the flame temperature was reduced and flame shear was increased, creating localized extinction. In all instances, HC emissions were below the detectable threshold, indicating excellent combustion efficiency.
Higher swirl caused increased coking and higher fuel temperatures at the nozzle because of increased recirculation, but the PLB flame was very sensitive to the amount of primary air swirl and if it was too low, flame instabilities would form and could lead to extinguishment. Higher swirl required an increased equivalence ratio to minimize emissions since with greater swirl, air turbulence and mixing were increased and less primary air was therefore required.

Atomizing air had a large effect on ignition and emissions. Above the optimal atomizing air set-point, CO emissions were negligible until blow-out because droplets were small enough to completely oxidize within/near the combustion region of the lifted, unstable flame. Even at blow-out, HC emissions were undetectable because the furnace was hot enough to at least partially oxidize the fuel. Conversely, if the atomizing air became too low, CO and HC emissions increased rapidly. NOx emissions decreased moderately in regions with an unstable flame, but were relatively consistent because fuel-NOx emissions were dominant.

A methane/oxygen pilot flame was used to anchor the flame during operation and improve ignition (especially during start-up). At steady-state conditions, the flame would lift off as the pilot energy was reduced below 0.3kW and increasingly destabilize as the pilot energy dropped below 0.15kW. However, CO and HC emissions were always both below their detection limits regardless of pilot energy (including without a pilot flame). Without the pilot flame, the PLB continued to burn in an unstable manner and so, was considered to be self-sustaining. The pilot flame increased the burner temperature and thus, marginally increased the NOx emissions. The pilot flame and primary air/fuel heater were necessary for ignition and combustor heat-up during the transient stages of combustion. Once steady-state conditions were reached, the air heater could be lowered or turned off, having no effect on CO or HC emissions, indicating that the combustor's insulative lining was effective at maintaining the internal temperature and preventing heat losses. However, low primary air preheating temperatures increased nozzle coking when below 88°C, worsening as the air temperature decreased further. Over time, the coking on the nozzle would build up and could interfere with atomization, increasing emissions. Lower primary air preheating temperatures caused only a small decrease in (thermal) NOx emissions.
Chapter 3

3 Internally Mixed Air-Blast Nozzle Spray Analysis

This study investigated the effects of various design parameters of an internally mixed air-blast nozzle (IMAB) in order to determine important trends for optimizing the atomization of pyrolysis liquid biofuel. Studies have shown that internally mixed nozzles are an effective strategy for PLB atomization [38], but the key design parameters that contribute to the nozzle's effectiveness have not been researched extensively. This study was conducted based upon previous PLB combustion research in a swirl burner [136]. Previous findings indicate that PLB is very sensitive to the atomizing airflow rate and tends to blow-out easily due to its low volatility, restricting atomization to low airflow rates/pressures. In these earlier studies [5], with low levels of atomizing air, PLB atomization was very poor and fuel coking occurred rapidly. Better atomization is clearly essential, but the fuel's sensitivity requires a knowledgeable and targeted approach to improve low-pressure atomization to enhance the flame's stability and emissions.

3.1 Design of Spray Apparatus

3.1.1 Spray Enclosure

A transparent enclosure (shown below in Figure 6), measuring approximately 55cm in width, 65cm in length and 55cm in height, made from plastic, was fabricated to contain the spray. The enclosure fit onto a plastic base that increased the total height of the enclosure to about 70cm. The enclosure had rectangular openings on either side to accommodate the laser modules from the measurement system and an air intake at the top to simulate combustion conditions where swirling primary air enters around the nozzle. The nozzle assembly was clamped into place on the top of the enclosure using a circular clamp fitting (McMaster-Carr item number: 9578T29) that screwed into the enclosure, tightening around the nozzle extension tube and allowing for angular motion while ensuring the nozzle assembly remained vertical. A shaft collar clamp (McMaster-Carr item number: 4591K18) with a set-screw was then used to fix the height of the nozzle in place. The nozzle was designed to spray vertically downwards. The lateral
attachments at the base of the enclosure were used for clamping it to the table to prevent movement or laser misalignment during measurements.

For all experiments, a towel was placed on the bottom of the enclosure to help prevent any errant spray droplets from bouncing back into the air or measurement volume. In addition, a black covering was placed over-top of the enclosure to ensure overhead lighting did not influence the measurements.

![Figure 6: Design of spray enclosure](image)

### 3.1.2 Extraction System

A Shop Vac Heavy-Duty Portable Wet/Dry Vacuum was used to prevent the buildup of fine droplets within the enclosure. The vacuum was plugged into a Veriac Variable Transformer to allow for an optimized level of suction based on preliminary tests, detailed in Section 3.2.7.

A funnel was affixed to the end of the vacuum hose within the enclosure and placed directly underneath the nozzle, below the laser measurement volume. The chosen funnel was the widest available diameter that was shaped in a way to prevent droplets from bouncing off the sides and back into the measurement volume. Visual confirmations were conducted to ensure that the funnel contained the spray adequately.
3.1.3 Air Control

Airflow rates were controlled with an Omega FL-3840ST rotameter. This rotameter was rated to have an accuracy of ±0.83SLPM (2% of full scale) and a repeatability of ±0.10SLPM (0.25% of full scale) at standard conditions. Testing with a calibrated flow meter found a maximum deviation of 1.3% rather than 2%. Downstream of the rotameter was a 0-15PSIg Ashcroft 1084 Test Gauge with a rated error of ±0.075PSIg which was used to measure air pressure. The atomizing air line was pressure controlled by an upstream regulator and free from oil and particulates because of new filters installed just prior to the commencement of experiments.

3.1.4 Liquid Supply

These experiments were conducted with room temperature (21°C) distilled water supplied by Canadian Springs. Flow measurements were conducted using an OHAUS Adventurer Pro AV8101 scale (rated repeatability of 1.0g and linearity of ±0.2g) and a stopwatch. Measurements were done at 30mL/min corresponding to 30g/min, matching the fuel flow rate in previous combustion experiments [5]. Confirmation of scale accuracy and calibration was conducted with standard weights. A Cole-Parmer Gear Pump, model 74014-02, was used for the experiments. Water flow rate measurements were conducted during every test so calibration error is not a factor. At the nozzle's liquid inlet, another 0-15PSIg Ashcroft 1084 Test Gauge with a rated error of ±0.075PSIg was used to measure liquid pressure.

3.1.5 Nozzle Assembly

The nozzles used in these experiments were supplied by BEX Spray Nozzles [156] and are classified as internally mixed air-blast nozzles. The full assembly was comprised of a back-connect body where the atomizing air and water inlet attached, a 6" extension tube (0.75" in diameter), around which the assembly was clamped onto the enclosure, and an air and liquid cap which atomized the liquid into a spray with the use of high-speed pressurized air. The liquid cap (Figure 7) was made of 316 stainless steel, had three air outlets, each 2mm in diameter and one central liquid outlet that measured 0.51mm or 1.0mm in diameter depending on the model. The air cap was affixed to the liquid cap with the use of a threaded retaining ring as illustrated below in Figure 8. The standard air cap (Figure 7) had six holes at a full outlet angle of 70°, designed to produce a hollow cone spray pattern. The outlet holes measured 0.51mm or 0.94mm
depending on the model and were brass or 316 stainless steel. Nozzles in either material should have been otherwise identical (within manufacturing tolerances). When the nozzle was assembled, just downstream of the liquid outlet and within the air cap was an air/liquid mixing chamber measuring 1.7mm or 3.6mm in diameter depending on the model.

![Figure 7: JPL26B air cap (left) and liquid cap (right) [156]](image)

Figure 8: Schematic diagram of BEX's JPL26B internally mixed air-blast nozzle [5]

Standard purchased nozzle models included the JPL26B nozzle (JL40100 liquid cap and JPG60 air cap) and the JPL16 nozzle (JL2050 air cap and JPG15 air cap). The JPL26B nozzle has the larger dimensions listed in the previous paragraph (1.0, 0.94 and 3.6mm respectively), while the JPL16 nozzle has the smaller dimensions (0.51, 0.51 and 1.7mm respectively). Other than the dimensions specified (and those associated with them), the nozzles are otherwise generally
equivalent from an atomization standpoint. Many customized nozzle assemblies were produced to test various geometric design parameters. Some modifications were made to purchased standard stock items to customize them for experiments while other items were purchased as undrilled blanks to allow for the machining of specific designs. Liquid caps were always purchased as a stock item while air caps varied depending on the design requirements. Detailed manufacturing drawings for custom air cap designs can be reviewed in Appendix B.

3.2 Experimental Methodology

3.2.1 Laser Diffraction

Experiments were conducted using the Spraytec machine from Malvern Instruments Ltd. as depicted in Figure 9. The Spraytec device used laser light diffraction based on Mie theory to determine spray particle sizing and distribution on a volumetric basis. The system formed a 10mm diameter collimated beam produced by a helium-neon laser with a wavelength of 632.8nm. The laser was emitted from the transmitter module through the spray where droplets diffract the incident light mostly towards the receiver module. Based on the light's angle of incidence at the receiver, which resulted from its interaction with the droplet(s), a Fourier lens focused the light onto a set of concentric optical detectors. Large particles diffracted light at smaller angles and this light was focused near the central detectors while smaller particles had a larger diffraction angle and this light was focused more towards the outer detectors. These angles were independent of the droplet's motion [157].

![Spraytec System Diagram](image)

Figure 9: Spraytec system secured to the optical support bench [158]
All measurements were conducted with a 750mm lens which had 33 detectors and could resolve droplets as small as 2μm at a maximum distance of 500mm from the receiver module. If the droplet was further than 500mm, the light would not have been captured by the receiver. The 750mm lens could also detect droplets as large as 2mm in diameter. The software had the ability to extrapolate beyond either limit based on available data [157].

Once the laser light passed through the spray volume, it formed an overall diffraction pattern within the receiver and the system analyzed the light intensity as a function of the distance (incident angle) from the centre of the laser beam as demonstrated in Figure 10. The software then iteratively derived a particle size distribution from this scattering intensity pattern using optical models [159]. This process is depicted below in Figure 10.

![Figure 10: Laser diffraction pattern (left) and iterative particle size derivation procedure](image)

Prior to every measurement, the Spraytec system took a measurement of the ambient light or noise, called the dark background and a measurement with the laser active but no spray, called the light background, which accounted for any optical contamination and ensured a proper baseline light scattering on the optical detectors. This allowed the machine to differentiate between background light/noise and diffracted light from droplets. The machine also aligned itself prior to every experiment to ensure accurate results and remained stationary after alignment because it was affixed to an optical support bench running between the two laser modules,
imaged above in Figure 9. Each module could be moved along the bench, but was secured by clamps prior to each experiment [157].

Experiments were all conducted on a continuous basis, meaning that one measurement was taken every second. The Spraytec system had a performance verification before any experiments were conducted, and was deemed to be in proper operating condition. During all tests, the pump and extraction system were on a separate table from the Spraytec and no part of the enclosure had direct contact with the Spraytec, all in an effort to prevent and minimize vibrations from affecting the measurements. In addition, no bright lights or screens were near or visible from the perspective of the receiver.

3.2.2 Experimental Setup

The set-up involved two separate inlet lines (liquid and air) into the nozzle and an extraction system pulling the spray out of the enclosure. All connections were secured with Teflon tape where required to ensure that no leakage could occur. Prior to the commencement of measurements, all connections were leak tested and no leaks were found.

The atomizing air was delivered through a compressed air line, passing through a regulator to moderate the incoming pressure. Downstream of the regulator, the air then passed through a rotameter to precisely control the flow rate, followed by a pressure gauge and finally into the nozzle inlet. The distilled water was pulled into the pump from a basin, past a pressure gauge and then into a separate nozzle inlet. The rotameter's scale was calibrated twice, on separate days, with respect to pressure, in units of SLPM using a MesaLabs Bios DryCal Definer 220H Primary Flow Calibrator (with a rating of 1% accuracy) in order to properly measure airflow and ensure consistency between experiments and nozzles. Hence, using the rotameter's scale and an air pressure reading, the airflow through the nozzle could be calculated in SLPM. The pump was not calibrated since liquid flow rates were monitored and measured during each experiment using a scale.

3.2.3 Nozzle Designs

A total of 11 nozzle designs (air/liquid cap combinations) were manufactured and tested to examine the effects of internal liquid orifice diameter, air/liquid relative velocity, air/liquid
impact configuration and the number, total surface area, diameter and shape of the external spray outlet holes. In initial testing, the standard JPG60 air cap was observed to atomize the spray very poorly at the flow rates anticipated in the burner (Figure 11) and also at higher flow rates, the nozzles showed poor repeatability and significant variation, even between different outlets on the same air cap. For some holes, a visible liquid jet was evident. Preliminary tests showed that results were more consistent at higher air pressures and flow rates, therefore to improve initial findings, three of the six holes were covered with PC-SuperEpoxy. This allowed for more suitable airflow rates to be tested (closer to burner conditions) as a result of the higher air pressures and in addition, outlet spray variability and repeatability were also significantly improved (Figure 11). The epoxy was applied to the external surface of the air cap only and care was taken to ensure that it did not enter the mixing chamber.

Figure 11: Comparison of a standard JPG60 air cap (left) at 15SLPM with poor atomization and a customized design of the same air cap with half the outlet surface area providing good atomization at 14SLPM (right)

The standard JL40100 liquid cap was used with a standard JPG60 nozzle with three (S3B) and four (S4B) holes blocked to test the effect of external outlet area on spray SMD. The standard liquid cap was used in all experiments unless otherwise stated. A customized JPG60 nozzle was manufactured with six holes (S3B6), but an equivalent total external outlet area to the three blocked hole nozzle (S3B), each hole being 0.66mm in diameter to test the effect of outlet hole
size on atomization. A similar custom nozzle with six holes of 0.80mm diameter (S2B6) was also fabricated to simulate two blocked holes of the standard JPG60 nozzle, to further analyze the outlet area trend. The latter two nozzles were tested in the previous PLB combustion research [5] of which this body of work is a continuation. A nozzle with five blocked holes was determined to be incompatible with the current spray measurement set-up.

Another custom JPG60 air cap was created with an equivalent external outlet area to the S3B design, but this air cap had slots rather than holes (S3B-slot). The slots allow for smaller cross-sections with a much lower risk of clogging when using PLB and this nozzle was also designed to determine if outlet shape has an effect on atomization.

An internally mixed air-blast nozzle atomizes a liquid jet within a mixing chamber. Research shows that air-blast atomization can be enhanced by atomizing a liquid film rather than a jet [111]. To explore the applicability of this theory to the current type of atomizer, a novel air/liquid impact configuration was used by inserting a pin into the mixing chamber just downstream of the liquid orifice (S4B-Pin) as shown below in Figure 12. In theory, the liquid would spread out across the head of the pin and spill over the sides as a thin film to be broken up by the high-speed air within the mixing chamber. In addition, because the pin reduces the cross-sectional area of the mixing chamber, the air would be at an increased relative velocity when interacting with the liquid further improving atomization.

![Figure 12: The JPL26B nozzle with a pin (highlighted) inserted into the mixing chamber to turn the liquid jet into a thin film](image)

To test the effect of the liquid jet itself, the internal diameter of the liquid orifice was reduced on a JL40100 liquid cap. This was accomplished by inserting J-B Weld Underwater Epoxy
(McMaster-Carr item number: 7605A16) into the orifice and then drilling through the epoxy on a lathe once it had cured. The internal orifice diameter was decreased from 1.0mm to 0.57mm (JL40100-57). This liquid cap was then used with the S3B, S3B6 and S4B-Pin nozzles during a second round of tests.

Finally, to test the effect of relative air/liquid velocity when the fluids interact within the mixing chamber, customized JPL16 and JPL26B nozzle configurations were compared. The major difference between these air caps/nozzles from an atomization perspective was the diameter of the internal mixing chamber, as shown in Figure 13, which was 3.6mm for the larger JPL26B nozzle and 1.7mm for the smaller JPL16 nozzle, a 78% reduction in cross-sectional area. The JPL26B nozzle had a customized JPG60 air cap (SB72) with three 0.72mm holes so that its total outlet area matched that of the smaller JPG15 air cap with six 0.51mm holes (Section 3.3.3 shows that hole sizing did not affect the spray SMD when the total outlet area was constant). In addition, both liquid caps were altered to have matching liquid orifice internal diameters of 0.72mm. The JL2050 liquid cap was expanded from 0.51mm to 0.72mm on a lathe (JL2050-72) and a JL40100 liquid cap was modified again as specified in the previous paragraph (JL40100-72).

![Diagram of the internal mixing chamber diameter of the air cap.](image)

**Figure 13: Internal mixing chamber diameter of the air cap, varied to influence the air/fuel relative velocity during primary atomization**

All nozzle air cap and liquid cap specifications and combinations are presented below in Table 3.
Table 3: Air and liquid cap summary table

<table>
<thead>
<tr>
<th>Air Cap  (material*)</th>
<th>Liquid Cap</th>
<th>Number of Holes</th>
<th>Hole Diameter (mm)</th>
<th>Mixing Chamber Diameter (mm)</th>
<th>Liquid Orifice Inner/Outer Diameter (mm)</th>
<th>Used With</th>
</tr>
</thead>
<tbody>
<tr>
<td>S3B (SS)</td>
<td>-</td>
<td>3</td>
<td>0.94</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>S3B6 (Br)</td>
<td>-</td>
<td>6</td>
<td>0.66</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>S2B6 (Br)</td>
<td>-</td>
<td>6</td>
<td>0.80</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>S4B (SS)</td>
<td>-</td>
<td>2</td>
<td>0.94</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>S3B-slot (Br)</td>
<td>-</td>
<td>3</td>
<td>0.80 x 0.56</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>S4B-Pin (SS)</td>
<td>-</td>
<td>2</td>
<td>0.94</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>JPG15 (SS)</td>
<td>-</td>
<td>6</td>
<td>0.51</td>
<td>1.7</td>
<td>-</td>
<td>JL2050-72</td>
</tr>
<tr>
<td>SB72 (Br)</td>
<td>-</td>
<td>3</td>
<td>0.72</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>- JL40100</td>
<td>-</td>
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<td>-</td>
<td>1.0/2.6</td>
<td>-</td>
</tr>
<tr>
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<td>0.72/2.6</td>
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</tr>
<tr>
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<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.72/1.3</td>
<td>-</td>
</tr>
</tbody>
</table>

* SS – 316 stainless steel, Br – brass

3.2.4 Spray Visualization

Each nozzle setup was filmed with a 10 megapixel Kodak EasyShare Z1012 IS digital camera with the distilled water flow rate at 30mL/min and varying airflow rates. Filming was done with and without the laser. The laser helped to illustrate the shape, location and density of the spray.

3.2.5 Nozzle Alignment

To make comparable measurements, repeatable alignment of the laser with the spray was critical. The detailed methodology by which accurate alignment between the laser and nozzle spray jets was achieved is specified in Appendix C.

3.2.6 Laser Distance from Nozzle Tip

The design of the enclosure allowed the nozzle tip to be positioned about 37.5-125mm from the centre of the laser. An ideal measurement height was determined to be where the spray reaches a minimal value, also known as the fully developed length. This length denotes the end of
secondary atomization, beyond which droplet collision and agglomeration can become dominant, increasing the average SMD [118]. Testing at progressively larger distances showed that most nozzles reached their fully developed lengths around 47.5-57.5mm. The magnitude of the secondary atomization varied, but was often minimal, especially beyond about 40mm, which is in agreement with findings in the literature [118]. The fully developed length could vary drastically if a jet showed poor atomization, but testing was not being optimized for this scenario.

A more important consideration with respect to the nozzle height was where the spray cone began to protrude beyond the edge of the funnel, allowing more droplets to remain within the enclosure, potentially becoming suspended in the air and biasing measurement results. Droplets carried by air streamlines are disproportionally smaller and can affect measurement results or deposit on optical surfaces. The nozzle configuration with the widest cone angle was the S4B air cap. At conditions facilitating the widest spray cone, the spray hit the edge of the funnel, but was still contained when at a distance of about 5cm from the laser. Since this was close to the average fully developed length of most nozzles, 5.25cm was selected as the optimal measurement height. This height also happens to be about 50 times the standard JPG60 outlet diameter, matching the fully developed length proposed in a study by Li et al. [121]. However, testing air caps with smaller diameters confirmed that 5.25cm was the optimal measurement distance with no relationship to the proposed equation by Li et al. All spray measurements were made at 5.25cm for consistency purposes.

3.2.7 Extraction System Strength

As previously mentioned the extraction system power was controllable and could therefore be tailored to the measurements. The vacuum employed in the setup was very powerful, utilizing a 6HP motor. High extraction airflow rates could potentially pull fine particles more rapidly through the measurement zone biasing results towards the larger droplet population. On the other hand, if the suction was too low, fine particles could remain suspended in the air or potentially escape around the funnel and bias results towards the smaller droplet population. As such, testing was conducted to ensure suction was in an optimal range where results were not sensitive to the suction power.
Preliminary testing looked visually at the amount of fine particles passing through the laser beam on either side of the funnel, at deposits on both the transmitter and receiver windows and at the spray SMD with consistent nozzle positioning as the power was cycled from high to low, waiting 60 seconds at every increment of 10% (between 30-100%) of power. Testing showed that the buildup of fine particles was not a concern above 50% suction and that SMD and droplet deposition factors were minimized between 50-70% for different nozzles. An average power of 60% was chosen to be used during all experiments.

3.2.8 Vignetting

Vignetting occurs when fine droplets diffract light at large angles and at a distance too far from the receiver to be collected (i.e. the light does not reach the receiver's lens). This would act to bias the results towards the larger droplet population in the spray. This usually tends to be a concern for smaller sprays than what is studied in this thesis. The 750mm lens could detect 2μm droplets at a distance of 50cm which should have presented no concerns for the sprays in this research. At the height of the laser beam, the widest spray cone studied was measured to be 13cm in diameter, with the centre of the spray located less than 40cm from the receiver module, totaling about 46cm. During measurements, vignetting is indicated when there is a discontinuity in the scattering pattern on the outer optical detectors or they show a positive slope [157], [160]. Neither indicator was present on the smallest sprays measured. In addition, studies have recommended that to avoid vignetting, the entirety of the spray body be no further apart than 1.5 times the focal length of the lens, which was the case in this research [161].

3.2.9 Beam Steering

Beam steering is caused by a small change in the continuous medium's index of refraction which causes the laser beam to be slightly steered onto the innermost detectors. This would cause the Spraytec to think that there is a large concentration of coarse particles which do not actually exist. The most common causes of this measurement artifact are temperature variations and evaporation [157], [160].

Beam steering was found to be a considerable problem in these experiments. The cause of the significant extent of beam steering was not entirely clear, but was most likely caused by a combination of air turbulence, humidity from rapid evaporation and the temperature variation
between the compressed air used within the nozzle to atomize the water and the room air. Besides the water just affecting the humidity of the air, the evaporation may also have acted to cool it, increasing the temperature variation around the nozzle. Evaporation was a likely contributor to beam steering in this case as the volume percentage of artifacts sharply rose with finer sprays as tested with different nozzles at the same atomizing airflow rate, eliminating the effect/contribution from the atomizing air itself. Strong scatter was also visible on the innermost detectors when the extraction system was turned on without any spray or atomizing air, indicating that there was a significant contribution from the turbulent inlet air. To account for the extraction system, it was activated during background measurements and system alignment so that the machine could account for the beam steering effect and attempt to eliminate it. Since the turbulence generated was not constant, this was a useful approach, but did not solve the problem entirely. A similar approach was considered with the atomizing air, but testing showed that having it on during alignment gave no improvement with respect to beam steering, but having it on generated small amounts of fine particles during background measurements that could then reduce detector sensitivity to them during measurements, negatively affecting data accuracy.

Originally, the experiment was setup to have air entering from the top of the enclosure to mimic a combustion chamber as well as around the laser modules to act as an air curtain to prevent water from depositing on the optical windows. However, this setup resulted in extremely high air turbulence within the enclosure and beam steering artifacts accounted for 70-90% of the spray data which is unacceptable and likely made the real data inaccurate. Instead, it was found that having a single inlet from the top of the enclosure was preferable and reduced beam steering to between 5-50% depending on the SMD of the spray. To prevent air from entering around the laser modules, shrouds were placed around them and tape was used to create a seal so that no air could penetrate. The shrouds were positioned 1-2mm from the plastic enclosure to prevent any vibrations from reaching the laser system. Preliminary testing of identical sprays showed that results were consistent regardless of whether or not the suction was active during the background and alignment or what percent power the suction was set at, giving confidence that the beam steering was no longer adversely affecting results. This consistency of results did not occur prior to the implementation of these beam steering reduction methods. Of the available lenses, the
750mm lens is better able to handle beam steering issues due to its larger separation between the inner and outer detectors. This means that beam steering artifacts would affect fewer detectors [162].

The protocol for removing the remaining beam steering inherent in the experimental setup (as recommended by the manufacturer) was to examine the data and remove the inner detectors one-by-one until no coarse artifacts are visible. With experience, beam steering artifacts were clear, as depicted in Figure 14 below. Each experiment was analyzed separately for the artifacts and they were removed. Since the inner detectors control the coarse droplet population and SMD is a measure that is heavily weighted towards the finer droplets, in cases where there was some ambiguity as to how many detectors to remove, the effect was negligible on the results.

![Figure 14: Common indications of beam steering (highlighted in green) in spray data](image)

### 3.2.10 Sources of Error

Random errors are inherent within experimental procedures and are therefore unavoidable. In order to quantify this error, its various contributing sources need to be identified and minimized to the extent possible. Air calibration showed that results are generally accurate within 1%, agreeing with the rotameter's specifications. For all error determinations, the S3B nozzle was
used at its minimum airflow rate (about 14SLPM). Given that preliminary testing indicated that larger sprays were less consistent and would therefore display a higher degree of error, the minimum airflow rate for the S3B nozzle represented a below average spray and a reasonable upper bound for the spray SMD data. Any nozzles that performed worse or resulted in a larger SMD were unlikely to provide important data. Errors will be given in percentages and were assumed to remain as a consistent fraction of the spray SMD magnitude.

Atomizing air was set at the beginning of each experiment and the value was also recorded at the end to establish the average airflow rate during an experiment in case any change occurred. During almost every experiment, the airflow tended to drop slightly or remain constant. For a typical coarse spray SMD of about 55μm using the S3B nozzle, where size variability is likely higher than for finer sprays, a ±0.5 unit (as etched on the rotameter) change in airflow was allowable which resulted in a +2.6%/-1.5% change in SMD. The largest recorded rotameter deviation at the end of an actual experiment was -0.3 units, corresponding to an average error of -0.15 units or -0.5% SMD error during the test. A similar test for liquid flow was conducted allowing for ±1mL/min and it corresponded to an SMD error of ±0.4%. As previously discussed, the liquid flow rate was measured for every test based on the mass of water used over the course of the experiment.

One final minor source of error was from multiple scattering through the spray. The Spraytec system assumed that the angle of incident light was from a photon hitting a single spray droplet, however if this was not the case than this assumption will cause experimental error. The system allowed for these errors to be corrected using a "multiple scattering algorithm". Preliminary tests showed that when active, the algorithm increased SMD results by about 1μm for sprays between 24-52μm. Independent studies have indicated that multiple scattering is only a real issue in dense sprays where laser transmission is less than 40%, otherwise this algorithm creates more error than it prevents [161]. As such, the multiple scattering algorithm was not used in any experiments conducted for this research since laser transmission was almost always above 70%.

The stability of the data is hereby defined as the length of time required for the average SMD of a continuous spray to be consistent within a predetermined deviation from the actual mean value. To determine this, the laser was aligned with the centre of the largest spray jet (with respect to
SMD) from the S3B nozzle and the spray was measured for five minutes after a suitable warm-up period. At increments of 30 seconds (nine segments in total), the average spray SMD was determined for a period of 5, 10, 15, 20, 30, 45, 60 and 90 seconds and compared against the five-minute average SMD. A 2% deviation from the five-minute average in this test was deemed acceptable and this test was run on two separate days. The tests required 45 seconds for the maximum deviation to be within 2% of the overall average. Hence, each individual spray measurement required a duration of 45 seconds for accurate results.

The final key error contributor was repeatability. Every day a baseline measurement was taken with the same nozzle configuration and alignment procedure. A single air cap and liquid cap was used for this, never being disassembled throughout the test campaign. It was essential that the nozzle was in the same orientation each day so that the same outlet hole(s)/spray jet(s) were being measured. The test was similar to the other nozzle tests (outlined in the next section), except that the nozzle was left stationary during data acquisition for a full three minutes, comprising one minute of warm-up and then two minutes of useable data collection. In theory, this repeatability testing should account for all the other sources of error as liquid and air consistency and data stability would be incorporated by this test. This test was conducted twice per day with the average reported, 11 days in total. The repeatability/random error for this experiment was calculated to be ±9.0% with a standard deviation of 3.4μm on an average spray SMD of 53.4μm. The daily variation, average and standard deviation are all shown graphically in Figure 15. Furthermore, the difference with respect to the baseline average between the first and second round of experiments was 3.3%. For all graphs within this chapter, spray measurements will have error bars of ±9.0%. Looking at the actual experimental data, only a single test had a percent difference that exceeded ±9% between the first and second rounds of testing, indicating that the conclusions of this error analysis are likely conservative. In addition, the test that displayed the high variability had very poor atomization as evidenced by liquid jets visibly protruding from the nozzle so the disparity in results would be expected. While the independent error sources should be accounted for in the daily repeatability measurements, one textbook [163] recommends that as part of an error propagation analysis the elemental errors be added as the root of the sum of the squares. In doing so, the total error sums to 9.3% which is virtually unchanged since the daily repeatability measurement is dominant.
3.2.11 Testing Procedure

All testing was conducted with distilled water so any droplets that deposited on the laser module windows would evaporate without leaving a residue or affecting results. Spray measurements were only conducted with water since the set-up is a very time consuming and difficult process. Setting up the experiment for another fluid would have required all preliminary testing to be repeated and given the likelihood of fluid deposits on the laser windows if the fluid was non-distillable, some airflow would have likely been required around the laser modules as a preventative measure. In allowing this airflow, beam steering artifacts would have greatly increased and results would have been affected and not comparable to the water measurements. While studies examining more complex fluids and more realistic spray surrogates could be advantageous, the spray would likely still differ in performance from PLB and previous research highlighted that even the best surrogates can have questionable accuracy [79], requiring further testing for verification. Furthermore, in a combustion environment there are many additional factors that can greatly affect a spray such as temperature and thermal feedback from the flame [164] which cannot be replicated regardless. As such, this phase of the research was solely designed to elucidate major trends (present regardless of the liquid) on which to focus the combustion research.

Figure 15: Daily repeatability measurements with the average (green) and one standard deviation (red) indicated
Experimental analysis focused on two main sets of data for each nozzle at each atomizing airflow rate. Most importantly was the average spray SMD, followed by the average percent by volume of particles larger than 100μm in diameter (which would be most likely to cause emissions to form from incomplete combustion). Prior to conducting actual experiments, the entire system was checked to ensure that there were no air leaks. For each nozzle, three airflow rates were tested to establish a trend. A common airflow rate (14.4SLPM) was used across all nozzles which was the base-point in preceding PLB combustion tests [5]. Most tests were conducted twice (on separate days) to ensure consistent results with a baseline measurement conducted every test day for repeatability and error determination. The only sets of tests not conducted twice were the ones using the contracted liquid orifice on the JL40100 liquid cap. Three sets of tests were conducted in round one all indicating similar results and so only one of these was conducted a second time to confirm the trend. Various angular measurements were taken for each nozzle (as described in the following paragraph) with rotational accuracy ensured with the use of a protractor affixed to the top of the enclosure and indicator markings made on the outside of the shaft collar clamp allowing for a rotational accuracy within 1°.

There were two main nozzle categories. The first was nozzles with blocked holes that could be visually aligned with the laser due to the higher density of the spray jets. The second group had a greater number of external outlet holes and therefore a more diffuse spray and had to be aligned with the alignment pin. The nozzle alignment methodology is described in detail in Appendix C. The entirety of the spray should be measured and compared between nozzles. Larger fuel droplets at the spray periphery are less likely to be fully combusted and therefore contribute largely to pollutant emissions. Hence, just the centre of the spray jet is not enough to properly characterize the spray. For nozzles with clearly defined jets, preliminary tests showed that a rotation of 10° put the laser beam close to the edge of the spray jet with a noticeable increase in laser transmission percent, indicating a region of lower spray density. With a rotation of 15°, the laser was no longer within the main jet and the transmission percent was very high, indicating a small droplet population where the data was likely no longer a proper representation of the spray. Lastly, a 5° rotation showed little change from the central measurement likely because the spray volumes overlapped significantly. Measurements at the spray jet centre along with ±10° seemed to give the most representative results and a proper characterization of the
spray so these three measurements were repeated for each spray jet from each nozzle within a given experiment, ensuring the data was collected for a full 45 seconds at each angular position. For the more diffuse sprays (nozzles with six outlets), a similar increase in transmission percent occurred with rotation away from the outlet as the measured SMD changed to a maxima or minima directly between the holes (30°). Even right in-between the holes, both the transmission percent and the visual droplet population was significant so for these nozzles, one measurement at the centre of the outlet and one directly in-between was conducted totaling six measurements, each 30° apart. Since the Spraytec system measures along a cylindrical path through the entire distance between the transmitter and receiver, any measurements at or above 180° of rotation would be redundant for these six-outlet nozzles. Measurements at the outlets are critical as this is where flame jets emanate, but the off-centre or between hole measurements (assuming the spray density is high enough to be relevant) are important too since these droplets could potentially escape direct combustion and form pollutants, especially with a low-volatility fuel like PLB.

A sample experimental procedure for the nozzle testing was as follows:

- If the Spraytec or other systems have been unused for more than 30 minutes, run the spray, laser and associated systems as a warm-up for 10-15 minutes
- Setup all equipment for the next test
- Film the spray if necessary
- Turn off the room lights and turn on the extraction system
- Allow the Spraytec to take background measurements and align the laser
- Turn on the water pump and the lights and wait for the water to drip out of the nozzle
  - Water is started first to wet all internal surfaces and form most even spray possible
- Turn on the atomizing air and set the rotameter to the correct airflow rate
- Using a stopwatch measure the water flow rate until it is at 30mL/min
- Confirm the air flow rate is stable at the desired value
- Record the air and liquid pressure readings and the pump's RPM
- Confirm spray jet alignment with the laser if necessary
- Turn off the room lights and initialize data acquisition
- Allow the system to take measurements and warm-up for one minute
- Start the stopwatch to measure water flow rate and record the initial water mass
- Begin taking spray measurements for at least 45 seconds in duration at each angular location
- Once all spray locations have been measured, stop the data acquisition and turn on the lights
- Stop the stopwatch, record the final water mass and calculate the average water flow rate
- Check the rotameter and record the final airflow reading
- Make any additional notes or observations required and reset for the next experiment
3.3 Results and Discussion

The results presented below were directly used to guide the combustion experiments detailed in Chapter 4 of this research which sought to optimize the combustion stability and reduce the emissions of a pure PLB flame while understanding the effects of atomization and spray pattern on the flame. Spray measurements themselves were conducted to better understand the relationship between nozzle design and spray characteristics in order to formulate a targeted approach with which to optimize the PLB flame.

For the results detailed below, two analytical methodologies were examined. The first being that all measurements made within a given spray were weighted equally, providing a straight average around a nozzle for average SMD and large droplet volume percentage results. The second method gave the central spray jet measurements twice the weighting of other measurements conducted off-centre or between spray outlets. The logic behind this second method is that the central spray jet measurement would have a higher droplet density than other measurement locations and should therefore be weighted accordingly. It was found that the overall trends of both methods were identical with a difference of only 2.1% for average SMD with a maximum difference of 3.9%. Similarly, for the large droplet population the average difference was 1.9% with a maximum deviation of 6.7%.

3.3.1 Spray Cone Angle

Cone angle tests were conducted by letting the spray briefly fall onto a sheet of cardstock for several seconds and measuring the average spray width from the outside edge. The spray was diverted from the paper until the air pressure had risen and stabilized forming a proper spray. The cone angle increased with increasing air pressure, but the effect was minimal. The S4B nozzle, at a maximum airflow of 21.1SLPM and air pressure of 13PSIg, had an average half-cone angle of 49.3° at the height of the laser. When the airflow rate was reduced to the minimum value of 8.0SLPM and a pressure of 2.4PSIg, the spray angle remained fairly consistent at 48.0°. For the S3B nozzle, the variation between minimum and maximum pressure (3.2-8.9PSIg) and airflow (14.3-26.2SLPM) was between 43.9° at low airflow and 45.5° at high airflow. Nozzles with six holes had noticeably narrower spray cones with the S3B6 nozzle having a half-cone angle of 39.9° at 26.3SLPM and 9.0PSIg.
3.3.2 External Outlet Area of the Air Cap

For this set of experiments, air caps with differing external outlet areas were tested to understand the effect this has on atomization. Two types of air caps were used for these tests, while all used the same standard JL40100 liquid cap. Two nozzles (S3B and S4B) used the standard JPG60 air cap with the outlet area changed by blocking three or four outlets with SuperEpoxy. Two other nozzles (S3B6 and S2B6) used custom-made JPG60 air caps from previous PLB combustion tests on the swirl burner, providing an opportunity to better interpret those combustion results. The latter two nozzles both had six holes, but reduced total outlet area/diameter to match that of the standard JPG60 air cap with two and three blocked holes. As previously mentioned, the nozzle characteristics are summarized in Table 3.

These experiments therefore examined the effect of varying the outlet area from one-third to two-thirds of the standard air cap (two to four blocked holes out of six) and the effects were drastic. At 14.3 SLPM, using the S3B6 nozzle as a baseline, the S3B6 nozzle had an average SMD 68% smaller than the S2B6 nozzle. At 26.2SLPM, the SMD reduction was 30%. Similarly, restricting the outlet area from three to four blocked holes further reduced the average SMD by 40% at 14.3SLPM and 10% at 21.1SLPM (by interpolation) when the S3B nozzle was used as a baseline. As expected, the results were more exaggerated at lower airflow rates. In addition, a preliminary test of the standard JPG60 six-outlet nozzle at 26.4SLPM formed an average SMD of 56.3μm. The same nozzle after having three holes blocked then provided an average SMD of 26.5μm at the same airflow, a SMD reduction of more than half. The results are presented graphically below in Figure 16 and Figure 17.
Clearly, the reduction of the air cap's external outlet area had a dramatic effect across the measured parameters. By reducing both the average SMD and the population of larger droplets, the combustion efficiency can be raised and the pollutant emissions can be lowered in
subsequent combustion testing. Effects were more pronounced at lower airflow rates and equilibrated where the graphs began to show an asymptotic progression. These effects were due to the increase in air pressure which was evident when the graphs were examined versus air pressure rather than airflow as shown in Figure 18 where all four graphs collapse onto a single curve, indicating that pressure is the driving force behind this trend of enhanced atomization. The benefit of this approach is that similar air pressures and spray SMDs can be created with smaller amounts of air. However, the effect of higher air pressure and the improvement in atomization is coupled nearly proportionally with an inevitable increase in spray outlet velocity due to the reduction in outlet area (Figure 19). Spray velocity is also coupled to flame shear which promotes lift-off and blow-out and is a critical issue for PLB, due to its low volatility. The outlet spray velocity was calculated using the following equation directly below. Normally, converting SLPM to a volumetric flow rate requires a correction for the temperature, but since the flow rate was calculated at the rotameter, the air temperature was at room temperature and could be excluded from the calculation with a negligible effect. This is the case for both spray and combustion outlet velocity measurements.

\[ U_o = \frac{14.7(p_a)}{60000(p_{a,a})(\pi N_h r_h^2)} \text{ (m/s)} \]

Figure 18: Average SMD versus air pressure for the customized JPG60 air caps
Figure 19: Average SMD versus outlet air velocity for the customized JPG60 air caps

Figure 18 demonstrates the characteristic atomization curve for a twin-fluid nozzle. At low levels of atomizing air/pressure, the average droplet size changed exponentially while at high levels of atomizing air/pressure, the average droplet size changed asymptotically.

This experiment therefore demonstrates that atomization within this nozzle is directly dependent on air pressure, which can be dramatically increased via the reduction of external air cap outlet area rather than requiring higher airflow rates. However, this effect is mitigated by the concurrent change in outlet spray velocity which would affect flame shear and stability. At what airflow rate (or within what range) the seated flame lifts off from the nozzle or destabilizes for the various air caps can be used to show flame sensitivity, indicating whether this method is effective for enhancing combustion stability for low-pressure PLB injection systems. Based on re-analyzing preceding combustion research with PLB and the S2B6 nozzle [5], the flames began to lift off when the outlet spray velocity was around 80m/s.

3.3.3 Number/Diameter of External Outlet Holes of the Air Cap

In the previous section, the results of the S3B and S3B6 nozzles were shown graphically. The results had almost identical average spray SMDs (within experimental error ranges) in Figure 16, indicating that as long as total outlet area (and therefore air pressure) is maintained, the spray
SMD will be equal. Furthermore, the data showed that with more air cap outlets, higher levels of atomizing air can correspond to a reduction in the percent volume of large droplets, indicating the potential for reduced emissions. However, based on previous research, lower airflow rates are more critical since the flame detached above 14.5SLPM and blew out at 20SLPM [136], so combustion improvement would likely be minimal, at best, given the error bar overlap below 20SLPM. It is more likely that at the airflow rates of importance during combustion, the spray parameters will be unaffected by the number of outlet holes on the air cap.

Nozzles with a greater number of smaller holes (equivalent outlet area) formed a much more diffuse and even spray, indicating a higher spray dispersion for each jet. A spray less dominated by dense jets would improve air/fuel mixing and combustion. However, if the burner imparts a large degree of swirl (which also improves mixing), it is possible that the effects from a more dispersed spray would be inconsequential. In addition, dense sprays of PLB have shown a tendency to agglomerate, forming larger particles with a slower burnout, requiring greater combustor hot-zone residence times [101] so spray diffusivity could prove to be an important factor. How the spray diffusivity/density affects the flame's stability and emissions was examined during combustion testing. A larger number of holes while likely beneficial, also required a reduced hole diameter that if too small could lead to clogging issues due to fuel solids and polymerization as described in the literature review and previous PLB combustion research [5], hence a compromise would be required. Furthermore, as previously mentioned, a greater number of smaller diameter holes also corresponded to a reduced spray cone angle during tests.

3.3.4 Air/Liquid Relative Velocity

Twin-fluid nozzles are highly dependent on the interaction between the liquid and air, with greater forces between the fluids (due in part to their relative velocity) corresponding to enhanced atomization. This explains the beneficial effect of higher air pressure described earlier. The previous section affected the outlet spray velocity, but it is likely more effective to influence the relative velocity within the air cap's mixing chamber, where the air and liquid first interact. For this reason, a smaller air cap was tested which had a smaller internal mixing chamber diameter, corresponding to a higher relative air/liquid velocity. The smaller air cap had a reduced airflow cross-sectional area by 78% relative to the larger one (used in previous sections).
For this test, a standard JPG15 air cap was used with the JL2050-72 liquid cap and the JL40100-72 liquid cap was used with the SB72 air cap (a customized version of the JPG60 air cap) in order to match the external outlet area of the air caps. The liquid orifices of both liquid caps were equalized and other design aspects of the liquid and air caps affecting atomization were also equal so that the airflow cross-sectional area and therefore the internal atomizing air velocity would be the only variable.

The results, depicted graphically below in Figure 20, show a 16% difference in average SMD at 14.4SLPM for the smaller nozzle relative to the larger one, indicating a significant effect from the higher relative air velocity. This effect increases to 31% at 8.0SLPM and so results are again larger at lower atomizing airflows which is beneficial for PLB combustion. The total surface area of these nozzles was less than that of the S4B nozzle by about 11% so the enhanced atomization effect was significant given that it was on top of the improvement already instilled by the reduced outlet area. The effect is similarly beneficial with respect to the population of large droplets as shown in Figure 21. Based on these graphs, the JPG15 air cap and associated liquid cap appear to provide the best atomization with respect to both the SMD and large droplet population. Moving forward, the mixing chamber diameter appears to be an important design characteristic, contrary to what Kim et al. [123] concluded.

![Figure 20: Average spray SMD versus airflow rate](image-url)
As in earlier sections, results collapsed onto a single air pressure curve (Figure 22), again indicating that this is the dominant factor affecting SMD for this type of atomizer and a decrease of the mixing chamber diameter resulted in a further pressure increase. However, the results no longer all collapse onto the same outlet velocity curve which is important, as shown in Figure 23. A smaller internal mixing chamber diameter and higher relative velocity shifted the outlet velocity curve to the left. This signifies that an equal spray SMD can be achieved with a lower outlet velocity, and hence reduced flame shear, by instilling higher relative velocities at the point of air/fuel mixing, making the smaller nozzle a superior design from a combustion standpoint. These effects from relative velocity are in agreement with published spray literature. Improvements in spray atomization from the air/liquid relative velocity can also be achieved in conjunction with external outlet area reductions, as these are independent from one another.
Figure 22: Average SMD versus air pressure

Figure 23: Average SMD versus outlet air velocity

It should be noted that air accelerates and decelerates within a finite time and distance which the calculations in Figure 23 do not account for. These calculations assume that the air is able to
accelerate to its full speed based on the given airflow rate and cross-sectional area. The distances involved with these nozzles are small however, on the order of a millimeter. If the air, upon exiting the air cap, has not yet reached its full speed, increasing the relative velocity within the mixing chamber could instead act to increase the final exit spray velocity and therefore act to impart additional flame shear. Hence, these results would need to be confirmed in the combustor before saying unequivocally that higher relative velocities impart beneficial results.

3.3.5 Air Cap External Outlet Shape

Given that nozzle-clogging problems have been prevalent with PLB in published literature, a slotted outlet air cap design could be a potential solution if smaller holes were deemed to be beneficial. While air cap outlet size has been shown to be inconsequential for spray SMD (with total outlet area being the important parameter), a greater number of smaller outlet holes formed a more dispersed spray which might be beneficial. Additionally, the effects of slots rather than holes presented an interesting design consideration to understand if outlet shape has any significant role in spray atomization. The slotted air cap (S3B-slot) was designed with an equivalent outlet area to the S3B nozzle. For slotted outlets, the data showed a minor increase in average SMD at low airflow rates while having no effect at high airflows. The slotted design also reduced the large droplet population at high airflows while having little to no effect at lower airflow rates of greater importance. In addition, the slots had no visually apparent effect on spray diffusivity as compared to the S3B nozzle and were a far more complicated design to manufacture, so overall the slotted design was not worth pursuing any further. Again, the average SMD measurements from the S3B-slot air cap collapsed onto the same air pressure and outlet velocity curves as the S3B air cap.

3.3.6 Effects of the Internal Liquid Orifice Diameter on the Liquid Cap

Given the strong influence of air pressure on the spray SMD, it was thought to be prudent to determine if the liquid pressure also played a critical role in the nozzle's atomization. In many plain-jet air-blast atomization correlations and papers (but not necessarily internally mixed), the thickness of the jet was found to be an important characteristic [100], [113], [128], though papers regarding IMTF nozzles (but not necessarily of the air-blast variety) have shown no effect from the liquid jet diameter [119]. For the JPG60 air cap, outlet holes are eccentrically spaced about
1.4mm from the centre of the mixing chamber, so given the liquid jet's proximity to the outlets and its 1mm diameter, it was hypothesized that the liquid jet diameter would have an effect on the nozzle's atomization characteristics. Regardless though, it was thought that with a narrower liquid jet diameter, the water could be broken up more easily by the atomizing air. The diameter of the liquid orifice on the liquid cap directly affects the liquid pressure. As previously mentioned, a JL40100 nozzle was modified to have a reduced liquid orifice internal diameter from 1.0mm to 0.57mm in order to understand its influence on the resulting spray. No other modifications were made to the liquid cap and no changes were made to any air caps used for these tests. Experiments with the smaller orifice liquid cap also used the same airflow rates as those conducted with the standard liquid cap, allowing for direct comparisons to identify the effects from the liquid outlet/jet diameter and therefore the liquid pressure. Air pressure, outlet velocity and relative velocity were unaffected or changed negligibly with these experiments.

The results of these experiments indicated that the increased liquid pressure/decreased liquid jet diameter had no beneficial effect on atomization, providing equivalent or poorer results across all studied categories as demonstrated in Figure 24 and Figure 25 below. The reduced liquid outlet diameter would cause the liquid jet to emerge from the liquid cap slightly faster (from about 0.6m/s to 2m/s), negligibly reducing the air/liquid relative velocity within the mixing chamber, but the thinner jet should then have been broken up more easily by the atomizing air which would have improved atomization overall in theory. The mechanism of atomization was therefore unclear given these results and additional testing would be required. Given the lack of spray SMD sensitivity to the initial liquid jet diameter, some form of prompt atomization appeared to be the most likely mechanism for spray formation.
Figure 24: Average spray SMD versus airflow rate comparing liquid jet diameter

Figure 25: Percent volume greater than 100μm versus airflow rate comparing liquid jet diameter
3.3.7 Air/Liquid Impact Configuration

As previously discussed, twin-fluid atomization is significantly dependent on the air/liquid interaction and maximizing the forces between the fluids results in finer atomization. Research has shown that atomizing a thin liquid film is more effective than atomizing a jet [111] and so, as previously shown in Figure 12, a splash pin was inserted in a standard JPG60 nozzle using a friction fit. During experiments, the head of the pin was positioned 0.45mm downstream of the liquid outlet. By design, the liquid would have pooled on the head of the pin and spilt over the sides where it interacted with the air as a thin film rather than a jet. In addition, along the length of the pin, there was less cross-sectional area available for the air to flow, increasing the air pressure and relative velocity at the air/liquid contact point. It was found that due to small defects in manufacturing, the spray preferentially flowed through three out of the available six holes. As such, three holes were blocked with epoxy similar to the S3B nozzle, but again one jet showed significantly poorer atomization while the other two holes performed well. The poor hole was then also blocked allowing for a direct comparison with the S4B nozzle and eliminating any concern for manufacturing defects. However, even with only two outlets, both of which had been atomizing the spray effectively, one hole was always significantly poorer than the other, especially at low airflow rates. At 8.2SLPM, one hole had an average SMD of 86.0μm while the other had an average SMD of 50.0μm. On the other hand, the S4B nozzle had one hole at 62.3μm and the other at 59.4μm.

For the S4B-Pin nozzle, average SMD values were comparable to the S4B nozzle, but the large droplet population data showed significantly poorer results, indicating an overall worse performance and that this nozzle would likely form higher amounts of pollutants in a combustion environment. Results are shown below in Figure 26 and Figure 27. In addition, the S4B-Pin nozzle is far more complicated from a design and manufacturing standpoint, so after reviewing this data, work on this nozzle was discontinued. It should be noted that once again, the S4B-Pin data did collapse onto the same air pressure and velocity curves as the S4B nozzle, indicating that for both nozzles, pressure is the dominant parameter and the atomization mechanism is the same.
Figure 26: Comparing the average SMD versus airflow rate of the S4B and S4B-Pin nozzles

Figure 27: Comparing the percent volume greater than 100μm versus airflow rate of the S4B and S4B-Pin nozzles
3.3.8 Nozzle Primary Atomization Mechanism(s)

Experiments with the S4B-Pin nozzle and the liquid jet diameter/pressure both provided poor and unexpected results, indicating an error in the underlying assumptions regarding the primary atomization mechanism. It had been assumed that the air was causing the water jet to breakup in some manner and so lower pressure atomization was poor due to the limited airflow rate as would be expected with an air-blast atomizer. Instead, these two test results indicated that the configuration of the liquid is actually unimportant to atomization quality. The most likely explanation for this is that the liquid jet was actually hitting the bottom of the air cap, causing the jet to break up/disintegrate, similar to research described by Kim [123], though the nozzle in that paper differed greatly in design and had eccentric outlets placed much further from the centre of the mixing chamber.

For the nozzle used in this research, once the liquid jet disintegrated from its impact with the bottom of the air cap, some water likely pooled there and spilled into the air cap outlets, being atomized by the air when entering the outlets. The remaining water then likely became deposited as a thin liquid film on the internal surfaces of the mixing chamber from strong air recirculation currents within the air cap and this water then flowed downwards towards the outlet holes. As the liquid film flowed into/over the outlets, it was broken apart by the atomizing air into a second population of droplets. Two distributions or populations of droplets were visible in most of the spray experiments, the relative magnitudes of which changed depending on the nozzle configuration and airflow rate (shown in Figure 28), which was evidence of two separate atomization mechanisms occurring within the nozzle. The smaller droplet population was likely the result of the thin-film atomization while the larger droplet population was probably from the pooling water spilling into the outlets from the bottom of the air cap. This demonstrates the primary atomization mechanism of this nozzle and explains why higher amounts of atomizing air/pressure resulted in a finer spray while a smaller liquid orifice (higher liquid pressure) and a more efficient air/liquid impact configuration had no meaningful or beneficial effect on the spray. The jet disintegrated in the same way regardless of size or pressure and so a thinner jet did not meaningfully contribute to the water's atomization. Furthermore, a significant portion of the water was already being atomized as a thin film and so the change in air/liquid impact configuration was ineffective. In addition, since the head of the pin in the S4B-Pin nozzle would
have partially shielded part of the outlets from direct/unobstructed airflow, the atomization of the pooled water would have been less effective than with the original design, explaining the higher population of large droplets shown in one of the graphs from Section 3.3.7. Now that the primary atomization mechanisms and the dominant atomization parameters of this internally mixed air-blast nozzle are understood, they can be used to predict the effect of any further nozzle design changes to optimize the spray SMD. Combustion results can also now be more easily interpreted and correlated to effects from the fuel spray.

**Figure 28: Examples of measured spray droplet volume distributions**

### 3.3.9 Investigation into Relevant Spray Correlations

Many studies have been conducted to correlate the spray behavior of nozzles with various fluid properties and design parameters. These equations can be a useful predictor of spray behavior, but since nozzle designs can differ with respect to many characteristics, the applicability and accuracy of such correlations is very difficult to ascertain without direct experimentation. Various correlation equations [106], [108], [113], [114], [122], [126], [128]–[130], [165]–[167] for air-blast (plain-jet and pre-filming) and internally-mixed nozzles were compared graphically using the data collected for this thesis from the S3B6, S4B and JPG15 air caps. The IMAB nozzle used throughout this thesis would be classified as a plain-jet nozzle, but the actual atomization mechanism was independent of the liquid jet as previously discussed. The mechanism of atomization would likely be described more as a "prompt-type" of mechanism where the water was atomized instantaneously from its interaction with a large force, in this case from the atomizing air, as the water slowly entered the air cap outlets. However, because the water was also atomized as a thin film, the nozzle classification is further complicated. The
The purpose of this analysis was to determine if any existing correlation served to accurately predict the data trends found in preceding experiments and could then provide a method with which to predict the change in SMD when PLB is atomized instead of water.

The predicted SMD results from the different correlations varied over an extremely large range between 30-1400μm while the actual experiments with the three nozzles only varied between a range of 22-61μm. Many of the plain-jet air-blast correlations were not designed for internally mixed nozzles and were therefore expected to give large spray SMDs with the low atomizing airflow rates/pressures studied. Most correlations formed a similarly shaped curve to the ones previously shown in this study when graphing the spray SMD versus airflow rate, but that was expected to be the case for the large majority of twin-fluid nozzles as their atomization improved with greater amounts of air, rapidly at first and eventually displaying an asymptotic relationship. As such, the shape of the trend alone was not sufficient to indicate any relevance between the data from this study and a specific correlation. Instead, any correlation that did not result in a similar magnitude as the data presented in this thesis (defined as less than twice the measured SMD at each airflow rate) was deemed to not be applicable and in addition, any correlation with a significantly flatter or sharper trend-line was also eliminated from consideration. An efficiency factor could have been used for the externally mixed plain-jet air-blast nozzles to reduce the predicted SMDs to more relevant magnitudes. However, because their primary atomization mechanism differed so greatly from what was believed to be occurring in the IMAB nozzle used in this thesis, it was therefore unlikely that they could be used to predict results with any reasonable accuracy and so this additional analysis was not conducted.

Given the basic criteria presented, all but three correlations were eliminated. The remaining correlations are shown in Figure 29-Figure 31. Out of the remaining correlations, the Sakai [122] internally-mixed nozzle was very close to the measured data, but was formulated with only water and thus had no validity with which to predict changes to the spray when using PLB and so this correlation was not examined any further. The remaining two correlations were from a paper on prompt atomization by Lefebvre [106] and a study using a pre-filming air-blast atomizer by Rizkalla et al. [108], [126] with no internal mixing (the basic equation was formulated by Rizkalla et al. [126] with the coefficients reported by Ashgriz [108]). The Rizkalla pre-filming nozzle correlation required the use of a characteristic dimension from the
atomizer and the authors of the paper recommended using the diameter of the pre-filming lip of the nozzle. There was no such dimension in the IMAB nozzle studied here, so the outlet hole diameter was selected as a replacement, providing results with a reasonable magnitude. The Lefebvre prompt equation contained a constant to reflect the efficiency with which a specific nozzle atomizes the liquid. This constant needed to be determined for each nozzle based on experimental data which also meant that results were likely to be of a relevant magnitude. To compare the two remaining correlations properly, the Rizkalla equation's characteristic dimension (pre-filming lip diameter) was changed for each nozzle to perform a similar function as the atomization efficiency constant in the Lefebvre prompt equation. As illustrated in the figures below, both correlations performed similarly for water sprays. Furthermore, it should be noted that previous combustion research [5], [36] with this type of nozzle utilized the correlation by Rizk and Lefebvre [128] to predict the spray SMD of PLB sprays. Based on the experiments in this thesis with distilled water, this correlation calculated SMD values three to eight times larger than the measured data. Hence, the actual fuel sprays in the preceding research likely had SMDs far smaller than previously anticipated.

Figure 29: S3B6 air cap measurements relative to predictive correlations for water and PLB
The Rizkalla and Lefebvre correlations were then re-analyzed with the viscosity, surface tension and density of 80°C PLB substituted for those of water. Results show that for all nozzles, the
Lefebvre prompt equation predicted a decrease in spray SMD by 55-59% relative to the water results, likely due to the decreased surface tension of the PLB. On the other hand, the Rizkalla equation predicted a 163-516% SMD increase relative to the water measurements, the most significant contribution to this likely being from the higher viscosity of the PLB. At this point in the research, it was unknown which of these equations was more accurate or both may have been incorrect, but these correlations were likely the best available spray predictors for the IMAB nozzle used with regards to the change in spray SMD when switching from room temperature distilled water to preheated PLB. More details on both correlations can be reviewed in Appendix D. Furthermore, additional comparative analysis and testing of these equations is presented in the next chapter.
Chapter 4

4 PLB Spray Combustion

4.1 Design of Combustion System

4.1.1 Combustion chamber

The steel combustion chamber (manufactured by Firebridge Inc.) was doubly insulated to protect against heat losses and was wide enough to prevent the fuel spray from depositing on the insulated walls of the combustor. While temperatures within the combustion chamber have been measured above 900°C, the outer steel walls of the combustor remain in the range of 50°C. The combustion chamber was mounted to a swirl box positioned atop the combustor and two viewports were located on either side of the chamber to monitor and observe the flame during experiments. Exhaust was pulled through piping at the bottom of the combustor and vented through a fume hood. There was a port box affixed to one side of the combustion chamber in order to mount instrumentation to measure the combustion environment. A schematic and cross section of the combustor is provided below in Figure 32 and additional information is available in previous research projects using this equipment [5].

Figure 32: Schematic and cross section of the combustion chamber [5]
The viewports of the combustor were 6.5" x 6.5" x 1/4" transparent quartz plates which provided a clear view of the flame and nozzle tip. In order to prevent any leaks of cold air entering the burner around the viewports, they were affixed with a gasket and an additional external layer of thermal tape.

The tubing for the pilot flame was inserted through the top hole of the port box. A thermocouple was inserted through the second hole of the port box (directly below the pilot flame) to monitor flame temperatures. Additionally, a pressure gauge was put into the third hole to continuously monitor the negative pressure within the combustor to ensure that no fumes vented into the laboratory.

4.1.2 Primary Air Heater and Swirl Generator

A stack fan at the end of the exhaust line controlled the primary air intake. This fan pulled air through the combustion chamber at a flow rate measured by a calibrated Master-Touch 8689 MPNH flow meter from Eldridge Products Inc. Just downstream of the primary air inlet, the air was heated by a 1kW Omega AHF-10120 air heater prior to entering a variable swirl generator. The swirl blocks, for the purpose of this experiment, were fixed at 80% of the maximum swirl (a swirl number of 3.38) which was found to be the optimal setting with respect to PLB flame stability and coking as determined by previous research with this combustor [5].

The swirl generator caused the primary air to enter the combustion chamber with a tangential velocity around the fuel nozzle at the exit of the burner throat. Upon exiting the throat, the primary air then expanded outwards away from the centre of the combustor, creating radial and axial pressure gradients. These gradients formed a low pressure region directly beneath the nozzle which caused hot product gases to recirculate towards the nozzle in what is known as a central recirculation zone [149]. A depiction of this process is illustrated below in Figure 33. Recirculation helped to increase air turbulence, mixing and temperatures within the ignition region of the burner as well as to reduce velocity, all improving ignition and flame stability close to the nozzle for a more compact flame [149]. Flame stabilization through swirl is particularly useful for PLB which requires higher ignition temperatures due to its low volatility and high water content. Calculations and additional details can be found in previous research on this combustor [5].
4.1.3 Fuel Injection System (Nozzle Assembly)

The nozzle assembly used in the combustor was essentially an identical design to that described in the previous spray chapter except that this assembly had a 13" extension tube rather than a 6" one. The same JPL26B and JPL16 nozzle assemblies were utilized in the combustor with some customization as described in detail in subsequent sections. Customized air cap manufacturing drawings can be found in Appendix B.

The fuel within the nozzle was heated by the primary air, which flows around the nozzle assembly. As previously mentioned, PLB should be preheated to a maximum of around 80°C to reduce viscosity and surface tension and increase volatility. However, temperatures can exceed this threshold during steady-state combustion causing fuel boiling, polymerization and combustion instabilities so a water-based cooling system was used within the nozzle assembly as depicted in Figure 34. This system was designed to maintain the PLB temperature at approximately 70-75°C. The cooling system is comprised of stainless steel tubing wrapped around the fuel line within the nozzle extension tube. The tubing has an internal diameter of 0.04" and an outer diameter of 1/16". A needle valve is used to control the water flow with a maximum continuous flow rate of 72mL/min [5].

Figure 33: Liquid flame jet stabilization via swirl induced recirculation zones [149]
4.1.4 Ignition System

To ensure stable PLB ignition, a continuous 0.3kW stoichiometric methane/oxygen pilot flame was utilized. The gas flow rate was controlled by two Matheson rotameters and the pilot system assembly was comprised of a Hoke jeweler's soldering torch body (part number 110-406), a 20" stainless steel extension tube with a ¼" outer diameter and a hi-heat torch tip from Grobet USA (part number 14.157) [5].

To ignite the methane flow through the pilot tip, an electric igniter was used within the combustion chamber. This allowed for ignition without opening the chamber door, which was particularly useful if the pilot extinguished during an experiment and had to be re-ignited. To ignite, the pilot tip was moved close to the igniter and an external button was used to generate an electric spark that hit the front of the pilot tip near the methane flow exit aperture. The pilot flame could then be repositioned close to the fuel nozzle outlet to allow for main system ignition. The system is illustrated in Figure 35 below.
Figure 35: A schematic of the combustor, emphasizing the pilot flame ignition system [5]

4.2 Experimental Methodology

4.2.1 PLB Analysis

Two batches of PLB were obtained from the fuel manufacturer to complete the required experiments. The manufacturer provided a certified analysis detailing the solid char, ash and water content of both batches of fuel. An elemental analysis of the fuel was carried out by the Analytical Lab for Environmental Science Research and Training (ANALEST) at the University of Toronto. The elemental analysis measured the carbon, hydrogen and nitrogen content of the fuel and the oxygen content was then calculated by subtraction, assuming that other elements are present only in trace amounts. Prior to the analysis, all fuel samples were thoroughly mixed to ensure that an accurate, representative sample was tested.

Density was calculated by weighing two thoroughly mixed 5mL samples of the fuel on a Sciencetech SM-128D Microbalance. This was repeated twice on two separate days and the results were averaged.
Kinematic viscosity measurements were conducted in accordance with ASTM standard D445. Calibrated Canon-Fenske viscometers were used within a temperature controlled hot water bath. Fuel temperature was measured prior to beginning measurements and timed carefully using a stopwatch. Each viscosity measurement was conducted at least twice to ensure accuracy and results were averaged since they were consistent. Once the fuel was heated to the appropriate temperature, suction was applied to one end of the viscometer to prepare the device for measurement. The viscosity is directly proportional to the time it takes for the heated fuel to move between two marked points within the viscometer under only the force of gravity.

The heat of combustion or higher heating value (HHV) was measured with the use of a Parr 6300 calorimeter in accordance with standard ASTM D240. This machine measures the energy content of a weighted sample of fuel. Previous researchers have confirmed the accuracy of this machine [5]. For proper ignition within the calorimeter, the PLB sample had to be mixed with ethanol. Both pure ethanol and the mixture (with PLB as a known weight percent) were then measured in the calorimeter, allowing the HHV of the pure PLB to be calculated. As a confirmation method, an analytical equation was utilized to estimate the HHV from the elemental analysis provided by ANALEST. This equation, written directly below, has been shown to be accurate within 2.5% with PLB from the same fuel manufacturer [5], [168]. In the equation, the HHV was calculated using the elemental mass fractions from the ANALEST results.

\[
HHV = 33.5[C] + 142.3[H] - 15.4[O] - 14.5[N] \left( \frac{M_J}{kg} \right) [72], [168]
\]

When analyzing the second batch of PLB, provided by the same manufacturer a month later, the calorimeter was unavailable from which to determine the PLB’s HHV. Instead, the manufacturer provided the HHV measurement. Detailed fuel specifications can be reviewed in Section 4.3.1.

4.2.2 Experimental Setup

A schematic diagram of the burner assembly and associated hardware is shown below in Figure 36. The same gear pump detailed in the spray experiments was used in the burner except that the gears were replaced with ones made from polyether ether ketone (PEEK) as found in Service Kit 74215-95, from Cole-Parmer. PEEK has been found to be the best performing polymer for use
with PLB [169] and no performance degradation of the pump was evident throughout the course of experimentation for this thesis. The fuel flow rate was monitored using the same scale detailed in Chapter 3. The fuel supply sat upon the scale and the change in mass was recorded by Excel in real-time and averaged every ten seconds, ensuring a consistent fuel energy supply to the burner of 10kW. The primary air flow meter was connected to LabVIEW which continually graphed the airflow in real-time while displaying 30 second and two-minute averages in order to maintain a constant equivalence ratio during experiments.

**Figure 36: Schematic diagram of the burner assembly and associated hardware** [5]

As previously mentioned, a heater was used to heat the primary air which then subsequently warmed the fuel and atomizing air prior to injection into the burner. A stack fan also pulled the primary air through the exhaust system ensuring the entire combustion system was under a slight negative pressure and thereby ensuring no pollution leaked into the laboratory. All connections and potential inlets on the combustor system were sealed with a gasket and/or thermal tape to ensure no air leaked into the burner or sampling lines. Where possible, the lines were tested for
leaks by pressurizing them with air and using a leak-testing compound. Gas-phase emissions were analyzed with a Fourier transform infrared spectrometer (FTIR) system while PM sampling was conducted by pulling exhaust through a filter assembly (both systems are further detailed in Sections 4.2.6 and 4.2.7 below).

A preliminary test was conducted to establish at what primary airflow rate CO emissions were minimized using the S2B6 nozzle (the same nozzle design used for preceding experimental research on this combustor [5]). CO emissions represent a simple indicator of combustion quality. An airflow of 280-295SLPM (equivalence ratio of 0.56-0.59 and 69-79% excess air) was then selected, matching previous research results [5], though the effect of primary airflow on CO emissions was minimal. This primary airflow rate was used consistently throughout all the combustion experiments since the primary airflow controls the swirl and recirculation dynamics of the combustor which were previously shown to be critical parameters for important combustion characteristics such as coking and flame stability [5]. This primary airflow range also gave the best results with respect to nozzle coking during preliminary testing.

4.2.3 Temperature Measurements

Several thermocouples were used to measure the temperature at specified locations and the sensor data was collected by LabVIEW software for real-time readouts. Some critical thermocouples were positioned as shown in Figure 37 below. Near the bottom of the nozzle, within the liquid cap, a 1/16in diameter, 24in long, PFA-coated, J-type thermocouple [5] was used to monitor the fuel temperature so that the cooling system could be initiated if overheating occurred. A K-type thermocouple was also used to monitor the exhaust temperature immediately downstream of the combustion chamber. Additionally, a second K-type thermocouple was inserted periodically through the port box to monitor flame temperature directly. This was a specially designed 24 inch, Nickel-Chrome-based super OMEGACLAD sheathed probe that was able to withstand temperatures of up to 1335°C [5]. Typically, this probe was positioned directly beneath the centre of the flame as shown in Figure 38 and left in place for 3-5 minutes to reach a stable temperature. The port entrance was sealed during these measurements to ensure that no cool air could leak into the combustion environment. Another thermocouple was used to measure the temperature in the PM sampling line and its placement is detailed in Section 4.2.7.
Figure 37: Burner thermocouple placement [5]

Figure 38: PLB combustion showing flame thermocouple placement (highlighted)
4.2.4 Nozzle Configurations

All nozzles used in this section were custom-made in a machine shop. The following chart (Table 4) outlines the air and liquid caps used during various combustion tests, all based on either the JPL26B or JPL16 standard nozzle and customized to isolate and test for specific parameters, spray characteristics and/or geometric design criteria. Liquid caps were made from 316 stainless steel while the air caps were mostly brass. Nozzle customizations are detailed in their respective results section and manufacturing drawings are shown in Appendix B.

Table 4: Summary chart for nozzle configurations used for combustion testing

<table>
<thead>
<tr>
<th>Air Cap (material*)</th>
<th>Liquid Cap</th>
<th>Number of Holes</th>
<th>Hole Diameter (mm)</th>
<th>Outlet Angle (*)</th>
<th>Mixing Chamber Diameter (mm)</th>
<th>Liquid Orifice Diameter (mm)</th>
<th>Used With</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard S0B6 (SS)</td>
<td>-</td>
<td>6</td>
<td>0.94</td>
<td>70</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>S2B6 (Br)</td>
<td>-</td>
<td>6</td>
<td>0.80</td>
<td>70</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>S3B6 (Br)</td>
<td>-</td>
<td>6</td>
<td>0.66</td>
<td>70</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>S4B6 (Br)</td>
<td>-</td>
<td>6</td>
<td>0.54</td>
<td>70</td>
<td>3.6</td>
<td>-</td>
<td>JL40100</td>
</tr>
<tr>
<td>sS3B6-70 (Br)</td>
<td>-</td>
<td>6</td>
<td>0.66</td>
<td>70</td>
<td>1.7</td>
<td>-</td>
<td>JL2050-72</td>
</tr>
<tr>
<td>sS3B6-90 (Br)</td>
<td>-</td>
<td>6</td>
<td>0.66</td>
<td>90</td>
<td>1.7</td>
<td>-</td>
<td>JL2050-72</td>
</tr>
<tr>
<td>sS3B6-60 (Br)</td>
<td>-</td>
<td>6</td>
<td>0.66</td>
<td>60</td>
<td>1.7</td>
<td>-</td>
<td>JL40100-72</td>
</tr>
<tr>
<td>sS3B4-70 (Br)</td>
<td>-</td>
<td>4</td>
<td>0.81</td>
<td>70</td>
<td>1.7</td>
<td>-</td>
<td>JL2050-72</td>
</tr>
<tr>
<td>sS3B8-70 (Br)</td>
<td>-</td>
<td>8</td>
<td>0.57</td>
<td>70</td>
<td>1.7</td>
<td>-</td>
<td>JL2050-72</td>
</tr>
<tr>
<td>sSoptB4-66 (Br)</td>
<td>-</td>
<td>4</td>
<td>0.71</td>
<td>66</td>
<td>1.7</td>
<td>-</td>
<td>JL2050-72</td>
</tr>
<tr>
<td></td>
<td>-</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td>-</td>
</tr>
</tbody>
</table>

* SS – 316 stainless steel, Br – brass

4.2.5 Flame and Nozzle Coking Visualization

A FUJIFILM FINEPIX F750EXR digital camera was placed on a tripod in front of one of the combustor's quartz viewing windows to continuously film the flame during experiments. All relevant PLB flame videos are being submitted electronically with this thesis and are listed in Appendix E. A schematic diagram of a resulting image is shown below in Figure 39.
Figure 39: A schematic diagram of a PLB flame image [5]

A PIXMA K-5 DSLR camera was used to take focused pictures of the nozzle surface to document the extent of coking at each set-point during each flame experiment.

4.2.6 FTIR Gas Phase Emission Measurements

A Nicolet 380 Fourier transform infrared spectrometer (FTIR) was used to measure carbon monoxide (CO) and nitric oxide (NO), the main constituent of NOx, emissions. The FTIR measured the infrared light absorbance of the exhaust gases. The spectral location of absorbency indicated the species in question and the magnitude of absorbency indicated its concentration. Two vacuum pumps in series were used to pull a fixed fraction of the exhaust gases from the combustor through a heated sampling line (with a temperature between 190°C and 200°C to prevent any condensation) and into the FTIR to be analyzed. The FTIR had a heated gas cell to prevent condensation with a volume of 0.19L [5]. Measurements were always conducted at the same absolute pressure of 86.3kPa with 24 successive scans to reduce noise. To ensure that the exhaust was free from particulates which could harm the instrument, a heated filter was installed along the sampling line as indicated in Figure 36.

Separate calibration curves were created for both CO and NO from certified compressed gas cylinders with multiple points generated (each measured at least twice and averaged) from
dilution with pure nitrogen, based on partial pressures. Results were verified a second time, on a separate day, for accuracy and the curves were averaged. Pre-existing FTIR quantification methods, used by past researchers, were shown to be outdated and inaccurate for CO (so a new one had to be created based on the new calibration data), but were still accurate for use with NO. NO is the main constituent of NOx and would therefore be representative of this pollutant family. Both CO and NO calibration curves were intended for use between 5 and 250ppm and used four points to plot a linear fit through the data. For no experiment was the NO concentration expected to be above 250ppm and for CO emissions, the precision of any values above 250ppm were unimportant as these points simply represented poor combustion conditions.

Based on the calibration, CO measurements were accurate, on average, within 8.1ppm, with a maximum error of 12.2ppm. In the region of greatest interest (below 30ppm), the measured error was about 6ppm and so the overall average of ±8ppm was used as a conservative error value for this pollutant. NO measurements were accurate on average within 7.5%, with a maximum error of 9.2%. In the most critical regions, the accuracy was closer to the average error, and therefore an error value of ±7.5% was used for this pollutant.

CO emissions were used to assess combustion quality rather than unburned hydrocarbons because CO is further along the chemical conversion chain (which ends in carbon dioxide) than unburned hydrocarbons (UHCs). Therefore, UHC concentrations should always be below that of CO, meaning that CO provides a greater measurement sensitivity for assessing combustion quality.

4.2.7 Particulate Matter Emission Measurements

The collection of particulate matter (PM) should ideally be done under isokinetic conditions. This ensures that the sampling line and the main exhaust duct have identical velocities so that collected samples are representative of the overall exhaust. This combustion system achieved this by ensuring equalized (null) pressure between the sampling line and the main duct. More information about this condition and the implementation within this system is described elsewhere [5]. A schematic diagram of the PM collection system as a whole is illustrated below in Figure 40.
A vacuum pump pulled the exhaust through the PM collection system (sampling line) which had a main line and a bypass line. The bypass line was used when changing the filter on the main line. 47mm diameter Tissuquartz filters were used from Pall Life Sciences (part number 7202) and secured by a stainless steel holder from Advantec MFS Inc. (model LS47, part 304700). A thermocouple positioned behind the filter in the main line monitored the temperature which was maintained above 115°C to prevent condensation on the filter. Downstream of the main and bypass filter assemblies, a condenser from Seakamp Engineering Inc. (part 2151414) cooled the exhaust prior to it entering the vacuum pump and being vented from the lab. Each filter was exposed to the exhaust for 4 minutes to avoid being overloaded and one dummy filter was used to heat up the system and bring it to steady state before actual measurements were conducted. For actual measurements, three filters were averaged for each data point. PM is comprised of ash and carbonaceous residue (CR). The PM analysis calculated the amount of CR (indicated as a weight percent of the total PM) in the exhaust in order to help determine the extent of fuel burnout during PLB combustion. This analysis does not require isokinetic conditions, but isokinetic sampling was carried out regardless because it is the preferred method for PM collection and analysis.

Figure 40: Schematic diagram of the PM collection system [5]
PM collection and analysis was based on ASTM D4422. The procedure was as follows:

- Filters were placed in an oven for two hours at 750°C the day before an experiment to burn off any moisture or organic residue that could be on them; they were then placed in Petri-dishes and covered overnight
- Prior to initiating testing, the filters were weighed on a Scientech SM-128D Microbalance ($M_0$)
- Testing was conducted as indicated in Appendix F
- After testing, the filters were again placed back in their Petri-dishes and covered overnight
- The next day, the filters were weighed again ($M_1$)
- The filters were then placed in an oven for two hours at 150°C to remove any moisture
- The filters were then weighed again ($M_2$)
- The filters were then placed in the oven a final time at 750°C for an hour to burn off any CR ($M_3$) before being weighed a final time

\[
\begin{align*}
    Total PM &= M_2 - M_0 \\
    Water &= M_1 - M_2 \\
    CR &= M_2 - M_3 \\
    Ash &= Total PM - CR = M_3 - M_0
\end{align*}
\]

It was not possible to quantify the CR sampling and measurement error since there were too many combustion variables that could fluctuate within a given range and therefore CR error could not be isolated precisely. As such, three filters were used and averaged for each nozzle data point and at least three weight measurements were averaged for each individual filter at each analysis step, all in an effort to minimize errors. CR results were also examined with respect to their overall trend and relative magnitude rather than their specific numerical values. With this methodology in place, CR results presented valuable information with which to judge respective nozzle designs relative to one another.

**4.2.8 Test Procedure**

During testing, the following combustion parameters were maintained within the given ranges:

- Primary air: 280-295SLPM (equivalence ratio of 0.56-0.59 and 69-79% excess air) to keep the air swirl and recirculation consistent; these values were established during preliminary experiments as they minimized CO emissions and are consistent with previous research [5]
- Swirl vanes: 80% of maximum angle (swirl number of 3.38) based on previous research [5]
- Pilot energy: 0.3kW-0.35kW based on previous research [5]
- Primary air temperature: 160-175°C based on previous research [5]
• Fuel preheat temperature: 65-80°C based on previous research with the nozzle insulated to prevent overheating from thermal feedback from the flame [5]
• Fuel flow rate: 10kW energy throughput

For each nozzle, the general experimental procedure was as follows:

• Carry-out the start-up procedure as outlined in the burner instructions in Appendix F and startup with ethanol at 10kW for approximately 30-40 minutes to preheat the combustion chamber
• Next, turn off nozzle cooling and initiate the flow of PLB, setting atomizing air to a level where the flame looks relatively stable; the nozzle cooling was turned on again at some point once the fuel line reached about 70°C
• Using the FTIR, take a background measurement and then let exhaust flow through the gas cell for 3-5 minutes, ensuring sample line temperature is above 120°C
• When ready, take two FTIR samples while recording relevant parameters (time, atomizing air/pressure, fuel flow rate, pilot energy, fuel temperature, exhaust temperature and primary airflow rate)
• Continue to take FTIR readings during the heat-up transient period every ten minutes and continually monitor all combustion parameters to ensure they stay within their allotted ranges
• When CO is below 100ppm, fuel temperature is above 60°C and the heat-up has been ongoing for more than 20 minutes, adjust the atomizing air to where the flame seems most stable, then find the nozzle height and angular position where stability is also maximized
• Next, increase the atomizing airflow via the rotameter until the flame just becomes unseated or unstable, noting the rotameter value, air pressure and relevant flame observations; do the same thing to find the minimal atomizing air for stability
• Set the atomizing air to 65% along the stability range (found during an initial test to give good flame stability and emissions) to provide consistency between experiments
• Continue to monitor CO readings from the FTIR until they become asymptotic, at which point the flame is reaching steady-state and the FTIR should be purged and nozzle coking should be observed and photographed for the transient period
• Next, take a new FTIR background, begin the exhaust flow to the FTIR and take two samples after 3-5 minutes (henceforth this process is used for all FTIR measurements and will not be specified in detail) while recording key combustion parameter values; this should confirm the CO emission's asymptotic progression
• Then take a measurement of the flame temperature directly below the nozzle as shown in Figure 38 ensuring that all air leaks are sealed with tape at the thermocouple insertion point; wait for readings to stabilize for about 4 minutes
• Take three PM samples, as outlined in the burner instructions in Appendix F, after using a dummy filter to allow the system to reach steady-state and become isokinetic
• At the end of the PM sampling, observe and photograph nozzle coking for the nozzle base-point
• Afterwards, take another two FTIR sample readings after purging the equipment and retaking a background
• Next, change the atomizing air to the next point, likely half way between the base-point and the maximum atomizing air where the flame lost stability
• Purge and prepare the FTIR equipment and ensure combustion parameters are still within their proper ranges
• After ten minutes observe and photograph coking and then conduct two FTIR samples while recording important combustion parameter values
• Again change the atomizing air set-point to the next value, this time likely half way between the base-point and where the flame lost stability at the minimum atomizing air; repeat the same procedure as for the previous point
• Repeat again for two more points at the maximum and minimum atomizing air values; the order of points may change depending on unique circumstances and how the experiment progresses
• Once complete, purge the FTIR one last time, turn off the air heating, turn on the nozzle cooling and switch back to ethanol to purge the fuel lines; follow the shutdown procedure in Appendix F to end the experiment

The common experimental base-point was determined during the first experiment (for the S2B6 nozzle) to be where the PLB flame was seated in the most stable manner on the bottom of the nozzle, biased towards higher atomizing air which tended to reduce pollutant emissions. This point happened to fall at 65% (closer to maximum atomizing air) between the highest and lowest atomizing air points of the stably seated flame range. To ensure a consistent comparison between nozzles and to establish reliable data trends, subsequent nozzle base-points were also placed at 65% along the range between each nozzle's own maximum and minimum atomizing airflow points.

4.3 Results and Discussion

4.3.1 PLB Fuel Properties

The results of the PLB fuel analysis (both batches) are listed in Table 5, followed by a detailed viscosity versus temperature graph shown in Figure 41 from the first batch of PLB. Furthermore, the results in the table are compared to property values presented in the literature and from the ASTM standard. Due to the large number of experiments conducted for this thesis, two separate fuel batches had to be ordered and results indicated that their fuel properties were similar. Every section below identifies the PLB batch used for each set of experiments. Results were only compared between experiments using the same fuel batch. Thus, the fuel batches were not mixed and fuel composition was not a variable.
Table 5: Fuel property summary and comparative chart [15], [19]–[21], [29], [32], [36], [54]–[56]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Typical Range of PLB</th>
<th>ASTM D7544, PLB Grade G and D</th>
<th>PLB Fuel Analysis for Batch 1</th>
<th>PLB Fuel Analysis for Batch 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water Content</td>
<td>wt%</td>
<td>15 – 30</td>
<td>30 max</td>
<td>21.9</td>
<td>22.3</td>
</tr>
<tr>
<td>Kinematic Viscosity</td>
<td>cSt at 40°C</td>
<td>10 – 90</td>
<td>125 max</td>
<td>36</td>
<td>32.1</td>
</tr>
<tr>
<td>Surface Tension</td>
<td>mN/m at 80°C</td>
<td>31</td>
<td>-</td>
<td>33</td>
<td>-</td>
</tr>
<tr>
<td>Acidity</td>
<td>pH</td>
<td>2 – 3</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Density</td>
<td>kg/m³ at 20°C</td>
<td>1100 – 1300</td>
<td>1100 – 1300</td>
<td>1197</td>
<td>1173</td>
</tr>
<tr>
<td>Solids Content</td>
<td>wt%</td>
<td>&lt;1</td>
<td>2.5 max (G), 0.25 max (D)</td>
<td>0.04</td>
<td>0.11</td>
</tr>
<tr>
<td>Ash Content</td>
<td>wt%</td>
<td>&lt;0.3</td>
<td>0.25 max (G), 0.15 max (D)</td>
<td>0.09</td>
<td>0.13</td>
</tr>
<tr>
<td>Carbon Content</td>
<td>wt%, dry (wet)</td>
<td>50 – 60</td>
<td>-</td>
<td>59.24 (46.27)</td>
<td>60.82 (47.23)</td>
</tr>
<tr>
<td>Hydrogen Content</td>
<td>wt%, dry (wet)</td>
<td>6 – 9</td>
<td>-</td>
<td>6.53 (7.55)</td>
<td>6.48 (7.53)</td>
</tr>
<tr>
<td>Nitrogen Content</td>
<td>wt%, dry (wet)</td>
<td>&lt;0.5</td>
<td>-</td>
<td>0.12 (0.09)</td>
<td>0.12 (0.09)</td>
</tr>
<tr>
<td>Sulfur Content</td>
<td>wt%, dry</td>
<td>&lt;0.05</td>
<td>0.05 max</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Oxygen Content</td>
<td>wt%, dry (wet)</td>
<td>30 – 40</td>
<td>-</td>
<td>34.11 (46.09)</td>
<td>32.59 (45.15)</td>
</tr>
<tr>
<td>Higher Heating Value</td>
<td>MJ/kg (from equation)</td>
<td>14 – 19</td>
<td>-</td>
<td>18.95 (19.13)</td>
<td>19.15 (19.57)</td>
</tr>
<tr>
<td>Lower Heating Value</td>
<td>MJ/kg (from equation)</td>
<td>13 – 18</td>
<td>15 min</td>
<td>17.30 (17.48)</td>
<td>17.51 (17.96)</td>
</tr>
<tr>
<td>Flow Rate for 10kW</td>
<td>ml/min g/min</td>
<td>-</td>
<td>-</td>
<td>29.6</td>
<td>29.2</td>
</tr>
</tbody>
</table>

Figure 41: PLB kinematic viscosity versus temperature
4.3.2 PLB Spray Test

To better understand the spray of PLB, an S4B nozzle (from previous spray experiments) was used within the burner to visually compare the water spray to that of the biofuel. The temperature of the fuel was varied to also examine the effect of fuel viscosity on the spray. While it was not feasible to use the Spraytec for a detailed analysis, as previously described, the visual comparison provided several interesting conclusions. The stack fan captured the fumes from the fuel and extracted fine droplets to allow for visual comparisons to be conducted.

At an equal atomizing air pressure (and spray SMD) to the water test, the PLB seemed to produce a visibly finer spray. This means that the Lefebvre prompt spray correlation [106] is likely the best indicator for PLB and this nozzle. However, a quantification of the correlation's accuracy is not possible at this time. In addition, this finding reinforces the conclusions from the previous chapter which stated that the water is likely atomized via a prompt mechanism. Prompt atomization is strongly dependent on fluid surface tension and PLB's surface tension is about half that of water, explaining the apparent SMD reduction seen here [106], despite the biofuel's much higher viscosity. Therefore, if comparing preheated PLB sprays to those of room temperature diesel (which many studies have done), atomizers that operate via the prompt mechanism should be ideal because the PLB's surface tension is far closer to that of diesel than its viscosity (which other atomization mechanisms rely upon more heavily) and so the spray size differential should be correspondingly reduced. For reference, as outlined in Section 2, preheated PLB’s surface tension is about 10% higher than room temperature diesel while its viscosity is about 200-400% higher.

The spray appeared to be finer at a temperature of 77°C (7cSt) than at 50°C (21cSt) based on the amount of mist generated by the atomization, so a reduced fuel viscosity still improved the spray, but the effect currently cannot be quantified. At both temperatures, the atomization looked excellent, but preheating is still important for fuel volatility and vaporization with respect to ignition. An image of the PLB spray at 77°C and 50°C is shown below in Figure 42.
4.3.3 PLB Spray Combustion

It has been well established that PLB burns in two main stages as depicted in Figure 43. First, the volatile components burn near the nozzle, followed by the solid char in a slower heterogeneous surface combustion process requiring longer hot-zone residence times for complete fuel burnout [85]. During combustion, fuel droplets that are caught in the burner's recirculation zone(s) can be deposited on the surface of the nozzle, polymerizing and forming solid coke as shown in Figure 44. This coke can then continually build up on the nozzle and, if too severe, can impinge or block the spray, negatively impacting the combustion process in many possible ways.

Figure 42: PLB atomization at 77°C (left) and 50°C (right) at comparable air pressures, both using the same nozzle
PLB combustion displayed several general trends with respect to flame behavior and emissions. It was observed that seated flames, throughout their stable atomizing airflow range, produced consistent and/or negligible CO emissions, as seen in Figure 45, and constant CR emissions. Therefore, for a stable flame, the finer spray and more rapid combustion with increasing atomizing air was counteracted by the reduced fuel residence time within the hot-zone or flame.
region of the burner as a result of its higher outlet spray velocity. Beyond this region, as the atomizing airflow/pressure was increased (further reducing SMD), the flame became unstable and lifted off from high shear well before blow-out occurred. In this region, the fuel burned with less visible flame in a more volumetric manner (i.e. with no discernible flame structure) along with visible pulsations as the flame attempted to reattach itself to the nozzle as shown in Figure 46. Near or above flame blow-out conditions, where spray SMD probably responds asymptotically to increasing atomizing air, CO emissions would likely progressively increase as residence time restrictions dominate. When the atomizing airflow decreased below a certain threshold, which was different for each nozzle, the CO emissions spiked (Figure 45) which indicated that the SMD was likely within a region where it exponentially increased with reduced atomizing airflow as shown in Figure 18 in Section 3.3.2. As the atomizing air decreased, the flame also became unseated and burned as a large, bushy, sooting flame (Figure 46), but still remained stable and well-anchored. Often, the bushy flame swirled around the nozzle near the exit of the burner throat. If the atomizing air was decreased too much, the fuel would begin to dribble out from the nozzle rather than being atomized. The PLB flame behaviour discussed above matches findings from previous research [5]. PLB flame behavior at high and low atomizing airflows for specific nozzles will only be discussed in later sections if it differed significantly from the behavior described here.

![Figure 45: Basic trend of atomizing airflow versus emissions; loss of stably seated flame near first and last atomizing airflow points](image)
NO emissions were stable as well, often trending in the opposite direction of CO emissions. The NO trend is small since the majority of NOx emissions are the result of fuel-bound nitrogen and therefore, largely unaffected by small changes in combustion efficiency. Therefore, any changes in NO concentration were likely from thermal NO formation which increases with combustion quality and temperature.

![Image of flame stability classifications](image)

**Figure 46: The PLB flame at high (left) and low atomizing air (right) from the sS3B6-70 nozzle**

There were three main classifications seen within the proceeding experiments with respect to flame stability. There were flames seated on the bottom surface of the nozzle, swirling flames around the exterior of the nozzle which did not make direct contact with the nozzle itself and detached flames where the visible flame often only burned near or below the pilot flame. Depending on the atomizing airflow and nozzle design, intermediate flames also existed between these three classifications along a spectrum. Detached flames would be the least stable or most prone to extinguishment should flame or environmental conditions become less favourable. Often these flames also had characteristic oscillations and pressure fluctuations, making them unstable. Flames seated on the nozzle would likely be the most stable and flames swirling around the nozzle or nearly attached/seated would be categorized as anchored flames assuming there were no unstable oscillations visible. A seated flame is by nature also anchored. In most cases, low atomizing airflows generated anchored, but unseated flames, even when fuel was dribbling out and poorly atomized (causing CO emissions to spike). This research focused on
stabilizing PLB flames and minimizing emissions, emphasizing ranges where stable and seated flames existed. It should be noted that if an anchored flame is required for a burner system, it is generally safer to favour lower atomizing airflow rates.

4.3.3.1 Effects of Nozzle Outlet Area

One of the key conclusions from the spray experiments was that SMD is determined solely by atomizing air pressure and by reducing the outlet area of the air cap, the pressure increases. Hence, when the outlet area was decreased, the same atomizing airflow rate corresponded to a significantly reduced spray SMD, or alternatively, to maintain the SMD, less atomizing air was required. It was also found that the spray outlet velocity, and therefore flame shear, is approximately proportional to the atomizing air pressure so a smaller SMD (achieved by reducing outlet area) corresponds to a higher outlet velocity.

Four nozzles were selected for this study and all nozzle configurations used the same JL40100 liquid cap. For this set of experiments, the standard Bex JPG60 (six 0.94mm holes) air cap and three others were used. The three customized air caps were: S2B6 (six 0.80mm holes), S3B6 (six 0.66mm holes) and S4B6 (six 0.54mm holes), having outlet areas of two-thirds, one-half and one-third of the standard nozzle respectively. Manufacturing specifications for the nozzles used in this section can be found in Appendix B. All experiments in this section were conducted with the first batch of fuel.

Results showed that the air cap outlet area had only a minor effect on the flame. As the air cap outlet area decreased, the flame stabilized at a higher air pressure, higher spray outlet velocity and lower atomizing airflow rate. The flame therefore stabilized in an area of increased flame shear, but reduced spray SMD. One of the main effects of reducing the outlet area was that it resulted in a narrower atomizing air range in which a stably seated PLB flame could exist, decreasing from 8.9SLPM with the standard (S0B6) nozzle to 6.6SLPM with the S4B6 nozzle. As the stability range decreased, the base-point atomizing airflow rate also decreased while the outlet velocity increased. A chart summarizing the nozzles' stable atomizing airflow rates and spray velocities is presented below in Table 6. The trends and relative magnitudes of the airflow rates and velocities in this table are important rather than the actual values, as the specific values would vary for each burner assembly and set of combustion operating parameters.
Table 6: Atomizing airflow and spray velocity summary chart for stably seated PLB flames

<table>
<thead>
<tr>
<th>Nozzle Configuration</th>
<th>Atomizing Airflow Range/Base-Point (SLPM)</th>
<th>Outlet Spray Velocity Base-Point (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S0B6</td>
<td>8.9 (8.6-17.5)/14.3</td>
<td>54</td>
</tr>
<tr>
<td>S2B6</td>
<td>7.1 (7.1-14.2)/12.0</td>
<td>64</td>
</tr>
<tr>
<td>S3B6</td>
<td>7.1 (4.5-11.6)/8.7</td>
<td>66</td>
</tr>
<tr>
<td>S4B6</td>
<td>6.6 (3.5-10.1)/8.1</td>
<td>86</td>
</tr>
</tbody>
</table>

The outlet area had little effect on the CO and CR emissions from the PLB flame as indicated by the data in Figure 47. The base-point CO was unaffected by the area change within the margin of error and the amount of carbon residue within the PM emissions was the same except for the smallest outlet area nozzle (S4B6) which showed a notable increase. CR is affected by spray SMD and hot-zone residence time. As the outlet area was decreased, base-point air pressure increased, reducing SMD, while increasing the outlet velocity, thus likely reducing residence time in the hottest combustor regions (in or near the flame). These effects seem to have negated each other (for CO emissions as well) until the reduction in hot-zone residence time became dominant for the S4B6 nozzle with respect to CR. This may indicate the region for this nozzle where the SMD response to atomizing air becomes asymptotic and could then no longer offset the increased spray velocity and reduced residence time near the flame.

Figure 47: Base-point nozzle comparisons with respect to air cap outlet area
It should be clarified that residence time always refers to the time that fuel droplets and residues spend in or near the flame, in the hottest regions of the combustor, where temperatures are high enough for oxidation reactions to form carbon dioxide. Residence time does not just refer to the time spent within the combustion chamber itself. Chemical reaction rates exponentially increase with temperature and so the time spent within the flame or "hot-zones" are critical to fuel burnout/oxidation.

An increased outlet area also increased the flame temperature and NO emissions almost proportionally which are correlated through thermal NO formation. Additionally, higher outlet areas corresponded to lower spray velocities which could have increased thermal NO production through longer flame region residence times. The increased temperature and NO emissions for the S3B6 relative to the S2B6 nozzle, which fell outside of the overall trend, were likely the result of a longer than normal transient heat-up period (determined by CO concentration) due to an issue with the fuel line temperature that took some time to resolve.

As the outlet area decreased, the flame tended to become a little more compact as shown in Figure 48, likely the result of the reduced spray SMD. Base-point seating stability, brightness and flame size all peaked with the S2B6 nozzle while the S0B6 nozzle had the least stable seating.
Reduced outlet area also corresponded to increased coking on the nozzle surface at the base-point as shown in Figure 49 below. This was likely because nozzles with smaller outlet areas tended to operate at higher internal air pressures, forming finer sprays whose droplets could then be more easily entrained within the burner's recirculation zone(s) and deposited on the outer surface of the nozzle where the fuel then polymerized to coke. This indicated a negative correlation between the spray SMD and nozzle coke formation. Additionally, the change in spray angle accompanied by the change in outlet area as indicated in Section 3.3.1 could have affected the coking, but the effect of this angle will be investigated in greater detail in Section 4.3.3.3. No trend was observed with respect to the heat-up transient time between nozzles to reach steady-state conditions. It should also be noted that all of these PLB flames were found to be optimized with the same distance between the nozzle and the pilot flame.
In conclusion, the S2B6 nozzle was chosen as the best design from this round of experiments. It had the strongest and most stably seated flame and low nozzle coking, along with equal CO and CR emissions compared to most of the nozzles. The S0B6 nozzle had slightly less coking and a wider stability range, but suffered from higher NO emissions and a much less stable flame when seated at its base-point. The S4B6 nozzle had much higher coking and CR emissions that could not be offset by its reduced NO emissions. Additionally, the S3B6 nozzle had worse coking.

4.3.3.2 Effects of Nozzle Air/Fuel Relative Velocity

Another key finding from the spray measurements was that a decrease in mixing chamber diameter, which resulted in an increased air/fuel relative velocity, could reduce the spray SMD significantly without affecting the spray outlet velocity. Therefore, the same spray SMD could
be achieved with a lower outlet velocity and thus lower flame shear. The S3B6 and sS3B6-70\(^2\) air caps were used for this section along with the first batch of PLB and the corresponding manufacturing drawings can be found in Appendix B. The S3B6 nozzle was chosen as a baseline despite the slightly better performing S2B6 air cap (mainly due to coking) because of the outlet area size restrictions on the smaller air cap. Other than the internal mixing chamber diameter, the only real difference between the S3B6 and sS3B6-70 nozzles was the liquid outlet diameter on the liquid cap which differed by 0.3mm, but was shown in the previous chapter to be inconsequential to atomization. A smaller liquid outlet is required for the smaller nozzle due to size constraints.

The effect of the smaller mixing chamber diameter and larger relative velocity was to greatly increase the intensity, brightness and seating stability of the PLB flame at its base-point as shown in Figure 50 below. The smaller mixing chamber size resulted in the base-point of the smaller nozzle (sS3B6-70) actually being established at a higher outlet air velocity and pressure than the larger nozzle (S3B6). However, the correspondingly large reduction in spray SMD likely overcompensated for the higher velocity and shear creating a stronger, but longer, flame. With the improvement in atomization, the smaller droplets could vaporize faster, allowing for the fuel's heat release to occur closer to the nozzle outlet, which resulted in a more intensely seated flame with higher stability. The smaller nozzle also took less than half the time to reach steady-state conditions with respect to CO emissions than the larger nozzle and the intensity of the flame generated much higher flame temperatures for the smaller nozzle of 860°C versus only 814°C for the larger nozzle. The only disadvantage of the smaller nozzle was its reduced atomizing air range in which a strongly seated and stable flame could exist. The smaller nozzle only had a seated stability range of 4.7SLPM (9.3-14.0SLPM with a base-point at 11.7SLPM) while the larger nozzle had a range of 7.1SLPM (4.5-11.6SLPM with a base-point at 8.7SLPM).

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\(^2\) The "70°" in the sS3B6-70 nozzle designation denotes the outlet angle of the smaller air caps, which varied in subsequent experiments. All larger air caps had 70° outlet angles.
The smaller nozzle had a base-point outlet spray velocity of 82m/s and the larger nozzle had a base-point velocity of 66m/s.

Figure 50: PLB flame comparison between the larger (left) and smaller (right) nozzles

From an emissions perspective, the smaller nozzle performed very well, giving off no measureable CO emissions until the atomizing air was dropped low enough that the fuel was no longer being properly atomized, however, even in this condition, the CO was minimal and efficiency was high, all a result of the nozzle's finer atomization. A comparison between the emissions from the larger and smaller nozzles is shown below in Figure 51. Due to the increased flame temperatures, thermal NO emissions were increased with the smaller nozzle which is unavoidable without a specific NO control strategy in place. The percentage of CR in the PM was also reduced with the smaller nozzle to 10.1% from 13.3%. This reduction was likely from a combination of the increased flame temperature, allowing for better fuel burnout, and the smaller SMD from the increased internal pressure of the nozzle, compensating for any increased outlet velocity and potential loss of hot-zone residence time. Additionally, both the higher flame temperature and finer atomization from the smaller nozzle would contribute to a higher fuel heating rate which has been shown to form less non-volatile residue [37], [76] and therefore would result in lower CR emissions. However, the enhanced atomization was probably the largest contributing factor to the reduced CR. It was expected that, in most cases, the trends for CR and CO emissions would be in the same direction and opposite to that of NO emissions.
Figure 51: Comparison of the sS3B6-70 and S3B6 nozzle emissions

In the previous section, the S4B6 nozzle appeared to have the least amount of burning char emanating from the flame, but had the highest CR emissions. Conversely, in this section, the burning char density from the sS3B6-70 nozzle downstream of the flame appears to be less than that of the S3B6 nozzle, but the sS3B6-70 nozzle has lower CR emissions. Therefore, visual indications of burning char are not necessarily indicative of CR performance.

In addition to a more stable flame with lower CR and CO emissions, the smaller sS3B6-70 nozzle had significantly less coking as shown in Figure 52. At all points tested, there was little coke around the outlets or above; some coke did form on the underside of the air cap, but at no point did it affect the fuel spray. Comparatively, thicker layers of coking formed all around the larger nozzle, occasionally impinging on the spray. The reduction in coking with the smaller nozzle appears to buck the established trend because finer sprays were shown in the previous section to increase coking. The likely reason behind this change for the sS3B6-70 nozzle was that the small droplets which used to get caught in the recirculation zone(s) and then deposit and polymerize on the nozzle surface, were now small enough to completely burn out before reaching the surface because of the nozzle's improved atomization and the increased flame temperature/intensity. In addition, as previously mentioned, higher fuel heating rates from the
hotter flame could have reduced the formation of non-volatile residue during polymerization and therefore also could have contributed to the lower amounts of nozzle coking.

![Figure 52: Coking comparison between the larger (left) and smaller (right) nozzles](image)

In almost every aspect, except for NO emissions and the stability range, the smaller nozzle (sS3B6-70), which generates a higher internal air/fuel relative velocity, was a far superior design to that of the larger (S3B6) nozzle.

4.3.3.3 Effects of Nozzle Spray Cone Angle

Using the smaller nozzle design, which has thus far given the best results, the effect of varying the spray angle was examined. The nozzles used were identical except for the angle of the outlet holes on the air cap, which were custom machined. The standard nozzles from Bex had an outlet angle of 70°, but angles of 60° and 90° were also manufactured. Manufacturing drawings for the nozzles are provided in Appendix B. After manufacturing, the customized nozzles all had a consistent internal pressure, and therefore SMD, at a given rotameter demarcation as evidenced by Figure 53. Therefore, internal atomization between the nozzles was unaffected by the change in outlet angle. All experiments in this section were conducted with the first batch of PLB.
The outlet angle had significant effects on the nozzle coking and stability. As the angle increased, the coking increased drastically and the experiment for the 90° nozzle even had to be stopped prematurely when it became completely covered in coke and the outlets became blocked. Comparatively, the 60° nozzle had effectively no coking. This is because the smaller cone angle directed the spray more axially, potentially weakening the recirculation zone beneath the nozzle and/or causing less of the spray to be entrained within it. Coking for these three nozzles can be viewed below in Figure 54.

For the 60° nozzle, while the coking was negligible, at no point was the flame properly seated on the nozzle and instead sat in a stable/anchored manner about 2cm downstream of the nozzle. On
the other hand, the 90° nozzle never became fully unseated, even at the maximum atomizing air from the experimental setup (23.0SLPM) one compact jet was still seated while the remaining jets were mostly detached. At low levels of atomizing air for the 90° nozzle, the flame did unseat due to poor atomization, but remained anchored as was typically observed from flames with low atomizing airflows. Therefore, as the outlet angle increases on the air cap, the seating range also increases. Visually, the PLB flames were quite distinct and can be viewed below in Figure 55. The 70° nozzle formed the brightest and most intense flame with the most stable seating (strongest flame) on the nozzle. The 70° flame also had a well-formed symmetrical conical structure owing to the hollow cone spray pattern formed by the nozzle. The 60° flame did not show the same flame structure and was unseated because of the poorer recirculation zone underneath the nozzle. As previously discussed, the recirculation near the nozzle was used to increase the local temperature in order to improve ignition and to reduce air/fuel mixture velocities (and shear) so that a seated flame could form. The 90° flame was much wider with distinct jets, but had less visible flame overall than the other two nozzles. The seating of the 90° nozzle was also less stable and intense than the 70° nozzle at their respective base-points.

![Figure 55: Comparison of PLB flames with changing air cap outlet angle](image)

There was no seated stability range for the 60° nozzle (base-point at 14.4SLPM), the 70° was seated stably within a range of 4.7SLPM (9.3-14.0SLPM with a base-point at 11.7SLPM) and the 90° nozzle was seated, though less stably and intensely, within a range of 16.4SLPM (6.6-23.0SLPM with a base-point at 13SLPM). Similarly, the base-point outlet spray velocity of the 60° nozzle was 89m/s, 82m/s for the 70° nozzle and 85m/s for the 90° nozzle. Again, these
numbers should only be examined with respect to the overall trend and relative magnitudes as previously described.

For all three nozzles, CO emissions were effectively zero, though CO may have slightly trended upwards with the outlet angle as shown in Figure 56. This trend was within the error range of the CO measurements and is therefore insignificant. NO emissions appear to have decreased slightly overall with increasing angle, but in a fairly insignificant manner.

![Graph](image.png)

**Figure 56: Base-point nozzle comparison for air cap outlet angle**

Flame temperature measurements peaked for the 70° nozzle, but otherwise showed no meaningful trend in the graph above. The flame temperature measurement location was fixed while the position of the flame, relative to the thermocouple, changed with the design of the nozzle. Flame temperatures should be positively correlated to thermal NO formation, but based on large changes to the flame pattern and location, it is understandable why that trend is not occurring in the results of this section (previous nozzle design changes had less effect on the position and pattern of the flame). Hence, flame temperature measurements were used as an indicator for the results rather than an accurate comparative parameter.
CR emissions within the exhaust were similar for 70° and 90° nozzles, but drastically increased for the 60° nozzle. This was likely because the decreased outlet angle gave the fuel more axial velocity and therefore less residence time in the hottest zones of the combustor. Additionally, less fuel was likely captured by the recirculation zone(s) because of the greater axial velocity, reducing solid fuel burnout and leaving more unburned carbon in the exhaust. One final interesting result from this dataset is that while the PM emissions increased drastically for the 60° nozzle, the CO emissions remained effectively constant. Generally, these two emissions should trend in the same direction as they are both indicators of combustion efficiency. However, carbon monoxide to carbon dioxide is a rapid volumetric process while CR burnout is a slow diffusion-based process, greatly dependent on hot-zone residence time and fuel/air mixing, and so the CR emissions were dramatically affected by the change in angle while the CO emissions were not. Moving from a 70° to a 90° nozzle likely increased fuel residence time because the spray would have had a higher proportion of radial velocity, keeping it in the hotter, upper regions of the combustor and allowing fuel droplets to be better entrained by the recirculation. Hence, there was a small corresponding decrease in CR (1.5%), but this is likely within the experimental error and therefore insignificant.

Nozzles with wider outlet angles were also tested briefly, but due to the size constraints of the combustion chamber, they could not be tested accurately because the flame jets and/or burning char would hit the chamber walls creating unreliable results. However, the data collected indicates that an increase in outlet angle above 90° would unlikely be beneficial.

The main conclusion from this set of experiments was that the cone angle had a major effect on the recirculation below the nozzle, similar to changing the amount of primary air swirl. From this series of tests, the 70° nozzle was still the best performing design. It appeared to provide the strongest flame with the highest stability when seated in addition to forming comparatively low levels of coking and emissions. Furthermore, the 70° nozzle had the shortest heat-up transient time by far, but no transient trend was observed with respect to spray angle. The only downside of this nozzle was that its stability range was relatively narrow and therefore its seating was more sensitive to the atomizing airflow, but this could probably be improved through additional design optimization. It is likely that an optimized spray angle would be somewhere above 70°, perhaps
in the 75°-80° range, where flame intensity and seating is still strong, but where the flame is also stable over a wider range.

4.3.3.4 Effects from the Number and Size of Nozzle Outlets

Spray experiments with water showed that changing the number and diameter of the outlets affected the nozzle's spray pattern rather than the SMD of the spray. Measurements showed that as long as the total outlet area was equivalent, the spray SMD was unchanged, but a larger number of smaller outlet holes reduced the spray angle and made the spray better dispersed and more evenly distributed. Alternatively, a fewer number of larger holes created more discrete, higher density spray jets.

Two additional custom nozzles were created for this round of experiments, similar in design to the sS3B6-70 nozzle, but differing in the number of outlet holes. All nozzles in this set of tests had an equal outlet area to the sS3B6-70 nozzle (six 0.66mm holes) and outlets were at an angle of 70°, however one nozzle was manufactured with eight 0.57mm diameter holes (sS3B8-70) and the other had four 0.81mm diameter holes (sS3B4-70). All experiments in this section were conducted with the second batch of fuel. The sS3B6-70 nozzle was also retested with the second fuel batch to ensure the consistency of results between the nozzles in this section. Manufacturing drawings for the air caps used in this section are provided in Appendix B.

To better understand the effects of the nozzle outlet number/size on the resulting spray patterns, a preliminary non-reacting test was conducted. This showed that at the sS3B8-70 nozzle's base-point, the spray was in a solid-cone pattern with a full cone angle of 74° as measured from the outer edges of the spray. The sS3B6-70 nozzle had a similar 74° full-cone angle at its base-point, but with a well-defined hollow cone pattern. Lastly, the sS3B4-70 nozzle formed an 86° full-cone angle at its base-point, also in a hollow-cone pattern.

Since all nozzles had an identical total outlet area and internal geometry, the comparatively large decrease in internal pressure for the four-outlet nozzle, as shown in Figure 57 below, was unexpected. Changes to internal airflow dynamics could have affected the atomization pressure slightly due to the customization between the nozzles, but then an overall trend would be observed, rather than just affecting the four-outlet nozzle. Outlet diameters were confirmed after
manufacturing so the most likely explanation for the pressure differential is some internal coking on the six and eight-hole nozzles which have smaller diameter outlets. Both of these nozzles did experience minor clogging towards the end of their experiments and while the pressure measurements were made during combustion tests prior to any evidence of clogging, some internal coking may have driven up the pressure beforehand.

Figure 57: Internal air pressure of customized nozzles, measured early during combustion tests

The most dramatic effect from the customized air caps was visually on the flame itself as illustrated below in Figure 58. The eight-outlet nozzle burned as a large, centralized, bushy flame that swirled around the nozzle rather than being seated on it, but it was anchored. Regardless of the atomizing airflow, the flame was never seated on the nozzle. This was likely due to the dispersed, solid-cone spray pattern produced by the nozzle which interfered with and weakened the recirculation zone below the air cap. The other two nozzles burned in the usual hollow-cone pattern with jetted flames, seated stably on the nozzle's bottom surface. The four-outlet nozzle had a more stable and intense seating with more intense and compact flames while the six-hole nozzle had a more bushy flame structure and weaker seating. The four-hole nozzle also had more visible burning char emanating from the flame, but is better compared through the accompanying videos listed in Appendix E. All three flames seemed relatively stable with the
sS3B4-70 nozzle being the best. Therefore, the main conclusions that can be drawn with respect to the outlet pattern are that fewer outlets increase flame jet compactness and seating stability, likely though only up to a point with respect to stability as a single outlet would probably be unstable and perform poorly. This result was unexpected given that denser spray jets (resulting from fewer outlets) would tend to reduce air/fuel mixing and thus the four-outlet design was actually predicted to form a poorer flame. However, it is probable that the poorer mixing from fewer outlets was nullified by the strong swirling primary air.

![Image](image_url)

**Figure 58: PLB flame comparison with differing outlet size/number**

At high atomizing airflows, the flame from the eight-outlet nozzle was detached and unstable (oscillating below the pilot flame), the flame from the six-hole nozzle was also detached, but anchored by the pilot and the flame from the four-outlet nozzle was mostly seated with only small oscillations. Therefore, the four-outlet nozzle is by far the most stable, even at high levels of atomizing air, likely because of its wider spray cone angle. Given the success of the four-outlet nozzle with its wider spray angle, it reinforces the conclusion from the previous section that an optimized outlet angle for a six-hole nozzle would lie somewhere between 70° and 90° with likely a steep performance drop-off when too high.

With respect to nozzle coking, the six-hole nozzle provided the best results as shown in Figure 59. Minimal coking was observed above this nozzle's outlets with almost none forming around or below them. With more nozzle outlets, the amount of coking greatly increased above the holes and with fewer outlets, the amount of coking greatly increased below the holes. This was because of the effect of the spray on the recirculation dynamics near the base of the nozzle. The solid-cone spray structure from the eight-outlet air cap may have weakened the recirculation at
the base of the nozzle (similar to the 60° nozzle design discussed in the previous section), preventing fuel from depositing on its bottom surface. As well, the heat generated by the swirling flame around the exterior of the nozzle was likely responsible for polymerizing some of the fuel there and forming the thick coke deposits above the sS3B8-70 nozzle's outlets seen in Figure 59. On the other hand, the wider hollow-cone spray pattern formed by the four-hole nozzle potentially increased the strength of the recirculation, providing the most stable and intensely seated flame along with significant coke formation on the nozzle's underside. The increased coking was also consistent with the wider spray from the 90° nozzle from the previous section. Both the four and eight-outlet nozzles could potentially develop coking problems under prolonged use, though coke often did burn off when it grew and interacted with the flame, assuming it did not first impinge the spray or block the nozzle outlets.

![Figure 59: Nozzle coking comparison with differing outlet size/number](image)

As mentioned, the flame from the eight-outlet nozzle was never seated, but its base-point was at 16.3SLPM. The six-hole nozzle was seated for 9.4SLPM (11.8-21.2SLPM with a base-point at 17.5SLPM). Finally, the four-outlet nozzle was seated for a much wider range of 13.8SLPM (5.2-19.0SLPM with its base-point at 13.1SLPM). In addition, the base-point outlet spray velocity of the eight-hole nozzle was 101m/s, 105m/s for the six-hole nozzle and 89m/s for the four-outlet nozzle. The observed trend was that a decreasing number of nozzle outlets increased the stability range, likely at least in part to the widening spray angle. The distance between the nozzle and pilot flame was also inconsequential for these nozzles.

The base-point flame temperature measurements were only useful for comparing the six and four-outlet nozzles which were found to have approximately the same temperature as shown in
Figure 60. This measurement, combined with the preliminary spray data showing the much wider spray angle (and therefore greater flame distance from the thermocouple) of the four-outlet nozzle, indicates that the flame from the four-outlet nozzle was probably hotter than that from its six-outlet counterpart. On the other hand, the flame shape of the eight-outlet design caused the temperature probe to sit directly within the flame during the measurement which was therefore much higher than the other nozzles and so this single measurement was not comparable. All nozzles had similar NO emissions with no significant difference between them. The four and six-hole nozzles also produced no measureable CO emissions at their respective base-points, while the eight-hole nozzle did produce a small amount. However, the difference between the six and eight-outlet nozzles was within the error range and therefore insignificant.

![Graph showing emissions and temperature vs number of outlets](image)

**Figure 60: Base-point nozzle comparison for differing outlet size/number**

The CR emissions were affected significantly by this design change. The six-outlet nozzle formed the least CR, but effectively equal to the amount from the eight-hole nozzle. On the other hand, the four-outlet design had far higher CR emissions than the other two nozzles despite its better stability, low CO and high temperature. The larger cone angle of the sS3B4-70 nozzle should also have helped to increase residence time, thereby reducing CR levels. However, this nozzle's internal pressure was significantly below that of the other two nozzles at its base-point (5.6PSIg versus about 10PSIg), meaning that the spray SMD of the four-outlet nozzle was much
larger and this was the likely culprit for the higher amounts of CR in the PM emissions indicated above. It is also possible that the smaller number of nozzle outlets and resulting higher spray density caused fuel droplets to agglomerate downstream of the nozzle which can occur with PLB [101]. Agglomeration would lead to larger droplets (effectively increasing the spray SMD or the population of large droplets), requiring additional hot-zone residence time for complete burnout and resulting in more CR. CO emissions were likely unaffected since CO oxidation is far more rapid than heterogeneous CR oxidation and therefore, CO emissions were less sensitive to the effects of spray SMD.

Clogging in these nozzles did become an important consideration, possibly because of the increased solids content in the second batch of fuel. This could also explain why the CR emissions from these nozzles were higher overall as compared to earlier experiments. The four-hole nozzle was the only one that did not clog while the other two clogged after base-point measurements were taken. The transient heat-up times were similar for the six and four-outlet nozzles and both were significantly shorter than the transient time of the eight-hole nozzle.

Clearly, the eight-outlet nozzle performed the worst out of this grouping. On the other hand, the four-outlet nozzle performed the best, having a larger stability range, a higher flame temperature, no instances of clogging and better seating/stability as compared to the six-outlet nozzle; both had no CO emissions. However, the six-hole nozzle did have better results with regards to coking and CR emissions. Given these findings, it should be noted that industrial-sized burners are much larger and so are their fuel residence times compared to the research burner used in these experiments, therefore CR emissions should be far lower in practice and consequently CR is one of the parameters of lesser importance in these tests. Since the sS3B4-70 nozzle performed very well and required performance enhancements with respect to only coking and CR emissions, it was chosen to be the basis for an optimized design moving forward utilizing the information gathered from all preceding experiments. Nozzle coking reduction was prioritized.

As this was the first series of experiments using the second batch of fuel, the effect of the PLB itself should be highlighted. While an analysis of combustion performance with respect to fuel properties is outside the scope of this research, the flames produced under identical combustor conditions with the same nozzle were very different as shown in Figure 61 below. The
standardization of PLB was noted in the literature review as a critical area of improvement required from manufacturers as this fuel becomes commercialized in greater quantities and these experiments presented a perfect example of why this is important. When designing a burner and combustion system, regardless of its purpose, flame size, radiant energy, the potential for clogging and many other parameters are critical to performance and fuel variation will cause significant issues if not properly standardized, even when the fuel is within current ASTM specifications as both of these PLB batches were.

![Figure 61: sS3B6-70 PLB flames under identical combustor conditions, comparing batch 1 (left) and batch 2 (right)](image)

4.3.3.5 Nozzle Optimization Results

4.3.3.5.1 Comparison with sS3B4-70 Nozzle

As a final stage in this nozzle design research, the trends previously observed throughout this thesis have been used to create a first-step optimized nozzle. Given the complexities of the fuel and its interaction with the large number of interconnected combustor parameters, proper optimization would be a lengthy process requiring a large number of iterations, which is beyond the scope of this thesis. A similar optimization process would also be required for each individual combustor, as significant variations would exist, resulting in a different final optimal nozzle design. This section describes the decisions and results of a simplified nozzle optimization process for the combustor used throughout this research. Based on the previous
section, the sS3B4-70 nozzle has provided the best results thus far, except with respect to coking and CR in the PM emissions. The design of the optimized four-outlet nozzle (sSoptB4-66) attempted to address these two areas, focusing on coking.

To improve coking, the outlet angle needed to be decreased, but in theory this would also tend to reduce flame seating by weakening the recirculation zone near the nozzle and increase CR by reducing the residence time. Based on the results from Section 4.3.3.3, the spray cone angle of the four-outlet design (sS3B4-70) likely fell between the cone angles of the six-outlet 70° and 90° nozzles (sS3B6-70 and sS3B6-90). Within this spray range, the effect of lowering the outlet angle was negligible for CR, but coking was significantly reduced. The CR fraction from the sS3B4-70 nozzle was probably elevated, compared to other nozzles examined within the same trend, due to its low base-point pressure and so to address this, the outlet area was decreased. Four outlets were still used, but they were smaller in diameter (0.71mm versus 0.81mm) to increase the nozzle's internal pressure and reduce the spray SMD. Furthermore, the reduction in outlet area had been previously correlated with an increase in coking, quite possibly because it increased the spray cone angle by several degrees. Based on all the preceding information, the outlet angle reduction was chosen to be 4° (from 70° to 66°) in order to decrease the spray cone angle overall, but also to remain far from a 60° outlet angle which previously gave quite poor results and an unseated flame. Also considered was the effect of these design changes on the base-point seating/stability and the stability range, but since these effects would have been hard to predict, they did not directly influence the design decisions. Given the parametric trade-offs involved with this design, complete optimization would likely require several iterations. The manufacturing drawing for this optimized nozzle design is available in Appendix B.

Coking was significantly reduced when using this optimized nozzle, as shown in Figure 62 below. This trend held at all atomizing air points examined as compared to the sS3B4-70 nozzle. There is no reason to believe that coking would represent an operational issue moving forward when conducting longer duration testing, i.e. continuously for multiple days, with the optimized nozzle. Previous experiments did show that coking increased when reducing outlet area (from the S3B6 nozzle to the S4B6 nozzle), but the outlet angle reduction incorporated in the optimized design, to which coking has been shown to be sensitive, seems to have offset this effect.
The optimized nozzle formed less intense, but longer flame jets because of its reduced outlet area which increased the outlet spray velocity, as shown in Figure 63. As a result of the optimized nozzle's reduced outlet angle, its seating intensity was correspondingly weakened due to the effects on the recirculation zone. Regardless, both nozzles formed a strongly seated and stable flame from a hollow-cone spray pattern.
For CR within the PM emissions, the nozzle design changes had no effect, meaning that the CR from the optimized nozzle was still elevated, but identical to that from the sS3B4-70 nozzle. However, as previously mentioned, the CR could be largely reduced or perhaps even eliminated when PLB is used in industrial systems. The design did have the desired effect on the internal pressure of the nozzle as shown in Figure 64, greatly increasing it above the sS3B4-70 nozzle and even above that of the sS3B6-70 nozzle, but CR was unchanged. At the base-point, the optimized nozzle had an outlet spray velocity of 103m/s compared to 89m/s for the sS3B4-70 nozzle. The reduced hot-zone residence time from the increased outlet spray velocity and the decreased cone angle, appears to have effectively countered any beneficial effect on CR emissions from the reduction in SMD due to the increased atomization pressure.

![Figure 64: Comparing the emissions and air pressure between the sS3B4-70 and sSoptB4-66 nozzles](image)

The optimized nozzle performed similarly with respect to CO emissions as compared to the sS3B4-70 nozzle, being near zero at the base-point (Figure 64). Eventually, as anticipated, CO emissions increased for the optimized nozzle at very high levels of atomizing air due to flame instabilities and localized extinctions from high shear rates along with lower hot-zone residence times. As such, the nozzle would not likely be operated at these higher atomizing airflow rates where measureable CO emissions were detected, so the poorer CO readings are inconsequential.
The optimized nozzle also had significantly decreased levels of NO formation, the reason for which is not immediately clear since NOx formation is complex and highly localized. However, the same trend occurred with the larger nozzles when the outlet area was reduced, comparing the S3B6 to the S4B6 design, so the trends were consistent. The reduction in NO could be from thermal NO due to the lower hot-zone residence time of the fuel as a result of the increased outlet spray velocity and/or perhaps could be from fuel-NO as reduced outlet area could form denser spray jets that could then create localized fuel-rich zones.

The flame temperature was 797°C for the optimized nozzle compared to 789°C for the sS3B4-70 nozzle. The higher temperature was attributed to the lower outlet angle of the optimized nozzle, positioning the flame jets a little closer to the tip of the thermocouple probe, though the small temperature difference likely also falls within the range of experimental error.

The optimized nozzle did have a wider seated stability range of 16.1SLPM (5.7-21.8SLPM with its base-point at 12.7SLPM) compared to the sS3B4-70 nozzle which had a seated stability range of 13.8SLPM (5.2-19SLPM with its base-point at 13.1SLPM). Right at the bottom of the atomizing air stability range (Figure 65), the optimized nozzle exhibited a wide, bushy flame structure that was unseated and swirling around the nozzle exterior, similar to other nozzles at low atomizing airflows. The flame was fairly symmetric and well anchored, providing stability. At this set-point, the coking was reduced on the bottom of the nozzle and more concentrated above the outlets, closer to the flame. Hence, coke deposits tended to form in higher temperature regions as seen earlier. At the maximum stable atomizing airflow (Figure 65), the flame’s seating was weaker, looking thinner and experiencing minor oscillations, but still clear. The flame jets were also dissimilar with one jet being bushy while the other was compact, though both jets remained anchored, seated to the nozzle and fairly stable. At this point, coking was more prevalent on the bottom surface of the nozzle. In preceding PLB flame research, the flame was lifted and near blowout at these same high atomizing airflow rates [5]. The current ability of a properly designed nozzle to form a stably seated PLB flame at high atomizing airflow rates and over a wide range of airflows indicates a reduced sensitivity to burner operating characteristics which was one of the main objectives of this research.
Figure 65: PLB flames at low atomizing air, 5.7SLPM (left), and at high atomizing air, 21.8SLPM (right)

Both flames from the four-outlet nozzles were sensitive to their rotational position relative to the pilot flame because fewer outlets caused the spray to become more concentrated and less dispersed. Poor rotational positioning generated oscillations in the flame jets and nozzle seating, reducing stability. Hence, the nozzle's rotational sensitivity increased with fewer outlet holes. On the other hand, both four-outlet nozzles were insensitive to their vertical distance from the pilot flame and both had approximately equal heat-up transient times as measured with respect to CO emissions.

The only remaining concern with this nozzle when used in the small-scale combustor is the amount of CR in the exhaust. The best way to address this problem without impacting coking would be to further reduce the nozzle's mixing chamber diameter to reduce the SMD without negatively affecting spray outlet velocity or residence time and/or to use five nozzle outlets (while maintaining the spray cone angle and perhaps slightly increasing the total outlet area) to reduce droplet agglomeration. However, both of these options would increase the risk of clogging.

In conclusion, both four-outlet nozzles had equal CR emissions, CO emissions and flame temperatures with the optimized nozzle having a greatly reduced coking propensity, lower NO emissions, an increased seated stability range and a weaker, but stable seated flame. Despite the less intense seating, the optimized nozzle's flame was very stable and well-anchored. Given the
notable benefits of both lower coking and NO emissions along with the wider seated stability range, the optimized nozzle was the best performing design. Its only potential disadvantage was the weaker flame seating, however there is no evidence to suggest that it actually caused any negative effects. Therefore, the optimized nozzle was used for the remaining experiments.

4.3.3.5.2 Cold-Start on 100% PLB

As previously described, experiments were typically initiated by running the burner on pure ethanol in order to heat up the combustion environment prior to beginning the flow of PLB. This is because PLB is not very volatile and has a high water content, requiring a large amount of energy input for ignition. Normally, combustor exhaust temperatures were above 500°C when the PLB flow was started. This startup procedure makes PLB less attractive for industrial use since fuel switching requires more complexity and ethanol is an expensive fuel [21]. Using the optimized nozzle and its much-improved atomization compared to previous research, a cold-start was attempted using the current combustion system. When beginning this research project and using early nozzle designs, ignition with PLB was difficult even after the combustor had been heated with ethanol, so this was an important step to see how far the nozzle design had progressed.

Before the test, the fuel line was purged with compressed air, but small amounts of ethanol were unavoidably present, estimated to be approximately 3mL. At the time of initial PLB ignition, the only sources of heat in the combustion chamber were from the 0.3kW methane/oxygen pilot flame and the 1kW air heater used to warm the incoming primary air and fuel. When beginning the test, the primary air was at a temperature of 144°C and the nozzle positioning and atomizing airflow matched that used for the base-point in Section 4.3.3.5.1. The experiment ran with the standard fuel energy throughput of 10kW.

During the cold-start, the PLB immediately ignited. The flame was initially unstable and for less than ten seconds after ignition, the flame appeared to contain a mix of PLB and ethanol. The flame stabilized after about 15 seconds and was fully developed by about 30 seconds (Figure 66), with its appearance changing little afterwards. The initial flame instabilities were likely the result of fuel boiling since the nozzle was very hot (105°C) before the fuel flow was initiated, dropping to below 80°C soon after.
During the cold-start, there were no issues with respect to nozzle coking. Heavier than normal coking was occasionally present, but burnt off without any external action. CR also built up on the insulative lining of the combustor early on, but burned away as the temperature within the combustion chamber increased. The heat-up on 100% PLB was very similar, but smoother, than when done with ethanol as shown in Figure 67. The flame established during this test was also very similar to that shown in Section 4.3.3.5.1 which used the same nozzle, indicating good experimental repeatability. The only noticeable difference between the flames was that in this experiment, the flame's seating was a little more intense. Just prior to the end of the test, at approximately 110 minutes, a possible minor clog within the nozzle was detected, but the flame was still stable and strong with the measured exhaust temperature continuing to slowly increase.
Figure 67: sSoptB4-66 nozzle heat-up transient profiles; one using solely PLB and the other warming up on ethanol until being switched to PLB at about 50 minutes

4.3.3.5.3 Pilot Flame Influence on Combustion Stability

Given the success of the optimized nozzle in improving PLB combustion, a final experiment was conducted to determine whether, during steady-state conditions, the PLB flame could be self-sustaining in a stable manner without the methane/oxygen pilot flame for support. Previous research in this combustor using a suboptimal nozzle design showed that without the pilot flame, the PLB continued to burn, but in a very unstable fashion, far downstream of the nozzle [5]. However, when using the optimized nozzle at steady-state conditions, the PLB flame was unaffected by the removal of the pilot with no decrease in stability. In fact, the PLB flame actually appeared to be slightly more stable without interference from the cross-flowing pilot flame. Pictures of the PLB flame with and without the pilot flame are shown below in Figure 68. Unfortunately, these pictures are not high quality because the combustor viewports were dirty near the end of the experiment when the images were taken. After 30 minutes without the pilot flame, the PLB flame was still stable, seated and unchanged, denoting that at steady-state conditions, a pilot flame is no longer required and combustion can be achieved with no secondary fuel input. These results are directly applicable to larger combustors which would have a reduced heat-loss fraction compared to this small-scale combustion system. The primary
air and fuel heater was on for the entirety of the experiment since the pilotless PLB flame would not likely have remained consistently stable without it.

![Figure 68: The stable PLB flame with a 0.3kW pilot flame (left) and without a pilot flame (middle); an unstable pilotless PLB flame (right) from previous research [5]](image)

The effects of the pilot energy on NO and CO emissions are shown below in Figure 69. CO emissions were effectively zero at all points, but did demonstrate a slight decrease within the error margin as the pilot energy was reduced. While this is not significant, the CO emissions could have been from the cross-flow shear of the pilot flame slightly interfering with the PLB flame. On the other hand, NO emissions decreased drastically when reducing the pilot energy due to the lower thermal NO produced without the intense heat of the methane/oxygen pilot flame. Based on the results of this experiment, at steady-state, the pilot flame should always be extinguished in order to reduce emissions and improve PLB combustion quality and stability.
Nozzle coking was unaffected by changes in the pilot flame energy. Furthermore, the PLB flames were identical in appearance at high and low levels of atomizing air regardless of the pilot energy, therefore the seated stability range of the PLB flame should also have been independent of the pilot flame. At all pilot energies examined, the base-point atomizing air pressure was equalized to maintain the spray SMD. It should also be noted that NO emissions were higher than in previous tests with the optimized nozzle (as evidenced at 0.3kW in Figure 69) because of reduced primary air inlet flow rates as a result of a mechanical issue with the stack fan. This would have increased thermal NO emissions because of increased combustion temperatures since there was less incoming primary air to heat up and the equivalence ratio was closer to stoichiometric.

**Figure 69: CO and NO emissions from a PLB flame as a function of pilot flame energy**
Chapter 5

5 Summary, Conclusions and Future Work

5.1 Summary

Distilled water was used to elucidate the key trends behind the atomization of an internally mixed air-blast nozzle. Findings indicated that a large improvement in spray quality (as measured by the SMD and the percent volume of droplets larger than 100\(\mu\)m) could be achieved by reducing the total area of the air cap outlets and by increasing the air/liquid relative velocity within the nozzle's mixing chamber. The effects of both were more pronounced at lower airflow rates and resulted in an increase of the nozzle's internal pressure. The internal air pressure of the nozzle was shown to be the dominant parameter influencing spray SMD as all of the data from various nozzles collapsed onto a single pressure curve. When the nozzle's outlet area was reduced, lower atomizing airflow rates could then produce a given spray SMD, but this was also coupled with a nearly proportional increase in spray outlet velocity. In a combustion environment, an increased outlet spray velocity also induces a higher flame shear, both of which can be particularly problematic for low volatility PLB that requires longer hot-zone residence times. Conversely, when the nozzle's internal mixing chamber was narrowed to increase the air/liquid relative velocity, a given spray SMD could be produced with a lower outlet spray velocity.

Having a larger number of smaller outlets with an equivalent total area did not affect the spray SMD and only reduced the population of larger droplets at high airflow rates. In addition, more outlets reduced the spray cone angle and formed a more dispersed and even spray, but would also increase the likelihood of clogging from the PLB solids content or polymerization. Furthermore, the shape of the outlets was inconsequential to the resulting spray SMD.

Within the nozzle, it is believed that the liquid jet disintegrated when impacting the bottom of the air cap and therefore, actions taken to reduce the liquid jet diameter and increase the liquid pressure had no beneficial effect on the spray. Some liquid then pooled at the bottom of the air cap while the remaining liquid was entrained by the atomizing air currents and deposited along the internal surfaces of the air cap's mixing chamber as a thin film. In both cases, the liquid was
atomized by the air within the air cap outlets, explaining why the atomizing airflow had such a large effect on the spray SMD and why there were two separate distributions evident within the spray data (the smaller distribution was likely from the thin-film atomization).

Given the primary atomization mechanisms within the IMAB nozzle and the apparent spray SMD decrease that occurred when PLB was atomized in place of water at an equivalent pressure, the prompt atomization correlation [106] was determined to be the best available spray SMD correlation for this fuel/nozzle combination. This attributes the spray SMD reduction to the lower surface tension of PLB as compared to that of water. Furthermore, to reduce the spray size differential between preheated PLB and diesel, atomizers that operate via the prompt mechanism should be utilized as the fuels' surface tensions are far more similar than their viscosities. However, lower fuel viscosities still improved the quality of the PLB spray.

CO and CR emissions were effectively independent of atomizing air when a stable flame was present because the effects of spray SMD and hot-zone residence time equally compensated for each other. Higher atomizing airflows caused the flame to lift off the nozzle and detach from shear, becoming unstable (often oscillating) and burning below the pilot with less visible flame as the SMD behaviour became asymptotic and residence time effects dominated. Lower atomizing airflows caused a spike in emissions below a certain point where the spray SMD likely grew exponentially. At low atomizing air, the flame became unseated and burned as a large, bushy, sooting flame, but remained anchored, swirling around the exterior of the nozzle. NO emissions were consistent because they were mostly the product of fuel-bound nitrogen with minor changes attributed to thermal NO.

Total air cap/nozzle outlet area was found to have only minor effects on the PLB combustion since as the outlet area was decreased, the flame would stabilize at a point where there was a smaller spray SMD and residence time, but increased flame shear. Reducing the outlet area caused the seated stability range of the flame to narrow, coking to increase and NO and flame temperature to decrease while causing the flame to become more compact. CO and CR emissions were mostly unaffected by the outlet area except that CR would increase if the total outlet area was decreased too much. For this trend, the S2B6 nozzle performed the best, producing the most stable and strongest flame while the S0B6 nozzle had the least stable seating.
Experiments with the smaller air caps used the S3B6 design due to size restrictions. Using a smaller nozzle to improve atomization through a higher air/fuel relative velocity resulted in a more intense and stably seated flame from enhanced ignition, but with a narrower allowable airflow range for stability. The flame also had a higher temperature and correspondingly higher NO emissions. Furthermore, through better atomization, CR, coking and heat-up transient time were reduced while CO emissions were eliminated. Therefore, the smaller sS3B6-70 nozzle performed much better than the larger volume nozzles.

When the spray outlet angle was increased, coking and seated flame ranges also increased significantly, likely due to the strengthening recirculation zone near the base of the nozzle. However, the 90° nozzle had a comparatively lower flame and seating intensity, so overall beneficial outlet angle effects appeared to peak below this point. The 60° nozzle was never actually seated at any point, but was anchored. All of the nozzles had negligible CO emissions and NO emissions were fairly constant. CR was effectively unchanged for outlet angles at or above 70°, but quickly increased below 70° from reduced hot-zone residence time. The sS3B6-70 nozzle was still the best design thus far, but an optimized design would have probably had a 5-10° higher outlet spray angle.

The number of nozzle outlets (with an equal total outlet area) had a large effect on the spray pattern. The eight-outlet nozzle formed an unseated, centralized, bushy flame because of its solid-cone spray which weakened the recirculation zone below the nozzle, forming minimal, but measurable CO emissions. The four and six-outlet nozzles formed hollow-cone sprays at varying spray angles with zero CO emissions and all nozzles had similar NO emissions. Fewer (larger) outlets, formed a more intense, compact, seated flame with a wider seated stability range as a result of its larger spray cone angle and stronger recirculation, but this also served to increase coking on the nozzle's underside. Fewer (larger) holes reduced the risk of clogging, but increased angular sensitivity to the pilot flame position due to more concentrated spray jets and CR was higher because of possible fuel droplet agglomeration and a higher spray SMD. The only moderate benefits of the six-hole nozzle was with respect to coking and CR, the latter of which would likely decrease significantly in a larger industrial burner. The four-outlet nozzle was the best design overall after this round of testing and was the basis for further optimization.
Based on the preceding results, a final optimized nozzle was manufactured having four 0.71mm outlets (the non-optimized design had four 0.81mm outlets) to decrease CR at a reduced angle of 66° from 70° to lower coking. Coking was greatly improved from recirculation effects while the flame seating was slightly weakened, but still very stable, and CR was unaffected as the reduced spray SMD was offset by the reduction in hot-zone residence time. Additionally, CO emissions were unchanged (still zero) while NO emissions were reduced significantly. The flame temperature was also unaffected, but the stable seating range was further increased. Overall, the optimized nozzle out-performed any previous design.

Using the optimized nozzle, a successful combustor cold-start was conducted using only a 0.3kW pilot flame and a 1kW primary air/fuel heater as energy inputs. The fuel immediately ignited, the flame stabilized within 15 seconds, coking was normal and the heat-up transient profile closely matched that using ethanol as a starting fuel. Finally, it was determined that when using the optimized nozzle at steady-state, a pilot flame was no longer required for stabilization because the pure PLB flame was fully self-sustaining. Without the pilot flame, there were no CO emissions, even after 30 minutes, and NO emissions decreased significantly without the thermal NO contribution from the pilot flame. Air cap coking and the PLB flame's seated stability range (with respect to atomizing airflow) were unaffected by the pilot and the stability of the PLB flame was slightly improved without the cross-flow shear generated by the pilot flame.

The objectives of this research project have been met and PLB combustion has been shown to be industrially viable with minimal emissions, only requiring secondary fuels in the form of a pilot flame during initial combustor operation. The seated stability range of the PLB flame has also been widened with a properly designed nozzle, so the flame is therefore far less sensitive to the burner's operating characteristics, especially with respect to the atomizing airflow rate.

5.2 Conclusions

The results of the combustion experiments indicated that with a properly designed nozzle, PLB is ready for use on an industrial-scale from a technical engineering perspective. It is capable of replacing heavy fuel oils and operating with high combustion efficiencies. Additionally, the effects of nozzle design and spray characteristics on PLB flame stability and emissions have been identified in order to guide burner designers looking to utilize this fuel. The examined
nozzle design criteria generated competing and unquantifiable effects, requiring trade-offs and an
iterative nozzle optimization process depending on the objectives of the application and the
specific characteristics of the burner. As a starting point, the following list identifies critical
factors for PLB combustion and the major parameters that correlate with them:

- CO emissions were negligible with a stable flame, a larger hot-zone residence time and
  reduced through better atomization, ideally by increasing the air/fuel relative velocity
  within the nozzle using a smaller internal mixing chamber diameter

- NO emissions were largely the result of fuel-bound nitrogen so to reduce NOx, fuel
  modification would be most effective, but thermal NO contribution was decreased with
  poorer atomization, by reducing the air cap outlet area to lower residence time and by
  reducing flame temperature and intensity; there should be no pilot flame active during
  steady-state operation

- Coking was reduced with better atomization from a smaller internal mixing chamber, a
  less intense seated flame, a smaller cone angle to reduce recirculation at the base of the
  nozzle and an increased air cap outlet area (possibly due to spray angle effects)

- CR emissions were reduced with a smaller spray SMD through better atomization and
  more air cap outlets to prevent fuel droplet agglomeration; hot-zone residence time was
  critical though, and could become the dominant factor, so the outlet spray velocity
  should be low with a wider cone angle if possible

- Nozzle seating and stability was increased with better atomization from a smaller
  internal mixing chamber, a wider spray cone angle (up to a point) to strengthen
  recirculation, fewer (larger diameter) outlets which also increased the spray angle and an
  increased air cap outlet area (up to a point)
5.3 Future Work

While substantial progress was made in understanding the atomization of this IMAB nozzle, time and instrument limitations prevented further study and more insights can be garnered by investigating the following topics:

1. It would be useful to study the effects of surface tension and viscosity on this nozzle in order to quantify their effect on the spray SMD and to confirm the qualitative results presented in this thesis. Customized fluids can be produced to isolate for and individually study these effects.

2. Spray measurements can be conducted to quantify the magnitude of the important trends identified on actual PLB sprays. Determining the base-point spray SMD and droplet size distribution for the optimized nozzle would also be beneficial. Furthermore, this would allow for the accuracy of the prompt atomization correlation to be determined with PLB sprays or a new correlation could be generated specifically for PLB.

3. Understanding how combustor conditions, such as thermal feedback and primary air swirl, influence the PLB spray would be useful in order to better connect the spray results with the flame observations and pollutant measurements.

4. Manufacturing inconsistencies are unavoidable, but their impact on the spray was not fully understood. A population of identically designed nozzles should be fabricated and tested to understand how sensitive the nozzle is to manufacturing tolerances and defects.

PLB has been shown to be a viable fossil fuel alternative, but progress on spray combustion and nozzle design can still be furthered through the study of these additional research avenues, precluded in this work by time and fuel limitations:

1. PLB flame and data repeatability seemed reasonable when using the optimized nozzle, but detailed repeatability and sensitivity experiments were not possible and would be useful for future work.
2. The two respective batches from our fuel supplier appeared to be fairly consistent with respect to the measured fuel properties, but caused results to differ quite drastically during combustion experiments. Understanding the specific fuel properties that most significantly impact combustion characteristics would be useful to address fuel standardization concerns as PLB fuel manufacturers look to increase industrial use.

3. Now that crude PLB is combusting well, it would be useful to compare it against different upgraded PLBs to determine whether they offer worthwhile benefits within burners, boilers and/or furnaces to justify their increased cost and carbon input.

4. While the final nozzle design operated very effectively, it was only one step in what should otherwise be a lengthy, iterative progress. Further optimization would likely lead to minor performance improvements, but valuable additional insights.

5. It is not well understood how the type of anchoring of the PLB flame affects its ability to withstand adverse environmental conditions. Flame seating stability and intensity were important observable characteristics throughout this research as unseated flames are thought to more easily blow-out or otherwise extinguish. Is a more intense flame seating always beneficial or only up to a certain point, after which increased coke formation can offset any advantages from improved stability? For stability, is it important whether the flame sits on the nozzle or can it simply be otherwise anchored nearby? Questions such as these are critical for PLB flames given their sensitivity to their environment and should be studied in the near-future.

6. When examining the combustion effects due to the changing number of outlets in Section 4.3.3.4, the four-outlet design had a more stable and intense, seated flame than the six-outlet design, but it is unclear whether this was due to the change in spray pattern and/or spray cone angle. A controlled experiment ensuring an equal spray cone angle (by adjusting the air cap outlet angle), but a differing number of outlets would answer this question.

7. For fuel oil flames, matching the fuel spray angle to that of the recirculation zone has been shown to optimize flame stabilization, combustion efficiency and emissions [149].
Computational fluid dynamics and analyses of the research combustor can be conducted to determine the recirculation characteristics to match the nozzle spray cone angle with the recirculation zone and determine if this optimization scheme also works for PLB flames.

8. Longer duration PLB combustion testing, on the order of days, would be beneficial to determine if any previously unidentified problems occur, data trends become inconsistent or coking worsens. Limitations of the small-scale combustor used for this research prevented continuous PLB run times longer than about six hours. Given the increased sensitivity of small-scale combustors, longer-term testing would be more applicable to industrial applications if conducted in a larger-scale facility.

9. During combustion experiments, the internal pressure of the nozzle would often slowly increase, likely from some internal coking or partial clogging, which could cause problems during longer duration testing. This issue stems from the small size of the nozzle and from fuel polymerization at the nozzle outlet (due to flame thermal feedback). Occasional flushing with ethanol could resolve the issue, but this would not be ideal. Instead, it should be determined whether this problem also exists within larger industrial nozzles and burners as it may simply be a consequence of the small-scale experiments being used for this research and not of practical concern.

10. This research showed that at steady-state, with a properly designed nozzle, PLB flames are self-sustaining and remain stable without a pilot flame. It is unknown at what time during the heat-up process the pilot flame can be extinguished and this should be investigated. Furthermore, once the PLB flame is burning without the pilot flame, it would be useful to determine whether the primary air heater is still required, and if so, what is the minimum allowable temperature to maintain flame stability and emissions.

11. It would be useful to connect the scale and gear pump into a feedback system to automatically control the fuel flow rate with the LabVIEW software already in use for burner sensor monitoring. Instead, during these experiments, averaged fuel flow rates were measured continuously in real-time with Excel using data automatically input from
a scale. The pump speed was then manually adjusted when necessary to maintain the proper flow rate.

12. The equipment used for these combustion experiments is aging and therefore, is in need of maintenance, but the results of this research were not negatively affected. The following is a list of equipment in need of servicing:

- The FTIR spectrometer requires a performance verification, end-plate realignment and a new laser and IR source as they are both now past their life expectancy
- The flame ionization detector, used to measure UHC emissions, was giving inaccurate readings, but was unnecessary for these experiments; the internal pump, which was originally thought to be the problem, was shown to be operating properly
- The USB module that sends sensor signals to the LabVIEW program for combustor monitoring can crash, requiring a restart; this unit may need to be replaced
- The exhaust stack fan, which controls the primary air, was unable to pull through the required airflow during the final combustion experiment, even after being cleaned, so the problem is believed to be related to age or an electrical malfunction
- The oxygen sensor did not appear to be providing reliable measurements and so it was not used for these experiments
References


[41] A. V. Bridgwater, “Renewable fuels and chemicals by thermal processing of biomass,”


assessment and economic analysis (NREL/TP-510-37779),” 2006.


Appendices

Appendix A. PLB Chemical Upgrading

The primary chemical upgrading methods are catalytic cracking and hydrotreating (or hydrodeoxygenation)[73]. Both methods act to deoxygenate the fuel and break down the HMW compounds to produce a biofuel with properties similar to that of typical transportation grade fuels, though subsequent refining through standard petroleum infrastructure is required [40], [42], [73], [83]. Both of these methods use a catalyst which becomes rapidly deactivated during testing, requiring frequent maintenance, and therefore research is still ongoing [13], [19], [83].

Catalytic cracking produces a chemically upgraded fuel at high temperature (about 450°C, but can vary) and atmospheric pressure, but reduces the maximum yield to only about 30% of the initial PLB. The resulting fuel is of comparatively poorer quality than when hydrotreated, but the process involved is simpler and therefore cheaper than the alternatives [19], [42], [73], [83].

Hydrotreating is considered to be a more viable option than catalytic cracking since hydrotreated fuel has a much lower final oxygen content (below 5wt%), a higher final heating value (more than twice that of the original biofuel) and a resulting yield of up to 65% of the initial PLB since no carbon is removed [73]. This process also improves ignition characteristics, reduces acidity, provides enhanced thermal stability and significantly reduces the fuel's water content and viscosity which are important for spray atomization and combustion [17], [70], [73]. For hydrotreating, a catalyst is used in a high temperature (up to 450°C), high pressure (up to 200 bar) and hydrogen rich environment. This process has also been used to reduce the nitrogen content of the fuel, through the formation of ammonia, which can reduce NOx emissions [83].

Both of these chemical upgrading methods require additional fuel processing, increased capital expenditure and result in a reduction of the fuel yield, all of which act to increase the cost of the biofuel which is just currently approaching economic viability in its crude state [32]. Additional processing also requires a higher energy input, which is equivalent to a higher carbon input, increasing the fuel's lifecycle carbon emissions and ultimately detracting from one of the main advantages of PLB, its carbon-neutrality.
Appendix B. Custom Air Cap Manufacturing Drawings

Figure 70: Manufacturing drawing for the S0B6 standard JPG60 air cap

Figure 71: Manufacturing drawing for the S4B6 custom JPG60 nozzle
Figure 72: Manufacturing drawing for the S2B6 custom JPG60 nozzle

Figure 73: Manufacturing drawing for the S3B6 custom JPG60 nozzle
Figure 74: Manufacturing drawing for the S4B custom JPG60 nozzle

Figure 75: Manufacturing drawing for the S3B custom JPG60 nozzle
Figure 76: Manufacturing drawing for the S3B-Slot custom JPG60 nozzle

Figure 77: Manufacturing drawing for the S4B-Pin custom JPG60 nozzle
Figure 78: Manufacturing drawing of the pin for the S4B-Pin custom JPG60 nozzle

Figure 79: Manufacturing drawing for the SB72 custom JPG60 nozzle
Figure 80: Manufacturing drawing for the standard JPG15 nozzle

Figure 81: Manufacturing drawing for the sS3B6-70 custom JPG15 nozzle
Figure 82: Manufacturing drawing for the sS3B6-90 custom JGP15 nozzle

Figure 83: Manufacturing drawing for the sS3B6-60 custom JGP15 nozzle
Figure 84: Manufacturing drawing for the sS3B8-70 custom JPG15 nozzle

Figure 85: Manufacturing drawing for the sS3B4-70 custom JPG15 nozzle
Figure 86: Manufacturing drawing for the sSoptB4-66 custom JPG15 nozzle
Appendix C. Nozzle Alignment Methodology

To make comparable measurements, repeatable alignment of the laser with the spray was critical. The nozzles were all unique in design and so it was imperative to compare the spray SMDs with a proper procedural methodology, otherwise the results would not have been meaningful. In order to achieve this, the laser must first pass through the centre of the spray. The laser itself on the Spraytec was biased towards the right side of the transmitter (left side of the receiver). Therefore, for proper alignment the enclosure was clamped parallel to the edge of the table with the legs of the Spraytec placed equidistant from the edge of the table so that the enclosure and laser were both parallel. An alignment bar was then put in place of the nozzle. The bar's width matched the diameter of the nozzle's extension tube so that it sat in the same position. The bar had a scale printed on its surface allowing the laser to be centred, thereby ensuring the nozzle was then centered with the laser. The alignment bar also allowed for a precise measurement of the height of the laser relative to the enclosure. Since the full width of the laser beam was wider than the nozzle's extension tube, the alignment device was comprised of two pieces magnetically attached. Once aligned, all components were secured throughout the entire set of experiments.

Aligning the spray with the laser was done with the use of an alignment pin. This was necessary since the nozzle and air cap were free to rotate. During alignment, the pin was pushed into one of the outlets on the air cap and a string was suspended from the pin with a small weight on the end acting as a plumb-bob. The string passed through the laser's path and then the nozzle was rotated to centre the string within the laser beam, establishing a datum. With the use of the datum and a protractor around the nozzle's extension tube, the nozzle was able to be rotated accurately within 1°. The pin was tapered at one end so that it could fit into all outlet hole sizes being tested. A piece of tape was placed around the tapered end in order to form a friction fit within the outlet to securely hold the pin in place without damaging the nozzle. Alignment in this manner was deemed to be accurate within ±4°. However, when some nozzles with blocked holes (from SuperEpoxy) were aligned in this manner, the spray jet emanating from the nozzle was clearly not aligned with the laser. In these cases, it was clear that the jets do not emerge straight from the nozzle and/or the turbulent air flowing into the enclosure was unavoidably distorting the spray. Therefore, a visual alignment of the jet with the laser was necessary, but
this was not difficult at high airflow rates as the spray formed dense, discrete jets. Visual jet alignment was actually deemed to be more accurate, within ±2°. Nozzles with six outlets created a more diffuse spray (increased spray dispersion per jet) and had to be aligned with the pin. However, diffuse sprays were much less dependent on alignment.

Daily baseline tests were conducted to determine experimental error. For these tests, the alignment pin was also used to ensure accuracy and repeatability. Since the pin would be used for this nozzle regularly, it was convenient to streamline the alignment process and so the other side of the pin was turned on a lathe to fit within this nozzle's outlets securely (no taper). The pin still used the same plumb-bob system to ensure alignment and accuracy was improved to within ±2°.

In cases where visual jet alignment was conducted, the laser only passed through a single spray jet between the transmitter and receiver. Since the air entering the enclosure was affecting the angle of the spray jet, when it was aligned with the transmitter, a 180° rotation of the nozzle did not yield identical results, rather 180±5° (depending on the rotational direction) was required. As such, all measurements were made with the spray jet in a consistent position. It was determined that having the spray jet closer to the transmitter was a better position since it would be less likely for any stray droplets to deposit on the receiver and in this position it was easier to view the jet, therefore allowing for a more accurate alignment with the laser. Measurement procedural consistency was critical.
Appendix D. Important Spray Correlations

1 Prompt Correlation

\[ D_{32} = 3 \left[ \frac{2}{d_o} + \frac{C \rho \frac{U_a^2}{2}}{4 \sigma (1 + ALR^{-1})} \right]^{-1} \] [106]

This correlation is for prompt atomization and was developed based on energy considerations, mainly the ratio of the energy required for atomization to the kinetic energy of the atomizing air.

C is a measure of the efficiency of the atomization process and varies between atomizer designs. It should be found experimentally and be well below unity [106], [124]. A good starting value for C is 0.00084 for jets [124] and 0.007 for thin sheets [106]. The value of C is larger with higher atomizing air pressures and more compact jets since the liquid is atomized more effectively, generating a smaller SMD. Comparing results between the equation and experiments in the paper showed a satisfactory agreement, especially at high air velocities where prompt atomization is favoured and at ambient atmospheric pressure [106]. The nozzle in the experimental validation of the correlation had the atomizing air impinging the liquid stream at a 30° angle [106], a smaller angle would reduce the efficiency of the atomization and thus, should correspondingly reduce the value of C.

The correlation had good accuracy with water and heating oils and where the absolute values were not accurate, the trends were still good [106]. Measurements were taken 5cm downstream of the nozzle exit [170]. Tested property ranges included: Water mass flow rates: 10-25g/s (0.6-1.5LPM); Heating oil mass flow rates: 10-20g/s; ALR: 0.4-1.4; Atomizing air velocity: 25-60m/s; Sheet thickness 102-305 microns; Ambient air pressure: 1-5atm [106].

The original paper was for pre-filming air-blast nozzles, but the author similarly developed an equivalent correlation for plain-jet air-blast nozzles, though no direct experimental data was given to corroborate the equation [106].
This correlation was designed for a pre-filming air-blast atomizer. The atomizer ejected liquid in a thin, conical sheet which was exposed to air-streams on both sides for disintegration. Results indicated that for low viscosity fluids, air velocity and density were the critical parameters (term one was dominant) with SMD being inversely proportional to both. The second term became dominant for higher viscosity liquids, meaning that in these circumstances, the liquid atomization was less sensitive to the air properties. Higher viscosities and lower ALRs degraded atomization. Additionally, the correlation had an accuracy of 5% compared to experimental results, except for high density liquids [126]. Please note that the constants in the correlation were left unsolved in the original paper by Rizkalla et al. [126], but were later solved by an intermediate party and published in the textbook by Ashgriz [108]. However, the textbook did not provide the derivation or experiments used to solve for the values of the constants. Furthermore, in the textbook's correlation, liquid density was used in the second term while the original paper used air density instead. The variables from the original equation were a better match to the experimental spray results from this research and therefore, it is assumed that the textbook made a simple mistake. Within this thesis, the original paper's variables were used with the textbook's constants. As previously described in Section 3.3.9, C was used as an atomization constant and varied for each nozzle, rather than as a characteristic dimension (pre-filming lip diameter), to make it similar to the prompt correlation for a better comparison.

Within the original paper, the correlation was considered to be accurate within the following range of properties: Liquid viscosity: 0.001-0.044Ns/m²; Liquid surface tension: 0.026-0.074N/m; Liquid density: 780-1500kg/m³; Air velocity: 70-125m/s; Air temperature: 296-424K; Air pressure: $10^5$-8.5*10^5N/m²; ALR: 2-6 [126].
Appendix E. PLB Flame Videos

1) SSoptB4-66 base-point (Figure 63)
2) SSoptB4-66 minimum atomizing air point (Figure 65)
3) SSoptB4-66 maximum atomizing air point (Figure 65)
4) Cold-start (after one minute and after one hour) (Figure 66)
5) SSoptB4-66, no pilot flame (Figure 68)
6) SSoptB4-66, 0.3kW pilot flame (Figure 68)
7) S3B4-66 base-point (Figure 58/Figure 63)
8) S3B6-70 (batch 2) base-point (Figure 58/Figure 61)
9) S3B8-70 base-point (Figure 58)
10) S3B6-90 base-point (Figure 55)
11) S3B6-60 base-point (Figure 55)
12) S3B6-70 (batch 1) base-point (Figure 50/Figure 55/Figure 61)
13) S3B6-70 (batch 1) minimum atomizing air point (Figure 46)
14) S3B6-70 (batch 1) maximum atomizing air point (Figure 46)
15) S3B6 base-point (Figure 48/Figure 50)
16) S2B6 base-point (Figure 48)
17) S4B6 base-point (Figure 48)
18) S0B6 base-point (Figure 48)
Appendix F. PLB Burner Instruction, Maintenance and Safety Manual

Test Preparation

1. Select and dry filters in the oven (the day before) for 2 hours at 750°C
2. Remove PLB (bio-oil) from the refrigerator and place it in the fume hood (the night before)
3. Using a Scientech SM-128D Microbalance, measure the mass of the three PM filters you will use (do this just prior to a combustion test)

FTIR and Heating Devices Preparation *(1-2 hours before running on fuel)*

4. Turn on the both computers and the FTIR power supply
5. Make sure the exhaust sample line is closed to the FID (the right-hand valve on the back of the FID should point to the right)
6. Turn on FID and wait
7. Open the vacuum pump line on the FTIR manifold (up position) and then turn on the vacuum pump and the UHV pump for the FTIR and draw vacuum to roughly -100kPa
8. Turn on the FTIR Cell Heating Jacket
9. Turn on the heating tapes and move the knobs to the levels indicated on each of them, note one is controlled by a Veriac (setting about 40%)
10. Put acetone and compressed air through the nozzle assembly fuel line to remove any PLB remnants
11. Attach nozzle caps and spray acetone on the underside of the bushing to remove any PLB residue
12. Cut ceramic (3.75x1.75") if needed and cover nozzle circumference, but not the bottom of the air cap so that the fuel can be heated; try to thin out and even out the ceramic before securing in place with metal wire
13. Confirm that the sleeve around the nozzle is sitting approximately concentric
14. Check that the pilot tip, yor-lok and fitting inside combustor are all tight so there are no leaks
   a. Scrape tip clean, wipe with acetone and blow compressed air through both sides
   b. Clean igniter with emery paper and align with the pilot tip
15. Remove insulation covering exhaust vent, check exhaust thermocouple placement and remove any ash on the thermocouple with compressed air
16. Check inside combustor to ensure nothing left in there or fell in
17. Seal door with rubber gasket (with the longer side near the handles to cover the corner), holding in place while door is closed, careful not to rock combustor
18. Once the combustor door is closed and the stack fan is ready to be turned on, turn on the temperature controllers for the filter and the transfer line: 408°F (209°C) and 378°F (192°C) respectively; turn on the Veriac controller for sampling line heating tapes and the power bar.

19. Turn on the air intake flow meter power supply before the stack fan is activated.

20. Turn on the stack fan in the other room and set the primary air to the desired flowrate (≈ 300SLPM); first rotate the fan to ensure it is not stuck (recommended using a hex key) and put the Veriac to about 85% slowly from 100% (here at start-up to prevent a blown fuse); open the bypass valve to get the right flow (if the fan does not rotate when activated, shut off immediately to avoid damage or electrical problems).

FID Preparation *(1-2 hours before taking samples)*

21. Turn the FID on and wait for 45-60 minutes
22. Press “F3” (Diagnostic) on the FID to see the temperatures
23. Once the “burner temperature” is above 165°C:
   a. Open the H₂/He and the Compressed Air cylinders outside the room (make sure the cylinder output pressures are at 20-25PSIG)
      i. 2000psi is a full cylinder, replace around 500psi
   b. Press “Main” → “F8” to ignite the flame in the FID (the burner temperature reaches ≥ 220°C)
      i. If ignition successful, temperature increases rapidly
      ii. If unsuccessful purge the analyzer (Main → F2) and check gas lines

Pre-Combustion (Air Intake, Exhaust and Pilot Flame) Preparation

24. Turn on the O₂ pump and maintain the exhaust flow rate at around R=9.8 (i.e. 1.8SLPM); if the steel ball gets stuck open the rotameter all the way and then set the flow rate.
25. Turn on the air heater on the right countertop and set it to 100% load (do not run if the stack fan is not on)
26. Open the Methane and O$_2$ cylinders outside the room for the pilot and the nitrogen cylinder for the FTIR (make sure the nitrogen valve is closed on the manifold); fully open the cylinder and flow needle valves, but do not touch the regulator valves
   a. Record starting pressures
27. Reattach the pilot flame tube, careful not to tighten heavily with the wrench or hit the igniter
28. Open the atomizing air valve and set the rotamer to the desired flowrate ($\approx R = 45-50$)
29. Move the pilot tip close to the electric igniter inside the combustor and ignite the flame; during ignition angle handle downwards to raise tip up close to igniter since tube not fully straight:
   a. Check pilot tip in a good position for a strong and consistent spark and mark the spot on the tube
   b. Open the Methane rotamer valve slightly and ignite methane with the electric igniter
   c. Open the O$_2$ rotamer valve to obtain a blue flame
30. Move the pilot flame to the desired position (likely at the edge of the sleeve) while the handle is lifted and tighten the yor-lok fitting to secure in place
   a. When changing the pilot flame energy: if increasing change methane first, if decreasing change the oxygen first; change both gases in small increments towards the desired flow rates
31. Increase methane and O$_2$ on the rotamer valves to obtain the desired pilot energy (0.3kW, based on steel balls)
   a. If at any time the pilot flame turns off stop the fuel pumps and stop the flow through both methane and oxygen rotameters immediately and then restart the pilot flame from step 26
32. Open the faucet to start the cooling water for the main heat exchanger and set it to 1.8GPM; keep the condenser line closed for now
33. Allow 10-15 minutes for air to flow through and heat up
34. Tape and seal combustor door
35. Check on FID and confirm oxygen pump rotameter flow

**Experiment Recording (LabVIEW)**

36. Wake up the computer on the right countertop and open the LabVIEW software, file is "burner monitoring (Sina).vi"
37. Click Run to start the measurements
Ethanol Warm up

38. Turn on hood fan by plugging it in
39. Put roughly 500mL of ethanol from the container pour into the beaker and start the scale software
40. Set the pump to $\approx 23g/min$ ($\approx 600$RPM depending on the nozzle) and prime the pump (do not run dry for longer than a few seconds); if fuel will not flow check fittings for air leaks and turn off atomizing air flow, then try again
41. Allow ethanol to warm up the combustor for 30-40 minutes
42. Start stop watch
43. The primary airflow should be around $285$SLPM as read on the flow meter
44. Pour bio-oil into container, place it on the scale and turn on the electric mixer if so desired
45. Calibrate FID and can run an FID measurement on ethanol to confirm calibration (the reading should be zero)
46. Confirm primary airflow and pilot energy and adjust if necessary, turn off nozzle cooling just before PLB switch

FTIR Preparation and Sampling
47. After at least 15 minutes (ideally 1 hour), align the spectrometer
   a. Go into the bench tab of experimental setup and set the velocity to 0.47 and the gain to 8.0
   b. Go into the diagnostic tab and click the align button

48. While the burner is warming up, purge the FTIR gas cell to get it ready for the measurements:
   a. Close the needle valve on the manifold
   b. Close the vacuum pump valve on the manifold and open the nitrogen valve
   c. Slowly open the needle valve and fill the gas cell to -15kPa with nitrogen (quickly)
   d. Close the nitrogen valve and open the gas cell to the vacuum pumps on the manifold
   e. Pull vacuum from the gas cell to roughly -100kPa
   f. Repeat steps (a)-(e) for a total of 5 times or more if the device has been sitting for a long period of time

49. Collecting a Background (do this close to the time of taking the sample):
   a. Open the OMNIC software
   b. Go to the Experimental Setup and select “collect background before every sample”; can select save interferogram if any post-processing is desired
   c. Click on “Collect Background” when pressure has stabilized (24 scans at a resolution of 1)
      i. If any anomalies in background such as a vertical line between 2000 and 2500 (on the x-axis), the background is poor and the FTIR should be purged and re-run
   d. After collecting the background, add the window and then name and save the file in a secure location
   e. Go back to the Experimental Setup and select “Use specified background file” and choose the path of the saved background
   f. Now the FTIR is ready to take samples

50. When the combustor has reached a steady state temperature, take FTIR samples:
   a. Ensure manifold needle valve almost closed
   b. Open the exhaust sample line to the gas cell and stabilize for 5 minutes while maintaining a pressure of roughly -15kPa in the gas cell by using the needle valve on the manifold
   c. Make sure the exhaust sample temperature is above 120°C
   d. Click “Collect Sample” and wait for the sample to be taken
e. After the sample is complete, add to window and save the data
f. Close the exhaust sample line to the gas cell and purge the gas cell (step 48)
g. Take a new background for the next sample (step 49)
h. Repeat steps (a)-(f) for the next samples with roughly 3 minute intervals to average samples, depending on experiment

51. Analyze the results:
   a. If result expected to be below 30ppm:
      a. Open the TQ Analyst software and open the desired calibration file (December 2009 Corrected CO PLS4.qnt for NO and use TQ method just CO for CO measurements)
      b. Press “Quantify” and select your sample file
      c. Close program without saving or can hurt calibration
   b. If result above 30ppm:
      a. Open both spectras and Ctrl-click to select both, then click subtract
         i. Find the proper subtraction factor and apply it to excel calibration; will need to zoom in near the appropriate wave-number range, but the subtraction result will automatically scale so some large constant peaks should be within the wave-number range to avoid scaling the window down to within the signal noise
         ii. In original window, match the y-axis of both spectra, zoom in and visually assess an approximate factor as a double check

FID Sampling and Calibration

52. Calibrate the FID after the warm-up stage when $T_{\text{burner}} \approx 315$-$330^\circ C$ (viewed by pressing F3 from main menu)
   a. Turn the left-hand valve (on the back of the FID) to point left
   b. Turn the right-hand valve to point right (close the gas sampling to the FID)
c. Press “Main” → “F4” → “F2” → “F1”
d. Open the brass valve to around 1-2 psi (>0)³

e. Once the value is stable, press “F1” and close the brass valve (if the value is unstable, stop the calibration and retry it when about to do the measurements)
f. Press “Back” → “F2” quickly
g. Open the CH₄-90ppm cylinder (on the floor) to around 1-2 psi
h. Once the value is stable, press “F1” and close both valves on the cylinder (not the regulator) then press back quickly after to protect the pump
i. Turn the left-hand valve to point right
j. Make sure that the measurement range is set to 0-300ppm; the uncertainty is ±3ppm
k. May need to repeat calibration to check values or if problems arise

53. For sampling, turn the right-hand valve to point to the left so that the exhaust is running through the FID
54. Measure the THC level: press “Main” and then “F1”; the FID burner temperature rises to about 370–380°C
   a. Check the exhaust temperature in the sampling line
   b. If you want to check the results you can unscrew the sampling line at the FID/FTIR inlet junction and allow it to pull in room air (exhaust will be pulled through the oxygen pump) and the HC readings should be <3ppm
   c. Once finished reattach sampling line though if a lot of HC were present it is good to allow room air to flow through the FID for a few minutes to ensure that it is clean
   d. While the sampling line is detached, the oxygen sensor will not be accurate
55. Turn the right hand valve to the right (towards the FTIR) when finished sampling
56. If finished, the FID can be put into standby (F7 from the main menu) or can be left and turned off after the experiment

**PLB Fuel Switch**

57. When ethanol warm-up is complete (>500°C exhaust), switch the fuel line to PLB and change to the calibrated RPM slowly in order to get the desired fuel flow rate when the PLB reaches the pump (not before):

³ Any pressure exceeding 2.0 psi can damage the FID pump
a. Lower the atomizing air flow to about 40 (depends on fuel batch and nozzle) when the PLB hits the nozzle
b. Using a digital scale and a stop watch (or the computer program), measure the fuel mass pumped at a certain RPM on the pumps to determine the fuel mass flow rate and accordingly the input energy of the burner
c. Set the RPM of the pumps to get 10kW energy input
d. If ceramic insulation is used around nozzle, turn off nozzle cooling unless required

58. Allow at least 30 minutes for warming up and reaching a steady state condition
59. Confirm the primary airflow rate is good

PM Sampling

60. Place 2 dummy filters in the main and the bypass lines and make sure you have enough filters ready to replace those during the experiment
61. Turn on the water for the PM Sampling Condenser and set it to approximately 0.25GPM
62. Open the main line (2 valves) and turn on the PM sampling pump on the floor

63. Run the first dummy filter in the main line for 5 minutes or until a significant pressure drop is observed across the filter:
   a. Open the main line while the bypass line is closed and let the exhaust flow through the PM line
   b. Maintain a null (zero) pressure difference on the manometer using the brass knob on the PM rotameter to find the isokinetic condition, which corresponds to 10.4% of the total exhaust flow rate (around 0.3-0.35 on the rotameter); it is better to have a PM sampling pressure a little below zero than above
   c. Warm up the PM sampling line and wait for the “Wet Gas” temperature to exceed 115°C; a higher rotameter flow rate gives a faster temperature increase, but the filter will also overload faster

64. Close the main line first and open the bypass line; at the same time (one hand on the main line red valve and the other on the yellow bypass line valve) then close the yellow valve on the main line which is redundant; run flow through the bypass line while placing a new dummy filter in the main line
65. When starting the main line, open the redundant valve first then open the main line valve and close the bypass line valve simultaneously
66. Repeat steps 63-64 one more time with new dummy filters in the main and bypass lines if needed, and find the isokinetic condition; when changing filters, do so fast since temperatures decrease and the flow patterns change when the lines are open as the pump will pull in the room air
67. Start collecting PM samples using the official filters:
   a. Place PM1 filter in the main line while exhaust is running through the bypass line
   b. Rapidly switch back to the main line and start the timer; prime by opening the yellow valve on the main line and then at the same time turn the remaining valve on the mainline and the bypass valve
   c. Adjust the PM flow rate and null pressure, and make sure the temperature is above 115°C
   d. Collect PM for 3-5 minutes. During this time, place a new dummy filter in the bypass line if necessary only since it affects sampling temperature
   e. When PM1 collection is complete, rapidly switch to the bypass line and place the PM1 filter in its Petri-dish
   f. Repeat steps (a)-(e) 2 more times for PM2 and PM3 filters
68. Turn off the PM sampling pump so the lines do not get clogged, close valves
69. Turn off the cooling water for the PM condenser
70. Weigh the loaded filters after storing them (covered) at ambient conditions for about 24 hours

**Flame Temperature Profile Measurements**

71. Insert the K-type thermocouple into the port box and position at the centre of the flame:
   a. Hold the thermocouple in place and record the temperature once it is steady after 3-5 minutes
   b. Seal the entrance to the port box with tape to prevent cold air from leaking into the combustor

**Borescope IR, Pictures & Videos (not currently functional)**

72. Connect the borescope to the IR adapter and the laptop
73. Open the borescope port on the port box, place it in its port, hook the cooling air to scope, and begin taking spectra (must do this rapidly because the cooling air can change conditions in chamber)
74. After taking IR, remove the IR adapter, connect the camera adapter, and take pictures and videos

**Shutdown Procedures**

75. Switch to ethanol for flushing the lines (increase pump RPM when the ethanol reaches it):
   a. Turn off the air heater; ensure it is not running when there is no primary air flow (the stack fan is off)
   b. Turn on nozzle cooling
   c. Purge the gas cell with nitrogen and maintain vacuum afterwards for a couple minutes before turning off
   d. Run ethanol for about 20 minutes
76. After flushing with ethanol:
   a. Turn off the pump
   b. Turn off the pilot flame; methane flow first
      i. If the pilot tip is red hot then push into the primary air flow to cool it down
   c. Turn off all the heating tapes on FID and FTIR (4)
   d. Empty water from the sampling line vacuum pumps; pumps should be on during water dump
   e. Turn off the FTIR vacuum pumps, the gas cell heater and the FTIR power supply
   f. Leave vacuum pump valve on FTIR manifold open until FTIR cylinder cools then close
   g. Increase the atomizing air flow rate to maximum
h. Increase the primary air flow by closing the stack fan bypass so all flow goes through burner and put the Veriac to around 110%

i. Turn off the FID:
   i. If exhaust was clean, no action is necessary; if it was dirty detach the sample line at the FID/FTIR junction and let room air flow through the FID or can pull air through the now extinguished combustor (if combustor dirty do the former) and can initiate the pump by conducting a measurement
   ii. Turn off all supply gas cylinders (starting with H₂/He and then compressed air); at this point can turn off all five gas cylinders (oxygen, nitrogen and methane); close the cylinder and needle valves without changing the regulator valves
   iii. Ensure both valves point to the right when the pump is off (it should turn off with the hydrogen/helium cylinder)
   iv. Press “Main” → “F2” (Purging) when you can no longer hear the pump or fine if the device was previously in standby mode
   v. Wait for 20-30 minutes and turn off the FID (when temperature, F3 from main menu, about 170-175°C or less)

j. Turn off the O₂ pump, heaters (including one controlled by a Veriac), and the power bar

77. Close all the cylinders outside the room (5) if not already done
   a. Record final pressure values

78. Remove door clamps, pilot flame (ensuring the tip does not hit the igniter during removal)

79. Put the unused fuel in the fridge, set the fuel valve to open to drain PLB in the line and place paper towel below the inlet/outlet to catch drips; detach fuel lines from the pump to ensure no bio-oil remains within the gear housing – run pure ethanol through the pump if necessary

80. Turn off/unplug the scale and pump

81. Once swirl box is cooled the door handles can be unlatched and the seals removed to allow additional air flow, but do not open the door until temperature lowers to 120°C

82. Stop labVIEW (the file is in the "Sina" folder on the desktop, arranged chronologically), then restart the program to monitor the cool down

83. Turn down the water flow so heat exchanger water flow rate is about 1.2GPM

84. Once the exhaust flange is around 70°C, turn off the atomization air, the stack fan (Veriac), the cooling water, the three computers and the flow meter power supply; unplug the fuel hood fan

85. Empty the water traps into a bottle once the stack fan is turned off; also empty water from the oxygen pump (with it on) now that the surroundings have cooled

86. Clean the media bottles, glassware, and utensils

87. Clean the nozzle:
a. Remove both nozzle caps and retaining ring, clean with a paper towel (before and/or after removal) and place the parts in acetone until all deposits are dissolved for about 5 minutes; cover the beaker since acetone is very volatile
b. Once deposits are removed, rinse the pieces under water, spray with acetone and lay on a paper towel to dry; seal up the acetone for re-use if not too dirty

88. Spray acetone on the underside of the nozzle bushing, only replace nozzle caps just before next test in case of residual bio-oil which can cause sticking
89. Clean the combustor viewports from the inside using a towel; need to do this after each test or the windows get progressively harder to clean; can use a little water and then dry if needed
90. Put blank PM filters into both the main and bypass lines
91. Close vacuum pump valve on FTIR manifold and confirm the FID is off

APPENDIX I: Temperature Limits

- FID sample gas: $160 \leq T_{gas} < 196^\circ C$
- FTIR sample gas: $120 \leq T_{gas} < 185^\circ C$
- Want to be careful not to exceed these temperature ranges which should be measured while air is flowing through the devices, otherwise temperature will not be accurate and could accidentally overheat the system, causing damage

APPENDIX II: Maintenance

Heated Filter Element: Located near the oxygen pump (a black cylinder with a knob affixed on its top), the heated filter must be changed every few (about 5) PLB tests when it becomes brown and can flick off ash build-up. Simply turn the knob and change the filter.

Coalescing Filter: Also near the oxygen pump, the collector must be drained if filled with water and change the filter if needed every few tests (about 5) when it look dirty or becomes soft. Drain and get at the filter by unscrewing clear casing.

Purge Sampling Lines: Line goes from near the PM filters, just prior to the water trap condenser to the valve between the FID and FTIR devices. Purge using compressed air diverted from the atomizing air set-up with the inlet attached near the FID/FTIR. The entire sampling line or just a section of it can be purged. Screw air tubing onto sampling line when unexpected readings are seen from the FID or when fuel dribbles out or cokes heavily, but should do every 2-3 tests.

Water Trap: After every few tests the water trap (silver cylinder) near the oxygen pump needs to be drained into a bottle. The pump does not need to be on when draining the trap. Water also may build in the line between the trap and the pump, needing to be drained.

Pilot Flame Cleaning: If the pilot tube is dirty or malfunctioning, run compressed air through the tubing and tip.

If water traps overflow, take off the worm gear below the hose adapter and be prepared to catch the water that falls out with a container or vacuum

Exhaust Duct: After a dirty test, remove the flow straightener and clean the area below with a paper towel and vacuum cleaner to remove deposits and material build-ups; ensure exhaust thermocouple properly positioned

PM Sampling Lines: Put compressed air backwards through the PM sampling lines after every few tests to clean the system as water will build up quickly
Burner Shutdown Safety Checklist:

Double-check the following have been turned-off

- Primary air heater
- Pump (and unplug)
- Scale (and unplug)
- Pilot flame with rotameters closed
- Four FTIR/FID heating tapes (touch)
- FTIR vacuum pumps, gas cell heater and power supply after purge
- FTIR vacuum manifold closed once cooled
- Atomizing air flow
- FID (with both valves pointing right) after purge
- Five gas cylinders and needle valves (He/H2, CH4, N2, air, CH4)
- Veriac for primary air stack fan, leave at 100% to avoid blowing a fuse during power-up
- Unplug fuel hood fan
- O2 pump, 3 heaters (one controlled by a Veriac), turn off yellow power bar (controls more heaters)
- Cooling water
- All (3) computers and screens
- Flow meter power supply
- Put away unused fuel (in fridge if PLB)
- Empty water traps, FTIR/O2 vacuum pumps
- Remove/clean nozzle
- Acetone/ethanol capped
- FTIR purge gas generator MUST BE KEPT ON
- Confirm FID methane gas cylinder closed
- PM vacuum pump off
- Turn off fuel mixer
- Oven for PM filters off and unplug
- Scale for measuring PM filters off