CHARACTERIZATION OF SPRAY AND COMBUSTION OF DIESEL-ALCOHOL BLENDS IN A CONSTANT VOLUME CHAMBER

BY

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THESIS

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Abstract

In this study, the spray combustion characteristics of Acetone-Butanol-Ethanol (ABE)/Diesel blends was investigated. An optical-accessible constant volume chamber capable of controlling ambient temperature, pressure and oxygen concentration was used to mimic the environmental conditions inside a real diesel engine cylinder. ABE fuel with typical volumetric ratios of 30% acetone, 60% butanol and 10% ethanol were blended with ultra-low sulfur diesel at 80% volumetric ratio and were tested in this study. The ambient temperature was set to be at 1100K and 900K, which represents normal combustion conditions and low temperature combustion conditions respectively. The ambient oxygen concentrations were set to be at 21%, 16% and 11%, representing different EGR ratios. The in-cylinder pressure was recorded by using a pressure transducer and the time-resolved Mie-scattering image and natural flame luminosity was captured using a high-speed camera coupled with a copper vapor laser. The results show that the liquid penetration was reduced by the high percentage of ABE in the blends. At the same time, the soot formation was reduced significantly by increasing oxygen content in the ABE fuel. Even more interesting, a soot-free combustion was achieved by combining the low temperature combustion with the higher percentage ABE case. In terms of soot emission, high ABE ratio blends are a very promising alternative fuel to be directly used in diesel engines especially under low-temperature combustion conditions.

In addition, in this work, a modified chamber system has been described, which features a new injection pump system with a new piezoelectric injector, an upgraded LabVIEW
control program and a new chamber head component. The new system has been tested and validated for the performance and consistency. Preliminary tests have shown that the repeatability of the upgraded constant volume chamber system is satisfactory.
Acknowledgments

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# Table of Contents

List of Tables ........................................................................................................................................ viii

List of Figures .......................................................................................................................................... ix

Chapter 1  Introduction .......................................................................................................................... 1

Chapter 2  Literature Review ................................................................................................................. 3

2.1  Review of Alternative Diesel Fuel and Blends .............................................................................. 3

2.1.1  Biodiesel ....................................................................................................................................... 3

2.1.2  Alcohol .......................................................................................................................................... 5

2.1.3  Acetone-Butanol-Ethanol Mixture .............................................................................................. 8

2.2  Review of Spray Characterizations in Constant Volume Chambers ..................................... 10

2.2.1  Design Considerations of Constant Volume Chambers ......................................................... 10

2.2.2  Optical Diagnostics for Spray and Combustion ...................................................................... 12

2.3  Tables .............................................................................................................................................. 17

2.4  Figures .............................................................................................................................................. 18

Chapter 3  Experimental System Setup ............................................................................................. 23
Chapter 3

3.1 Caterpillar Constant Volume Chamber Setup and Modification ........................................ 23

3.2 Data Acquisition and Control System ................................................................................. 26

3.3 Design of an Ultra-High Pressure Constant Volume Chamber ........................................... 27

3.4 Injector Delay Measurement ............................................................................................... 31

3.5 Injector Driving Current Profiling ....................................................................................... 32

3.6 Tables .................................................................................................................................. 34

3.7 Figures ................................................................................................................................. 35

Chapter 4

Data Processing and Calibration Experiments ............................................................................. 46

4.1 Combustion Pressure and Heat Release ............................................................................... 46

4.2 Liquid Penetration Length .................................................................................................. 47

4.3 In-cylinder Pressure-Temperature Relations ...................................................................... 48

4.4 Figures ................................................................................................................................. 49

Chapter 5

Experimental Study ....................................................................................................................... 51

5.1 Experimental Conditions and Fuel Properties ................................................................. 51

5.2 Experiment Results with HEUI Injector ............................................................................. 52

5.2.1 Liquid Spray Penetration Length .................................................................................. 52
5.2.2 Combustion Heat Release

5.2.3 Natural Luminosity and Flame Structure

5.3 Experiment Results with Siemens Piezoelectric Injector

5.3.1 Validation of Data Consistency

5.3.2 Combustion Heat Release Analysis

5.3.3 Comparison of Injection Triggering Strategies

5.4 Summary

5.5 Tables

5.6 Figures

Chapter 6 Conclusions

6.1 Recommended Future Studies

References
List of Tables

Table 2.1 Properties of biodiesel prepared from vegetable oils and used cooking oil ..... 17

Table 2.2 Properties of acetone, butanol and ethanol ................................................ 17

Table 3.1 Comparison of sapphire and quartz materials for optical windows.................. 34

Table 5.1 Experiment parameters and conditions......................................................... 66

Table 5.2 Statistics of injection pressure in all tests ......................................................... 67

Table 5.3 Statistics of ambient pressure ........................................................................ 67

Table 5.4 Comparison of experiment condition repeatability with different injection triggering strategies: a) without automatic adjustment; b) with automatic adjustment .................................................................................................................. 68
List of Figures

Figure 2.1 Schematic of pre-burn type constant volume chamber in NCSU [46]........... 18

Figure 2.2 Typical pressure trace during pre-burn type constant volume chamber operation ........................................................................................................................................... 19

Figure 2.3 Cross-section view of the quiescent chamber in Tsinghua University [47] ........................................................................................................................................... 20

Figure 2.4 Cross-section view of the constant flow type chamber in Universitat Politècnica de València [49] ........................................................................................................................................... 21

Figure 2.5 The flow field of a swirl injector measured by PDA [54].............................. 22

Figure 3.1 Schematic of the Caterpillar constant volume chamber......................... 35

Figure 3.2 Modified chamber head with Siemens piezoelectric common rail injector installed........................................................................................................................................... 36

Figure 3.3 Schematic of the manually operated high-pressure generator system........ 37

Figure 3.4 Cross-sectional view of the UHPCVC ...................................................... 38

Figure 3.5 Hierarchy Diagram of the LabVIEW control program .......................... 39

Figure 3.6 Schematic of the constant volume chamber control system............... 40
Figure 3.7 The final pressure of premixed combustion for various combinations of nitrogen dilution ratio and initial pressure (for stoichiometric oxygen) ......................... 41

Figure 3.8 The final temperature of premixed combustion for various combinations of nitrogen dilution ratio and initial pressure (for stoichiometric oxygen) .................. 42

Figure 3.9 Feasible range of initial operating condition demonstrated ...................... 43

Figure 3.10 A schematic of injector delay measurement and the photodiode driving circuit ................................................................. 44

Figure 3.11 Typical injector driving current profile ........................................... 45

Figure 3.12 Measured injector driving current profile of the Bosch solenoid injector..... 45

Figure 4.1 Illustration of combustion phasing definition based on cumulative heat release .................................................................................................. 49

Figure 4.2 Illustration of the liquid length extraction algorithm ............................... 50

Figure 5.1 Spray images of ABE80 and D100 at 900K ............................................. 69

Figure 5.2 Typical liquid penetration length history ............................................. 69

Figure 5.3 Liquid penetration length history of ABE80 and pure diesel .................... 70

Figure 5.4 Pressure trace and normalized heat release rate of ABE80 and pure diesel spray combustion ................................................................. 71
Figure 5.5 Ignition delay of ABE80 and pure diesel combustion.............................. 72

Figure 5.6 Combustion duration of ABE80 and pure diesel combustion.................. 72

Figure 5.7 Natural flame luminosity of ABE80 combustion under 1100K and 900K ...... 73

Figure 5.8 Spatial integrated natural luminosity of ABE80 under various conditions..... 74

Figure 5.9 Spatial integrated natural luminosity of pure diesel, ABE20 and ABE80 under 1100K, 21% oxygen concentration................................................................. 74

Figure 5.10 Average and standard deviation of pressure traces at various ambient conditions.................................................................................................................. 75

Figure 5.11 Spray combustion pressure trace at 1200K and 1000K............................. 76

Figure 5.12 Apparent heat release rate of spray combustion at 1200K and 1000K ...... 76

Figure 5.13 Close-up view of pressure trace and the standard deviation at two different injection triggering mode .................................................................................. 77
Chapter 1 Introduction

With the growing concern for environment issues and limited soil fuel productions, most countries throughout the world are adopting more and more stringent regulations on vehicle emission control. Researchers and engineers have to seek solutions that can reduce emissions and improve combustion efficiency at the same time.

Alcohol, such as methanol, ethanol and butanol, are considered as promising alternative transportation fuels. Quite a lot of works have been done in the research of ethanol/ethanol-blend fueled engines. In general, ethanol demonstrates great potential for the reduction of HC, CO, NOx and soot emissions of internal combustion engines [1]. The U.S. Department of Energy estimated that by the Year 2011, there are 862,837 vehicles fueled with E85 in use, which consisted 72% of the alternative fuel vehicles [2], marking the massive commercial use of bio-ethanol fuel and blends. There has been quite a lot research on the ethanol-diesel blends at various ratios and operating conditions. Hansen et al. reviewed the recent studies on ethanol-diesel fuel blends as an alternative fuel [3].

Compared to ethanol, recent studies consider butanol as a more advantageous alternative fuel source. For its longer carbon chain, higher heating value, and cetane number, which makes butanol more like fossil fuels than ordinary ethanol fuels. N-butanol is suitable for diesel LTC combustion and has great potential in decreasing soot and NOx emissions. Previous production of butanol has mainly relied on the pyrolysis process of fossil fuels such as coal, crude oil and natural gas. In 2004, Ezeji et al. showed that acetone-butanol-
ethanol (ABE) mixture (usually 60%: 30%: 10% in volume) can be produced via integrated fermentation process of biomass using Clostridium beijerinckii BA101 bacterium [4], which will greatly reduce cost and improve conversion efficiency. However, the separation process was still costly, which obstructed the industrial application of butanol as biofuels. If the application of “intermediate” product for butanol could be considered, production cost would be lowered.

The objective of this work is to explore the possibility of using high-percentage (up to 80%) ABE blends in diesel as an alternative transportation fuel. The motivation of this work is to explore the possibility of high-percentage ABE-diesel blends as a low-cost and low-emission fuel. A pre-burn type constant volume chamber is ideal for the research, because it can almost mimic real engine operation conditions. The optical accessibility provides possibility for the high speed imaging of spray and combustion processes, which is essential for the investigation of spray development, ignition characteristics, flame propagation, soot emission, etc.
Chapter 2 Literature Review

2.1 Review of Alternative Diesel Fuel and Blends

2.1.1 Biodiesel

Biodiesel is the collective name for methyl or ethyl esters prepared from vegetable oils or animal fat, which are suitable for fueling diesel engines. Biodiesel contains no petroleum products, so it is a renewable resource of energy. Typical sources for biodiesel include: soybean, peanut, palm, sunflower, linseed, used cooking oil and animal fat. Although the chemical and physical properties of biodiesel products are quite similar to conventional diesel (shown in Table 2.1), they are usually blended with diesel in order to minimize the need of engine tuning and calibration.

Biodiesel has 10% less heating value on weight basis compared to diesel. However, due to a higher specific gravity, the per-volume-based heating value of biodiesel is slightly lower but rather close to that of diesel. As a result, it can be expected that the brake fuel specific consumption of biodiesel-fueled engines will be higher. Zhang et al. [5] observed similar combustion behavior with various biodiesel fuels. The ignition delay for ester/diesel fuel blend was found to be shorter than neat diesel. Senatore et al. [6] observed an advanced combustion phasing with rapeseed oil methyl ester. As a result, a higher in-cylinder pressure and gas temperature was observed when using biodiesel. In terms of emissions, a general conclusion from previous studies with biodiesel fueled engines show reduced particulate matter (PM), hydrocarbon (HC) and carbon monoxide
(CO) emissions, but the NO\textsubscript{x} emissions will be increased with increasing biodiesel blending ratio. In a study by FEV Engine Technology [7], the NO\textsubscript{x} emissions were proportional to the blending ratio of biodiesel. For pure biodiesel case, an 8% increase of NO\textsubscript{x} emission was observed compared to the baseline diesel case. Schumacher et al. [8] performed experiments with 10%-40% soybean-oil biodiesel blends and observed a 15% increase in NO\textsubscript{x} emission for the highest blending ratio. Marshall et al. [9] tested the engine performance and emission under transient conditions and found out that the biodiesel fueled engine may increase NO\textsubscript{x} emission by up to 16% in transient condition. Some other studies also show increasing NO\textsubscript{x} emissions with the use of various biodiesels. The reason for the increased NO\textsubscript{x} emissions with biodiesel has also been discussed extensively in the previous studies. On the hardware side, some studies show that the injection and combustion timing of biodiesel is getting advanced due to the faster pump and injector response caused by the differences in viscosity and compressibility [10-13]. On the other side, there are some other experiments that keeps the start-of-injection precisely to be the same but also observe increasing NO\textsubscript{x} emission. Schmidt et al. [14] argued that the increasing NO\textsubscript{x} emission was mainly due to the higher availability of oxygen in the mixture. Monyem et al. [11] argued that the increasing cetane number of biodiesel will result in a more advanced combustion by shortening the ignition delay and thus increasing the temperature and favors NO\textsubscript{x} formation. The reason for the reduced CO, HC and soot emission is more well-established, it is commonly accepted that the fuel-born oxygen content of biodiesel accelerates the oxidation reaction of these incomplete combustion products [15, 16]. Some other experiments also measure and
investigate the changes in particle size distributions of biodiesel-fueled engines. A majority of studies have shown that the number of small particles can be observed when using biodiesel. Krahl et al. [17, 18] tested the engine with pure rapeseed biodiesel and two commercial diesels. It is observed that the population of small particles (10~40nm) was significantly increased compared to low sulfur diesel. Further investigations with other biodiesel fuels [19] also show similar conclusions. Tsolakis et al. [20] reported a decreasing mean particles diameter and increasing particle number with rapeseed biodiesel, which is consistent with the previous studies. They also attribute this change in particle size distribution to the changing injection pressure due to the difference in fuel property, higher injection pressure can lead to a finer liquid droplet and thus smaller soot particles. In addition, some researchers also pointed out that the use of biodiesel can have a positive effect in re-optimizing the NOx-PM trade-off [21].

As a brief conclusion, biodiesel have the ability of advancing combustion timing, and lowering PM, CO and HC emission. The NOx emission of engine fueled with biodiesel is usually higher.

2.1.2 Alcohol

Alcohol as a fuel additive might be the first alternative fuel that is commercially available on market. Most of the countries in the world sell ethanol-containing gasoline and diesel at gas stations. Apart from ethanol, methanol and butanol are also being investigated in depth as a potential fuel additive in diesel engines.
Methanol is the simplest saturated alcohol; it has relatively high toxicity and corrosion compared to transportation fuels. Methanol can be derived from bio-renewable resources such as corn starch, wood. Looking at the properties of methanol, it has lower viscosity, nil or no sulfur, so it can be expected that the addition of methanol in diesel can help to enhance atomization and reduce sulfuric gas emission. However, the heating value of methanol is only around half of diesel, which will increase the fuel consumption to maintain the same load. Another problem in using diesel with methanol is the miscibility. Previous studies [22] have shown that the methanol-diesel mixture will start to become unstable at volumetric ratio greater than 5%, when a higher blending ratio is desired, oleic acid (as a solvent additive) is added to maintain the stability of mixture. Some other studies [23, 24] used a MPI system to inject methanol into intake manifold to deliver methanol as a premixed charge with air, but the additional fuel injection system will increase the cost and requires modifications to the engine. Chu et al. [25] studied using methanol-diesel as a “drop-in” fuel without changing the original injection timing configurations, a decreasing power output was observed but the efficiency was improved. The NO\textsubscript{x}, PM and CO emission was significantly reduced with the methanol-diesel mixture, but the HC emission was slightly increased. Kulakoglu et al. [26] found that with the increasing methanol blending ratio, the NO\textsubscript{x} and fuel consumption were increasing proportionally, but the CO, HC emissions were reduced. Some more systematic studies showed that the performance and emission of methanol-containing fuel is dependent on fueling strategy and requires modification of injection timing to get the best operation condition [27, 28].
Ethanol (C$_2$H$_5$OH) is another common source of alcohol fuel additive. Compared to methanol, it has higher heating value but still the miscibility and corrosion remains an issue. The impact of ethanol to diesel engine emissions has been investigated by several previous studies [29, 30, 31, 32]. He et al. [31] discovered that, the soot emission was being significantly reduced with the increasing blending ratio, however, HC and NO$_x$ emissions were increasing. Li et al. [32] found the similar conclusion but also observed an increasing trend of HC emissions with increasing ethanol blending ratio.

Butanol (C$_4$H$_9$OH) is a four-carbon alcohol. It has four isomers: n-butanol, iso-butanol, sec-butanol and tert-butanol, among which, n-butanol is the most common used. In the recent years, butanol has been recognized as a better candidate for alcohol fuel additive, due to its similarity with transportation fuels such as higher heating value, cetane number and less corrosive. Butanol is fully miscible with diesel, which eliminates the need of solvent additive. Also, the solubility of water in butanol is far less than that of methanol and ethanol, so the amount of moisture getting absorbed in fuel mixture is greatly reduced. Zoldy et al. [33] found that when n-butanol is blended with diesel at a volumetric ratio of 5%, the cetane number, viscosity, flash point requirements can be met and the mixture can be directly used as transportation fuel without further calibration. Yao et al. [34] studied the pollutant emissions of a diesel fueled with 5~15% butanol with diesel. It was discovered that the combustion phasing and pressure rise did not change much at lower blending ratios up to 15%, while the soot emission had been significantly reduced, the HC and CO emission maintained at the similar level compared to neat diesel
combustion. Another study by Liu et al. [35] in constant volume chambers also showed that the butanol as a diesel additive has an effect of reducing soot emissions.

### 2.1.3 Acetone-Butanol-Ethanol Mixture

The mixture of acetone-butanol-ethanol (ABE), initially an intermediate product for bio-butanol production, recently received focus from diesel engine combustion researchers. ABE mixtures produced via integrated fermentation process of biomass typically has a volumetric ratio of 3:6:1 for acetone, butanol and ethanol respectively [4]. By eliminating the further distillation process to get pure bio-butanol, the production cost can be significantly reduced and the production rate of bio-fuel can be increased.

Table 2.2 summarizes the properties of components in ABE mixture as well as the calculated property of ABE mixture at volumetric ratio of 3:6:1, which is the most typical composition from fermentation process. It should be noted that the properties of ABE mixture itself does not qualify as an “appropriate” alternative biodiesel according to ASTM D6751 standard. As a result, most of the researchers use low-percentage blend of ABE-diesel mixture to investigate the influence of ABE additive to diesel engine performance.

Although the major species of ABE mixture is basically alcohol (ethanol, 10% and butanol, 60%), which have been studied in great depth. The influence of acetone together with these alcohols is significantly different from previous studied with pure alcohol additions into diesel fuels. The concentration of acetone plays an important role in the
determination of ignition delays as well as initial stage heat release rates. Wu et al. [36, 37] investigated the impact of acetone contents to spray combustion characteristics of ABE/diesel mixtures in a constant volume chamber, it was found that the addition of acetone concentration had a significant effect on advancing combustion phasing, i.e. shortened ignition delay time. Meanwhile, an accelerated initial stage combustion rate was observed with higher acetone concentration. This was further confirmed in engine experiments by Lee et al. [38], it was found that the premixed combustion rate of ABE mixtures is decreasing with the increase of acetone concentration. As the most redundant species in ABE mixture, the concentration of butanol and its impact on combustion characteristics were also studied by several researchers. Wu et al. [39] pointed out that in ABE mixtures, certain amount of butanol in ABE mixture are desired for the following purposes: (1) Increase energy density of the mixture; (2) Adjust the overall volatility of mixture to an appropriate level; (3) Counteract the retardation effect of acetone and ethanol to an appropriate level. It was also observed that increasing butanol content may lead to an increasing emission in soot. The effects of ethanol, as a minor species in ABE mixture, have not been studied thoroughly in literature. As a conclusion, the three components in ABE mixture shows different features when determining the mixture property: acetone has a predominant role in advancing combustion phasing; butanol mediates the overall heating value of mixture and counteracts the retardation effect caused by acetone.

The influence of ABE blending ratio with diesel was also investigated by several studies. In the following discussion, ABEx denotes ABE blended with diesel at volumetric ratio
of x%, for example, ABE20 means 20%vol. ABE blends with 80%vol. diesel. Zhou et al. [40, 41] performed experiments to investigate ABE20, ABE50 and ABE80 at low temperature conditions; Wu et al. [42] studied ABE20 at various temperatures and ambient oxygen conditions; Lin et al. [43] studied ABE80 and compared to previous studies by Wu and Zhou. It was found that, for the same composition of ABE mixture, there seems to be an optimum blending ratio for appropriate combustion phasing. Both ABE20 and ABE80 showed retarded combustion phasing compared to diesel, due to the lower cetane number and the charge cooling effect. However, for ABE50, the retardation effect seemed to be recovered and the mixture exhibited a similar combustion characteristic as diesel. In terms of emission, increasing ABE blending ratio will always result in a reduced soot emission.

2.2 Review of Spray Characterizations in Constant Volume Chambers

2.2.1 Design Considerations of Constant Volume Chambers

Constant volume chambers are being widely used in spray dynamics and spray combustion studies. It provides a wide range of pressure and temperature conditions that covers the operation points for both gasoline and diesel engines. In a cold chamber test (ambient temperature lower than 300K), the liquid spray dynamics and evaporation processes can be investigated. In a hot chamber test (ambient temperature higher than 800K), the simultaneous spray evaporation and combustion processes can be studied. Constant volume chamber isolates the complexity of in-cylinder turbulent flow, chamber
geometry and liquid fuel impingement on the walls. It focuses only on the spray itself, thus provides direct validation on the spray and evaporation models.

There are mainly three kinds of constant volume chamber designs: pre-burn type chambers, quiescent chambers and constant flow chambers. The pre-burn type (shown in Figure 2.1) chamber generates high pressure and high temperature condition by igniting a premixed combustible-gas mixture, and wait for the desired condition during the cool down process, as shown in Figure 2.2. The quiescent chamber (shown in Figure 2.3) directly controls the ambient condition by heating up the gas inside the chamber using heater cartridges to the desired condition. The constant flow chamber (shown in Figure 2.4) is similar to the previous one, but heating up a huge batch of gas externally to provide a constant flow through the experiment section. Compared to quiescent and constant flow type chambers, pre-burn type chambers have less accuracy in temperature control. In addition, due to a fixed p-T relation (closed system, constant density), it has less flexibility in varying combinations of pressure and temperature. However, pre-burn type chambers can provide a much higher pressure and temperature environment with less energy consumption. The structure and accessories for experiment system are also simpler than constant flow type chambers.

A summary of some examples of pre-burn type chamber can be found in the works by Sandia National Labs [44], University of Illinois [36, 41, 45, 63] and North Carolina State University [46]. An example of experimental work in quiescent chamber can be
found in Ref. [47]. The studies in constant flow chambers can be found in works done by CMT-Motores [48, 49].

2.2.2 Optical Diagnostics for Spray and Combustion

(1) Spray Dynamics

The dynamics of spray can be characterized by liquid spray penetration, spray angle, droplet velocity profile. High speed imaging with either shadowgraph or Mie-scattering configuration can be used to acquire real-time spray image and further extract liquid spray penetration and spray angle information.

Pickett et al. [44] studied the liquid spray penetration length of a common rail diesel injector with Mie-scattering approach. A Xenon lamp was used to illuminate the spray region, elastic scattering will occur on the surfaces of liquid spray droplet and can then be captured by a high speed CMOS camera. The framing period of the camera was set at 50µs and the exposure time was 18µs. The Mie-scattering image of spray show brighter signal at higher droplet density areas and dark signal at background. Huo et al. [50] measured the liquid length of combusting spray in a constant volume chamber with Mie-scattering approach. In this experiment, a copper vapor laser was used to provide high repetition rate, high intensity illumination on the spray area. A bandpass filter was used to isolate the scattered signal from liquid droplet from combustion chemiluminescence. In comparison, Klein et al. [51] performed similar high speed imaging experiment with shadowgraph setup. The images showed dark signals for liquid area and light signals for
background. Both these approaches provide instantaneous spray images and the liquid length can be further extracted from image processing. However, the dynamics of spray cannot be fully understood only with the knowledge of liquid penetration length, the velocity field of spray is another essential parameter to be measured in spray experiments.

Phase Doppler Anemometry (PDA) is being widely used in quantifying flow field velocities. The basic principles of PDA have been described in full detail in Bachalo’s paper [52]. It is basically correlating the fringe pattern from interfering laser beams that travels through the measurement point with the local flow velocity. Nouri et al. [53] used PDA to measure the flow field of a GDI swirl injector at various injection durations. The measurement was fixed at a single point downstream of the spray. Santolaya et al. [54] measured the flow field of a swirl injector at low ambient flow velocity, in this study, multiple measurement locations were selected to depict the full image of flow field. Figure 2.5 shows the measurement results from this study, it should be noted that even though multiple measuring points were used, the velocity information is still discrete in space, which reveals the drawback of PDA measurement.

(2) Spray Vaporization

The simultaneous measurement of liquid phase and vapor phase spray concentration field can be achieved by two approaches: schlieren imaging and laser induced exciplex fluorescence (LIEF).
The experiment setup of schlieren imaging is very similar to the shadowgraph imaging. The only difference in setup is that there is a schlieren stop at the focal point of collection optics, the schlieren stop is usually a knife edge. The use of schlieren stop is to increase the sensitivity of measurement to the gradient in refractive index of gas, so the image acquired is usually used to distinguish the vapor phase spray area from ambient air. Pickett et al. [55] investigated the vapor phase spray penetration with different schlieren stop setups: knife edge, round aperture, and no stop. It was discovered in this research that, although the use of schlieren stops increases the response sensitivity, but at the same time reduces the collected light intensity at the camera. It was recommended to use focused shadowgraphy instead of schlieren in high turbulence intensity conditions such as pre-burn type constant volume chambers. Although shadowgraphy is less sensitive to refractive index gradients, the huge refractive index difference of spray vapor and ambient gas allows for sufficient measurement accuracy.

Another method to measure spray vaporization is laser induced exciplex fluorescence (LIEF). The principal of LIEF was proposed by Melton [56, 57] Two dopants are added into the fuel, and these dopants can fluoresce upon excitation of incident laser. In liquid phase, two dopant react with each other and form exciplex molecule; while in vapor phase, the collision probability of two dopant molecules is low, so the dopant itself is getting excited to a higher electronic level and fluoresce at different wavelength than the liquid phase emission. By using different filters, liquid phase and vapor phase fuel distribution can be measured separately. Felton et al. [58] applied LIEF technique in the measurement of in-cylinder liquid phase and vapor phase fuel concentration. It was found
that the fluorescence signal was significantly dependent on the temperature, which sets
difficulties in the interpretation of data. Kim et al [59] performed experiments in a
quiescent constant volume chamber and calibrated the fluorescence signal to fuel
concentration. It was discovered that decomposition of exciplex molecules will become
dominant at temperature higher than 1000K. LIEF can be used as a tool to visualize both
liquid and vapor phase distribution field, but the quantitative measurement is difficult and
almost impossible.

(3) Soot Concentration

The methods to measure soot concentration include: light extinction method and laser-
induced incandescence (LII). The forward illumination light extinction (FILE) method
proposed by Xu et al. [60] is based on the principals of normal light extinction. In this
setup, a point source of light is being expanded to illuminate the spray area, a reflector is
placed behind the flame, the high speed camera captures the reflected light on the same
side of the light source. The interpretation of data is based on Lambert-Beer Law, where
light is being attenuated when traveling through the soot cloud. With a higher
concentration of soot, a weaker signal can be detected. This method can be used for time
resolved quantitative soot mass concentration measurement. The laser induced
incandescence (LII) was proposed by Melton in 1984 [61]. The principal of LII is to heat
up the soot particles with the energy from laser, and the particles will then emit
incandescence at higher temperature. However, this method “destroys” the soot particle
by heating up and thus enhances the chemical reaction rate. As a result, the time-resolved measurement cannot be done without proper correction and calibration.


### 2.3 Tables

Table 2.1 Properties of biodiesel prepared from vegetable oils and used cooking oil

<table>
<thead>
<tr>
<th></th>
<th>Kinematic Viscosity [cSt]</th>
<th>Cetane Number</th>
<th>LHV [MJ/kg]</th>
<th>Density [g/mL]</th>
<th>Flash Point [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASTM Standard(^1)</td>
<td>1.9–6</td>
<td>40 min</td>
<td></td>
<td></td>
<td>130 min</td>
</tr>
<tr>
<td>Peanut(^2)</td>
<td>4.9</td>
<td>54</td>
<td>33.6</td>
<td>0.883</td>
<td>176</td>
</tr>
<tr>
<td>Soybean</td>
<td>4.5</td>
<td>45</td>
<td>33.5</td>
<td>0.885</td>
<td>178</td>
</tr>
<tr>
<td>Palm</td>
<td>5.7</td>
<td>62</td>
<td>33.5</td>
<td>0.88</td>
<td>164</td>
</tr>
<tr>
<td>Sunflower</td>
<td>4.6</td>
<td>49</td>
<td>33.5</td>
<td>0.86</td>
<td>183</td>
</tr>
<tr>
<td>Linseed</td>
<td>3.59</td>
<td>52</td>
<td>35.3</td>
<td>0.874</td>
<td>172</td>
</tr>
<tr>
<td>Used Cooking Oil(^3)</td>
<td>5.16</td>
<td>36.59</td>
<td></td>
<td>0.887</td>
<td></td>
</tr>
</tbody>
</table>

\(^1\) ASTM D6751-15ce1 Standard Specification for Diesel Fuel Oils  
\(^2\) Vegetable oils data adapted from Srivastava et al. [62], viscosity data at 40°C.  
\(^3\) Used cooking oil for menthanalysis, data from Lapuerta et al. [21], viscosity data at 40°C.

Table 2.2 Properties of acetone, butanol and ethanol

<table>
<thead>
<tr>
<th></th>
<th>Kinematic Viscosity [cSt]</th>
<th>Cetane Number</th>
<th>LHV [MJ/kg]</th>
<th>Density [g/mL]</th>
<th>Flash Point [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetone</td>
<td>0.35</td>
<td>29.6</td>
<td>0.791</td>
<td></td>
<td>17.8</td>
</tr>
<tr>
<td>Butanol</td>
<td>2.63</td>
<td>25</td>
<td>33.1</td>
<td>0.813</td>
<td>35</td>
</tr>
<tr>
<td>Ethanol</td>
<td>1.08</td>
<td>8</td>
<td>26.8</td>
<td>0.795</td>
<td>8</td>
</tr>
</tbody>
</table>

* Properties data adapted from Lee et al. [63]
2.4 Figures

Figure 2.1 Schematic of pre-burn type constant volume chamber in NCSU [46]
Figure 2.2 Typical pressure trace during pre-burn type constant volume chamber operation
Figure 2.3 Cross-section view of the quiescent chamber in Tsinghua University [47]
Figure 2.4 Cross-section view of the constant flow type chamber in Universitat Politècnica de València [49]
Figure 2.5 The flow field of a swirl injector measured by PDA [54]
3.1 Caterpillar Constant Volume Chamber Setup and Modification

The constant volume chamber was designed to test the spray and combustion process with a HEUI injector from Caterpillar. The structure of the chamber is shown in Figure 3.1. During the experiment, a very lean mixture of acetylene, nitrogen and air is combusted to generate a high pressure and high temperature environment inside the combustion chamber. During the cool down process of hot mixture, the injector will be fired at the moment of reaching the desired pressure and temperature (as P and T are related). The high-speed camera will be triggered by injector signal. The captured images are used to acquire information about liquid penetration, flame luminosity, and soot formation. In-cylinder pressure traces are also captured simultaneously and are used to calculate heat release rate. The experiment procedures are automatically controlled by an in-house LabVIEW code (see detailed descriptions in Section 3.2). The full details of Caterpillar constant volume chamber system can be found in several previous literatures [45, 64].

In this work, a modification of the original chamber system was made, in order to accommodate a Siemens piezoelectric common rail injector in the same chamber. As shown in Figure 3.2, a modified chamber head was designed and fabricated to replace the current piece. A fixture bar was used to press the injector onto the chamber head with two M6 socket cap screws to ensure sealing between the injector and the chamber. According to Bosch Technical Guideline Y445 124 317, the maximum tightening force exerted on
the copper sealing washer is 15kN. To avoid overload while also ensure proper tightening force, a pre-set torque screwdriver with Allen wrench adaptor was used to provide 5N-m tightening torque on each screw, which converts to a tightening force of 8.3kN on the sealing washer.

The design of the new chamber head considered injectors with different exterior dimensions. When designing the hole that houses the injector, both axial and radial directions have some flexibility to fit in injectors of different size. In addition, there are two gas exchange ports with standard NPT 1/8 fittings on the bottom of the chamber head. It can be used for individual control of the intake and exhaust flows in the future, one of the ports may also be used for installing the thermocouple probe for in-cylinder temperature measurement.

In chamber spray experiments, only a small quantity of fuel is injected in each experiment cycle, the mass flow rate required is very small. Thus, a complete set of diesel engine dual-stage pump system is not necessary. The merits of eliminating the mechanical pump also include: more compact layout of the experiment system, avoid contaminating of fuel by lubricating oil inside mechanical pumps, reduce noise level during experiment.

In this work, a manually operated fuel pressurizing system was built. A schematic of the system can be found in Figure 3.3. The key component of the system is a high-pressure generator from High Pressure Company (Model No. 37-6-30), which is designed to generate a maximum pressure of 30,000psi (206.8MPa). Before the experiment, the fuel
reservoir should be filled with at least 200mL of test fuel. If the test fuel used is different from the previous run, flushing of fuel reservoir is also required prior to experiment. To suck fuel from reservoir to pump, shut off Valve 2 and open Valve 1, and then rotate the handle on the pressure generator counterclockwise until reaching the maximum range. To deliver fuel from pump to fuel rail, shut off Valve 1 and open Valve 2, and then rotate the handle on the pressure generator counterclockwise until reaching the maximum range. Every full stroke requires 84 revolution of handle to complete, and the volume of fuel sucked/pushed out in each stroke is 11mL.

In the first 3~5 strokes, it is desired to repeat the suction operation without fueling the fuel rail, this will help to eliminate the air bubbles from the fuel reservoir to the pressure generator. In the following 2~3 strokes, slowly fuel the fuel rail and wait for the pressure to drop, this will help to bleed the air bubbles from the pressure generator to the injector from fuel return line. If replacing fuel, fire the injector several times to flush the injector also. It will require about two full strokes to fill up the fuel rail completely. In the “pressurizing stroke”, every degree of handle rotation will generate a huge rise in the fuel pressure, due to the small compressibility of liquids. Thus, care should be taken in this stroke: rotate slowly and always observe pressure sensor reading.

The pressure sensor on the fuel rail is from Omega (Model No. PX41S0-30KG5V). It requires a regulated DC power supply ranging from 10~40V. The output is a differential-type signal; two output leads should be connected to a pair of differential signal ports on data acquisition board, connecting one of the leads to GND will lead to erroneous
readings in LabVIEW. Different DC power supply may change the intercept in voltage-pressure conversion equation, calibrate with atmospheric condition and modify equation accordingly.

3.2 Data Acquisition and Control System

The data acquisition and control of experiment operation is realized with an in-house LabVIEW code. The original code was built in 2000. Due to the discontinued support to older version of LabVIEW commands in data acquisition modules, in this work, the code was being upgraded to comply with the new format in LabVIEW Version 2012. Although the DAQ subroutine modules in software are being upgraded to the latest version, the hardware that is being used is still outdated and is gradually being discontinued by National Instruments, so it is also recommended to replace the DAQ hardware in the future. A hierarchy diagram of the LabVIEW code is shown in Figure 3.5, which is consisted of four levels: top level, functional level, sub-functional level and data I/O level. The top level of the program is the front panel, which shows the current status of experiment system and displays the current measurement for temperatures and pressures at different location. The functional level contains five subroutines, which are the five steps of the experiment operation. The sub-functional level subroutines are functions that are commonly being used by higher level programs. The function of the experiment control system is to perform designated actions in the correct order and timing, including: preparing combustible mixtures, pressurizing chamber with premixed gases, sending ignition signal, and performing scavenging and vacuuming at the end. As shown in
Figure 3.6, there are eleven solenoid valves in the system, which are controlled and coordinated by the LabVIEW code. Figure 3.6 also shows the timing when these solenoids are activated and disabled. The use of automatic control in LabVIEW greatly improved the experiment efficiency: it takes only 70 seconds to finish one whole experiment run.

During the experiment, various data are collected and recorded, these data include: fuel pressure, combustible gas mixture composition, ambient pressure at injection, and in-cylinder pressure trace. For the data that are not time-resolved, at least 1000 data points are measured at a sampling rate of 100kHz (which converts to 0.01s), and then averaged to eliminate fluctuation. For in-cylinder pressure trace, which is further used to calculate and analyze heat release rate, it is captured at a sampling rate of 100MHz for a duration of 12ms. For pressure trace data, at least five independent experiment runs are required for each case in order to average out fluctuations.

### 3.3 Design of an Ultra-High Pressure Constant Volume Chamber

In this work, an ultra-high pressure constant volume chamber (UHPCVC) is designed. The purpose of building UHPCVC is to investigate spray and combustion characteristics of diesel fuel at elevated ambient pressures up to 300bar. The pre-burn type constant volume chamber design was selected for UHPCVC.

A schematic of the chamber with accessories assembled is shown in Figure 3.4. The UHPCVC is cubic-shaped with three through holes drilled on each surface, the
cylindrical holes intersect at the center of the cube to form the experiment section, which has a volume of approximately 1.8L. There are six windows, one on each surface of the cube, to accommodate either a metal plug or a high strength sapphire optical glass. The reason for choosing sapphire as the material for transparent window is that sapphire has high mechanical strength (tensile strength: 300–400MPa), and an acceptable transmittance down to UV range (~0.75). Compared to quartz, sapphire has relatively lower transmittance at 266nm (usually >0.85), but the mechanical strength is greatly improved, as shown in Table 3.1. The metal plugs can be used to install intake/exhaust port, thermocouple, and the injector. Both the metal plugs and sapphire windows are being secured and tightened on the chamber body by a flange, which has 12 socket head bolts on it to provide evenly distributed tightening force on the windows to avoid excessive local stress that leads to cracking. The chamber is being heated up to 105°C before the experiment to avoid water vapor condensation on walls and optical windows and also to reduce heat loss. There are six tubular heating elements that fit into the grooves on each surface of the cube, each of the heating tube is 1kW. The switches that controls the on/off of heating tubes are controlled by a thermostat relay. Insulation materials are applied on the exterior surfaces to reduce heat convection and radiation to the environment, an aluminum panel is used to fasten the insulation materials.

The operation of the UHPCVC is similar to a typical pre-burn type constant volume chamber, the only difference is that the premixed charge has to be pressurized before ignition to provide even higher pressure after combustion. In order to calculate an accurate range for the composition of the premixed gases and the initial pressure
condition, thermodynamic analysis for the process was performed. The premixed combustion process can be simplified to a constant volume combustion problem. Here, the following assumptions were adopted:

(1) The system is a closed and insulated, the combustion process is adiabatic;
(2) The combustion is complete, chemical equilibrium is not considered;
(3) Dissociation is neglected;
(4) The specific heat is a constant during the process.

Based on previous experiments, it is shown that the combustion and the following cool-down process will only take less than 3 seconds, so it is reasonable to assume adiabatic. Also, as the mixture is very lean, it can be expected that the oxidation of C\(_2\)H\(_2\) is near complete.

The chemical reaction during the combustion process is:

\[
C_2H_2 + xO_2 + yN_2 \rightarrow 2CO_2 + H_2O + \left(x - \frac{5}{2}\right)O_2 + yN_2
\]

Here, \(x\) is the concentration ratio of oxygen to C\(_2\)H\(_2\), it will vary with the desired oxygen concentration condition; \(y\) is the concentration ratio of nitrogen to C\(_2\)H\(_2\).

Under the above assumptions, the premixed combustion process can be formulated as:
During the cool-down process, the ratio between pressure and temperature is to remain a constant. The desired condition for spray experiment is: pressure around 200~300 bar, temperature around 1000~1200 K. It is also required to control the maximum pressure inside the chamber to be less than 500 bar. As a result, the maximum temperature after combustion should be less than 1700 K.

Equations (1)~(3) were being solved iteratively. The specific heat and the enthalpies of species are estimated with the CHEMKIN format 7-coefficient polynomial. The range for initial pressure prior to combustion was set to 50~120 bar, and the range for nitrogen/acetylene ratio (y value) was set to 10~50.

Figure 3.7 and Figure 3.8 show final pressure and temperature of premixed combustion for various combinations of nitrogen dilution ratio and initial pressure (for stoichiometric oxygen). It can be seen that, the final temperature is dependent only on the nitrogen/acetylene ratio and does not change with initial pressure, which is reasonable due to the assumptions adopted. The final pressure is shown to be dependent on both initial pressure and nitrogen/acetylene ratio. The higher the initial pressure, the higher the final pressure; the higher the nitrogen/acetylene ratio, the lower the final pressure.
As described before, it is desired to have a final pressure lower than 500bar and final temperature lower than 1700K. Also, considering the lower flammability of acetylene with oxygen diluted by nitrogen, there will be a maximum allowable nitrogen/acetylene ratio. Under these constraints, there will be a certain feasible range for the initial condition of the premixed gases. Figure 3.9 shows a feasible range under the constraint of $p_{\text{max}}=500\text{bar}$, $T_{\text{max}}=1600\text{K}$, and nitrogen/acetylene ratio < 35. It can be seen that an initial pressure of 60~90bar, and a dilution ratio of around 30 will yield a desired post-combustion condition.

3.4 Injector Delay Measurement

The injector will not inject fuel immediately after receiving the trigger signal, there will be a delay both before and after injection due to the mechanical response time. As a result, the injector delay is an essential knowledge for the further comparison of experiment data with simulation result.

Figure 3.10 shows the experiment setup for the measurement of injector delay. A laser beam is passed through the spray area and then received by a photodiode, and the laser is located right above the injector tip. The photodiode will produce positive voltage when receiving the laser energy, however, when the laser beam is blocked by spray, there will be no voltage output. The injector trigger signal and the voltage output from the photodiode are monitored simultaneously on an oscilloscope to measure the delay between these two pulses. The photodiode has a rise/fall time of several nanoseconds, so
it can be deemed as an immediate response device and there is no additional delay in the measurement.

As a part of the calibration experiment, the delay time between actual injection and the rising edge of trigger signal was measured for the Caterpillar injector used in the experiment. The delay time for this injector is 0.5ms.

### 3.5 Injector Driving Current Profiling

The injector driving current profile is usually specified by injector manufacturer. A typical injector driving current profile is shown in Figure 3.11, which has a higher “peak current” followed by a relatively lower “hold current”.

In order to accurately measure the instantaneous injector driving current without changing the line impedance (injector resistance is usually 0.5~10 Ω), a current probe is required. Tektronix provides clamp-style current probe at the price of around $2500. In this work, a self-made current probe was designed to minimize the experiment cost while providing acceptable measurement accuracy. A Hall effect current transducer (LEM LTS 15-NP) is used, which provides a measurement range of 45A. A linear voltage regulator (LM7805AC) is used to supply regulated 5V power for the current transducer. The LTS 15-NP chip converts the current signal to voltage, which can then be directly measured by an oscilloscope. The voltage-current conversion equation with the current setup is:

\[ V = 2.5 \pm 0.0416I \]
Figure 3.12 shows the measured injector driving current profile of the Bosch solenoid injector.
### 3.6 Tables

**Table 3.1** Comparison of sapphire and quartz materials for optical windows

<table>
<thead>
<tr>
<th></th>
<th>Sapphire</th>
<th>Quartz</th>
</tr>
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<tbody>
<tr>
<td>Transmittance @ 266nm</td>
<td>0.75</td>
<td>&gt;0.85</td>
</tr>
<tr>
<td>Transmittance @ 532nm</td>
<td>0.83</td>
<td>&gt;0.95</td>
</tr>
<tr>
<td>Compressive Strength</td>
<td>2GPa</td>
<td>&gt;1.1GPa</td>
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<td>Tensile Strength</td>
<td>300–400MPa</td>
<td>50MPa</td>
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<tr>
<td>Thermal Expansion Coefficient</td>
<td>8.4e-6/K</td>
<td>5.5e-7/K</td>
</tr>
<tr>
<td>Max. Useful Temperature</td>
<td>2000 °C</td>
<td>1100 °C</td>
</tr>
<tr>
<td>Price</td>
<td>$5,000/each</td>
<td>$900/each</td>
</tr>
</tbody>
</table>
3.7 Figures

Figure 3.1 Schematic of the Caterpillar constant volume chamber
Figure 3.2 Modified chamber head with Siemens piezoelectric common rail injector installed
Figure 3.3 Schematic of the manually operated high-pressure generator system
Figure 3.4 Cross-sectional view of the UHPCVC
Figure 3.5 Hierarchy Diagram of the LabVIEW control program
Figure 3.6 Schematic of the constant volume chamber control system
Figure 3.7 The final pressure of premixed combustion for various combinations of nitrogen dilution ratio and initial pressure (for stoichiometric oxygen)
Figure 3.8 The final temperature of premixed combustion for various combinations of nitrogen dilution ratio and initial pressure (for stoichiometric oxygen)
Figure 3.9 Feasible range of initial operating condition demonstrated
Figure 3.10 A schematic of injector delay measurement and the photodiode driving circuit.
Figure 3.11 Typical injector driving current profile

Figure 3.12 Measured injector driving current profile of the Bosch solenoid injector
Chapter 4 Data Processing and Calibration Experiments

4.1 Combustion Pressure and Heat Release

During the experiment, a high-speed pressure transducer was used to capture in-cylinder pressure at a repetition rate of 100 kHz for duration of 12ms. The contribution to pressure rise from spray combustion is calculated by subtracting the initial ambient pressure. Here it is assumed that the contribution of ambient pressure does not change during the 12ms duration of spray combustion. The obtained pressure trace is averaged over at least five runs.

Heat release rate (HRR) was derived from pressure trace data via:

\[
\frac{dQ}{dt} = \frac{\gamma}{\gamma-1} p \frac{dV}{dt} + \frac{1}{\gamma-1} V \frac{dp}{dt} + dQ_w
\]

Eq. 4

Among which, \( Q \) is the heat released from system, \( p \) and \( V \) are pressure and volume respectively, \( \gamma \) is the heat capacity ratio of gas mixture, which is considered as a constant (\( \gamma=1.4 \)) during the whole process. Based on the fact that the experiment chamber is a closed-system, it can be determined that \( dV=0 \). The term \( dQ_w \) is the heat transfer to walls, since the process is rather quick, it is reasonable for it to be neglected.

Due to the nature of differential operation, the calculated HRR will suffer from low signal-to-noise ratio. In order to remove the noise, pressure data are being smoothed first before differentiate using 7-point moving average method (MATLAB syntax: `smooth`), then the calculated HRR is also being processed with a Savitzky-Golay smoothing filter to remove the high frequency noise (MATLAB syntax: `sgolayfilt`).
After HRR is calculated, start of combustion can be defined as the time when 5% of the total heat is released; while end of combustion can be similarly defined as the time when 95% of total heat released. Then, ignition delay can be defined as the time between fuel injection and ignition timing and combustion duration is the time between start and end of combustion. The definition to combustion phasing based on total heat release percentage is illustrated in Figure 4.1.

4.2 Liquid Penetration Length

The liquid spray penetration length provides important information on the evaporation process of the spray. In the experiment, spray images are captured by either Mie-scattering or shadowgraph methods using high speed camera. The image sequences are then being analyzed with MATLAB to extract liquid penetration length data.

In this work, an improved algorithm was implemented in the processing code for liquid penetration length extraction. The algorithm was based on automatic image recognition functions built in LabVIEW. The workflow of the algorithm is described as follows: (1) The very first step of data processing is to read raw video format files, the batch of images is stored in a three-dimensional matrix (MATLAB syntax: readcin); (2) Then, the images are being cropped and rotated to show only one of the plumes and align the centerline of the plume to horizontal position (MATLAB syntax: imrotate); (3) Before processing images with boundary-recognition algorithm, it is required to binarize the grayscale image to black-and-white. A threshold value of 0.1 is selected for binarization (MATLAB syntax: im2bw); (4) The boundary-recognition algorithm is then executed and it detects all the connected region in the field of view, the output contains morphologic
information of the recognized regions such as area, boundary coordinates, primary axis length, etc. (MATLAB syntax: `bwboundaries, regionprops`); (5) Select the spray region: the detected regions contain not only spray region, but also some small regions due to camera noise or false regions introduced in binarization. For the most of the cases, the region where spray plume exists is the region with the largest area, so the liquid length can then be extracted from the property of the selected region. Figure 4.2 shows how liquid penetration length is determined from a sample image.

4.3 In-cylinder Pressure-Temperature Relations

In the constant volume chamber, during the closed system operations, the ratio between pressure and temperature should be close to a constant. If assuming no heat loss to walls, no species changes before and after combustion, this constant is directly related to the mass of air inside the chamber. The pressure-temperature relation is an important knowledge to identify ambient temperature condition upon injection via pressure reading and to calculate the ambient density for the experiment.

On the modified Caterpillar constant volume chamber, there is an additional NPT1/8-thread port. A K-type thermocouple (OMEGA TJFT72-K-INC-116G-6-SMPW-M) with outer diameter of 1/16 inch can be installed with a compression fitting to measure the gas temperature inside the combustion chamber. The thermocouple has a sheath diameter of 0.02 inch, which will yield a fast response time. A heat transfer and radiation correction will be carried out to account for the delay caused by limited heat transfer rates and the inaccuracy caused by radiation.
4.4 Figures

Figure 4.1 Illustration of combustion phasing definition based on cumulative heat release
Figure 4.2 Illustration of the liquid length extraction algorithm
Chapter 5 Experimental Study

5.1 Experimental Conditions and Fuel Properties

In this study, the Caterpillar constant volume chamber (Figure 3.1) was used to simulate real diesel engine conditions upon TDC. As is applied by other institutions like Sandia and IFP, premixed combustible gases (C2H2, Air and N2) were ignited and burned to achieve high-pressure and high-temperature conditions up to 18MPa. The chamber is equipped with a fused silica quartz window with 130mm in diameter and 65mm in height to allow optical access. Quartz is higher in mechanical strength than ordinary glass and also provides high spectral transmittance down to 190nm. The visible area of the quartz window is 110mm in diameter. The chamber wall was heated to 380K prior to experiment runs using eight cartridge heaters and a thermostat controller, to prevent water condensation on either chamber walls or quartz windows.

The injector (CATERPILLER hydraulic-actuated electronic-controlled unit injector) was mounted at the bottom of the constant volume chamber with the injection direction towards the quartz window. The injector has a six-hole, valve-covered orifice (VCO) type specification, with the orifice diameter of each hole is 0.145mm. Operating parameters of the injector during the experiment are listed in Table 5.1. A high-energy plasma-coil spark plug was installed on the sidewall of the chamber, ensuring stable ignition for the relatively lean combustible gas mixture. The pressure trace inside the combustion chamber was recorded using a high-dynamic pressure transducer (KISTLER 6121) coupled with charge amplifier. During the cool-down process of combusted gas, injector will be triggered upon reaching the specified pressure and temperature conditions. The
controller program will automatically adjust the delay timing from ignition to injection, thus providing reliable and repeatable experiment conditions. The accuracy of ambient pressure prior to injection can be controlled within ±0.6bar range in all circumstances.

As mentioned before, ABE is the product of acetone-butanol-ethanol fermentation process, with the typical volumetric concentration of ABE is 30% acetone, 60% butanol and 10% ethanol. In this study, analytical grade (99.5–99.8%) chemicals were used to make up the specified ABE mixture, which was then further blended with baseline ultra-low sulfur diesel (ULSD) as 80% vol. ABE and 20% vol. ULSD using magnetic stirrer. This test fuel is denoted as “ABE80” in the following discussions. Stability of the mixture was verified through gravitational method, the blends were deposited in a test tube at room temperature and pressure for 14 days. The results showed a unified mixture phase, proving that the ABE-diesel blend under this ratio is stable. Besides, in order to setup the benchmark, baseline diesel (denoted as “D100”) was also investigated under the exact same condition as ABE80 and the injection duration was kept the same. The physical and thermo-physics properties of each component in the mixture are listed in Table 2.2.

5.2 Experiment Results with HEUI Injector

5.2.1 Liquid Spray Penetration Length

The image sequence showing liquid spray penetration of ABE80 and baseline diesel is shown in Figure 5.1. The image sets were acquired at 900K and 21% ambient oxygen concentration conditions. The grayscale had been reversed to show spray plumes more
clearly. Images shown here have not been averaged; they are acquired in a single injection event sequentially.

It can be seen that the spray plumes showed a typical cone structure, with growing wrinkles on the periphery of spray, which are results from the developing instability wave on the surface of liquid sheet. At the downstream of sprays, especially ABE80, a strong entrainment of air occurs to further “expand” spray plume, forming a well-mixed air-fuel mixture.

From the comparison of spray patterns, it can be found that ABE80 showed substantially more “pale” spray plume than D100, especially at the periphery and the tail section of spray. The higher volatility of ABE than diesel should be a direct interpretation of this phenomenon: a higher volatility of ABE80 causes the liquid droplets at the specified sections to evaporate faster, thus decreasing droplet diameter and number density in those areas, which then lowered the scattered light intensity.

Another attribution should be that ABE80 has lower viscosity and surface tension than diesel, which favors the growth of instability waves on the spray surface, enhancing the liquid sheet breakup process and speeding up the evaporation of ABE80 spray.

From the spray images, liquid penetration length can be derived. Figure 5.2 shows the typical liquid penetration length data acquired from single image processing. Notable shot-to-shot variation can be observed; also, due to the turbulence and non-uniform environment of premixed-combustion chamber and limitations of post-processing algorithm, fluctuations in liquid penetration length existed within every measurement. The bold line in figure is an average of 3 measurements, smoothed by 5-point moving
average algorithm. Repeatability and error due to resolution limitations are estimated to result in an overall inaccuracy of 20%.

It can be seen from Figure 5.2 that during the injection period, the penetration length seemed to first increase rapidly, due to the initial development of spray, then maintain approximately the same, followed by a gradually decrease. This decrease in the liquid penetration length can be related to the combustion process, because the combustion will first occur at the well-mixed tail section of spray; the burned gas will have a heating effect to the spray upstream, which further enhanced the evaporation process. Plus, the combustion process reduced the remaining liquid fuel quantity, resulting in a decreasing penetration length. Using the above method, ABE80 and diesel liquid spray penetration under 900K/1100K ambient temperature and various ambient oxygen concentration conditions were derived from the images, as presented in Figure 5.3. Each of the curves are averaged from at least 3 measurements and smoothed.

An obvious conclusion from the figures is that ABE80 had a relatively shorter liquid penetration length than diesel under all ambient temperatures and oxygen concentration conditions. This indicates that ABE80 can form a better fuel/air mixture than diesel under the same injection parameters and operating conditions.

Ambient temperature has a major influence on the penetration length. One of the reasons is that higher temperature favors evaporation, which reduces penetration length; another important aspect is that in the experiment, ambient density was kept as constant. Higher ambient temperature also leads to a higher ambient pressure, and according to the atomization theory, the liquid penetration length is shortened under high ambient pressure.
It should be noted that oxygen concentration also has some minor influence on the penetration length: higher oxygen concentration leads to shorter penetration length. A possible explanation for this is related to the combustion process. Higher oxygen concentrations can lead to a higher combustion temperature at the downstream of spray, which will have a heat-up effect for the upstream spray droplet to enhance evaporation and reduce liquid penetration length. In the case of ABE80 spray, under the ambient oxygen concentration of 11%, the penetration curve seemed to be “retarded”, which is not observed in pure diesel cases. There has been no widely accepted explanation for this retardation.

5.2.2 Combustion Heat Release

Because of the “equal-injection-volume” basis in the experiment, the total energy injected in each case would not be the same. Thus, a normalization process is essential for eliminating the differences and setting up benchmarks.

Pressure traces acquired in experiments were averaged (at least 5 measurements) and used to calculate the original HRR. The original HRR was then normalized by the total released energy, which is derived from the integration of original HRR curve. The value of normalized HRR represents the fraction of the total heat release per millisecond.

The spray combustion pressure traces and normalized HRR are shown in Figure 5.4. From the figures, it can be concluded that the combustion phase is influenced by both ambient temperature and ambient oxygen concentration. A uniform conclusion is that a retarded ignition timing and lower peak heat release rate will occur due to the decreased oxygen concentration. The result for diesel is a good example of the above conclusion.
and is consistent with prior investigations in the author’s lab. Compared to diesel, ABE80 generally showed more mild combustion characteristics, reflected in a lowered peak combustion pressure and a flattened heat release curve shape. This character is desired for reducing in-cylinder combustion temperature and the emission of NO\textsubscript{x}.

In terms of different ambient temperature, ABE80 showed quite complicated results. At ambient temperature of 1100K, the combustion phase and heat release rate were roughly the same between 21% and 16% ambient oxygen concentration conditions. However, at the ambient temperature of 900K, the curves for all three different oxygen concentrations are obviously separated, showing quite different ignition delay times, but the peak heat release rate and the shape of HRR curve remained almost the same under the various ambient oxygen concentration conditions. This indicates that ABE80 fuel may have better tolerance for the changes in ambient oxygen concentrations with the heat release characteristics to remain almost the same. However, the ignition delay of ABE80 under low temperatures are quite sensitive.

Furthermore, comparing combustion characteristics of ABE80 between 900K and 1100K conditions, it can be found that ABE80 exhibits a steeper HRR curve at lower temperatures, which means a faster combustion. This is usually attributed to a higher degree of premix-dominated-combustion. In this case, although the ambient temperature is lower, which reduced the evaporation rate of liquid fuel and ignition delay increased greatly (Figure 5.5), allowing more sufficient time for fuel/air premixing process.

The ignition delays for D100 and ABE80 under various conditions are listed in Figure 6. Here, the ignition delay is defined as the time difference between the rising edge of
injection pulse signal and the start of combustion. Start of combustion is determined by cumulative heat release and is defined as the time at which 5% of the total heat is released.

From the figure, a general conclusion that can be made is that with decreasing ambient oxygen concentration would result in increasing the ignition delay. Also, it can be seen that the ignition delay of ABE80 and diesel at ambient temperature of 1100K is rather similar, even at varied oxygen concentrations. This showed that the major influence factor of ignition delay is the ambient condition, although ABE is a kind of oxygenated fuel which will change the oxygen concentration while combustion, the effect seemed to be rather minor. Compared to previous work on low-percentage ABE in diesel blend (ABE20) [41], ABE80 has longer ignition delay time than ABE20 under the same condition and it is more sensitive to the ambient temperature: the ignition delay time increases more rapidly with decreasing temperature, owing to the lower cetane number of butanol and ethanol.

Figure 5.6 shows the combustion duration of ABE80 and baseline diesel spray combustion processes. Similar to the ignition delay, the duration of combustion is determined via cumulative heat release. The end of combustion is defined as the time at which 95% of the total heat is released. It can be concluded that, at the same ambient temperature of 1100K, ABE80 has a small increase in combustion duration than baseline diesel. Under the lower ambient temperature of 900K, the combustion duration of ABE80 was shortened. This can be attributed to the faster combustion rate due to better premixing processes allowed by longer ignition delay time. Although at lower
temperature, chemical reaction rates will be slower than that of high ambient
temperatures.

As a brief conclusion, ABE80 fuel has milder combustion characteristics at the tested
conditions than diesel; ABE80 has better tolerance to EGR than diesel at the 1100K
ambient temperature condition; but it becomes rather sensitive at the 900K ambient
temperature condition.

5.2.3 Natural Luminosity and Flame Structure

Figure 5.7 shows the natural flame luminosity evolution of ABE80 under ambient
temperatures of 1100K and 900K. The images were captured in single injection event
sequentially; no averaging or smoothing processes were adopted. The images shown are
pseudo-color with the brighter color showing higher luminosity intensity. As stated by
Dec [65], the intensity of natural flame luminosity mainly depends on the soot
concentration and temperature of the soot particle. The flame luminosity image can be
seen as an indicator of soot concentration during combustion process.

The field-of-view mainly showed one of the spray plumes and the interaction of spray
with the chamber wall. It can be seen that natural flame luminosity intensity was
evidently reduced under lower ambient temperature and lower ambient oxygen
concentration. This indicates that LTC and EGR can help to reduce soot emission during
combustion, which is consistent with prior research.

Also, compared to D100 and ABE20 combustion reported in previous work conducted in
the same chamber [41], ABE80 fuel always exhibits a cleaner combustion, showing
lower flame luminosity intensity and retarded initial soot presence. This is mainly due to the oxygen concentration in ABE, which helps to improve combustion in fuel-rich zones. Also, as stated in the above part, ABE80 has relatively longer ignition delay time, allowing for better fuel/air mixture preparation and resulting in a premixed-dominant combustion process.

In order to quantitatively analyze the soot emission from spray combustion, the spatial integrated natural luminosity (SINL) was calculated by integrating the intensity of the acquired images pixel-by-pixel; the result was averaged by at least 5 experiment results.

Figure 5.8 shows the SINL of ABE80 under various operating conditions. In accordance with the observed result in Figure 9, the SINL data further provides quantitative support to the fact that with a lower temperature and lower oxygen concentration, soot emission from spray combustion will be lowered. From the figure, it can be seen that a 200K decrease in ambient temperature can result in a huge reduction in SINL: the maximum intensity reduced 74% from 1100K to 900K, while the influence of oxygen concentration is relatively weaker. The maximum intensity reduced 64% from 21% to 11% oxygen concentrations at 1100K.

Another observation from the figure is that the decrease of ambient temperature and oxygen concentrations also retarded the initial presence of visible natural flame luminosity, which is due to the low temperature combustion and a longer ignition delay under these conditions.
In order to compare ABE80 with other kinds of fuels, Figure 5.9 presents SINL data for baseline diesel, ABE20 and ABE80 under 1100K and with a 21% oxygen concentration condition. (ABE20 data from [41])

It can be seen from the figure that blending ABE in diesel is an effective solution for the reduction of soot emission. The maximum SINL value of ABE20 reduced by 35%, compared to baseline diesel, and 54% for ABE80.

5.3 Experiment Results with Siemens Piezoelectric Injector

5.3.1 Validation of Data Consistency

The very first step of the experiment is to validate that the performance of experiment system is consistent between each runs. In the preliminary tests, 27 experiment runs were carried out, which can be grouped into 5 ambient conditions, the target injection pressure was set to be 10,000psi for all tests.

Table 5.2 shows the statistics of injection pressures in the preliminary tests. All data from the tests were used, without any data selection or elimination process. It can be seen that the consistency of injection pressure is very stable. And the repeatability of this injection pressure can be further reduced by improving operators’ skill.

Table 5.3 shows the statistics of ambient pressures at the injection event for each of the test groups (corresponding to a similar ambient pressure). There are 5~6 experiments for each case, and similarly, all acquired data were used. It can be seen that for all attempted conditions, the ambient pressure exhibits excellent repeatability (less than 1%), except for the low temperature one, yet it is still well below 5%.
Figure 5.10 shows the averaged pressure trace (red) from spray combustion contribution and the standard deviations (gray). Again, it can be seen that for almost all test conditions, the repeatability of pressure traces was excellent, except for the low temperature condition. This conclusion was also observed in the previous experiments in the similar chamber. The reason for the relatively poor consistency at low ambient pressure/temperature conditions is that the ignition delay and combustion efficiency at lower temperature range are more sensitive to temperature variations. Although great effort has been made to maintain the quasi-steady state and uniformity inside the chamber, there will still be some inaccuracies associated with these sources. However, this can be improved by applying appropriate data selection criterion (such as +/- 3σ rules, etc).

5.3.2 Combustion Heat Release Analysis

In the preliminary tests, the baseline diesel was investigated under two different ambient temperature conditions: 1200K (high temperature) and 1000K (medium temperature). The injection pressure was controlled to be at 10,000 psi (68.9MPa), with an injection duration of 3ms, the injected mass was around 90mg per cycle. Table 5.1 summarizes the experiment conditions.

Figure 5.11 shows the spray combustion pressure trace at two different conditions. Both pressure traces show a typical diffusion combustion pattern: the pressure trace increases slower at the beginning and accelerates in the later stage. With the consumption of all injected mass, the pressure became stable at the end, and started to decrease slightly due to the heat transfer to walls. It can be seen from this figure that, both cases have an ignition delay of around 1ms. The final combustion pressures are around 13bar, with the
lower temperature case having the higher final combustion pressure. This indicates that the lower ambient temperature case might have a better combustion efficiency than the case at higher ambient temperature.

In order to better visualize the heat release characteristics at two different ambient temperature, the apparent heat release rate from spray combustion was calculated from the pressure trace, with the method described in Section 4.1 and is shown in Figure 5.12.

The heat release rate traces can be divided into four sections: (1) Ignition delay, during which there is no obvious heat release; in this process, the liquid fuel evaporates into vapor phase and get mixed with air, and some of the chemical reaction starts to take place. (2) Premixed combustion, during which a sharp increase in heat release will occur; this is the result of the ignition of premixed vapor/air mixtures. (3) Diffusion combustion, during which the heat release rate tends to be stable and constant; in this period, the liquid fuel is still being injected from the injector orifice, and the diffusional combustion is the dominant mode. (4) Late combustion, in this period, the injection event has ended, and the heat release rate starts to drop until the available hydrocarbons get completely oxidized.

Comparing the heat release rates at two different ambient temperatures, it can be seen that the lower temperature case has a significantly stronger premixed combustion region, showing a more obvious peak at the initial heat release. This is because of the longer ignition delay at lower temperature conditions that allows for better fuel/air mixing. The diffusion combustion heat release is also stronger at lower temperature condition,
probably related to the higher turbulence induced by the initial premixed-dominant combustion.

5.3.3 Comparison of Injection Triggering Strategies

There are two injection triggering strategies: with and without automatic adjustment. The LabVIEW program is capable of adjusting the time period between spark ignition (for \( \text{C}_2\text{H}_2/\text{Air}/\text{O}_2/\text{N}_2 \) mixture combustion) and injector triggering signal based on the knowledge of the previous experiment cycle. In theory, this should be an effective way of improving repeatability. Here, a comparative analysis between the two methods is performed.

In this study, two triggering strategies were tested under two sets of identical ambient conditions. For each condition, five experiment cycles were attempted to evaluate the repeatability of the setup. Figure 5.13 shows a close-up view of the spray combustion pressure, it can be seen that the standard deviations of the second column (with automatic adjustment), is slightly larger than that of the first column (without automatic adjustment). Table 5.4 further provides more quantitative information on the repeatability of ambient pressure/ temperature condition upon injection event. In general, both methods yield reasonably low fluctuations and they are both suitable for the experiment purposes.

It should be noted however, that the method without automatic adjustment requires a precise estimation of what the delay time (between spark ignition and injector trigger) should be. This requires a calibration experiment to be performed before each set of experiment, as this delay time- ambient pressure relation changes with mixture composition (whether it’s 21%, 16% or 11% oxygen) and climate conditions. The
recommended delay time values for 21% oxygen conditions have been tabulated and is recorded in the lab book.

As a conclusion, as the inaccuracies introduced by enabling automatic delay time adjustment is small, and it is easier to operate without prior knowledge to the delay time-ambient pressure relation, it is recommended to keep using the method with automatic adjustment enabled for further experiments.

5.4 Summary

The spray and combustion characteristics of high-percentage ABE-diesel blend (ABE80) was studied in a constant volume chamber under 1100K and 900K ambient temperatures and 21%, 16%, and 11% ambient oxygen concentrations. The main conclusions are as follows:

Under various ambient operation conditions, ABE80 spray exhibited shorter penetration length and a weaker Mie-Scattering signal than diesel spray, because of the higher volatility of ABE fuel and its better atomization ability. These characters of ABE allow for a better fuel/air mixing process during injection.

From the study of the heat release rate of both fuels, although ABE has higher volatility and better atomization, its heat release mode is not as violent as ordinary diesel premixed-dominant combustion. The heat release rate of ABE80 is mild and it seems to be more tolerant for the change in ambient oxygen concentrations.

In terms of ambient temperature, ABE80 showed more premixed-dominant combustion modes under lower temperature conditions, due to an evidently prolonged ignition delay.
The reduction in soot luminosity intensity also showed that ambient temperature is the main factor influencing the soot emission of ABE80 combustion.

Compared to baseline diesel and ABE20 in previous work, ABE80 exhibited the cleanest combustion in terms of soot luminosity intensity. The ignition time for ABE80 is the longest among compared fuels.

In addition, the modified chamber has been tested and validated. Preliminary tests have shown that the performance and the consistency of the chamber system is within the acceptable range.
5.5 Tables

Table 5.1 Experiment parameters and conditions

<table>
<thead>
<tr>
<th>For HEUI Injector</th>
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<td>Injection Pressure (MPa)</td>
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<tr>
<td>Injected Volume (mm³)</td>
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<td>Ambient Pressure (bar)</td>
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<td>Ambient Density (kg/m³)</td>
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<td>Ambient Gas Conc.</td>
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</tr>
<tr>
<td></td>
<td>N₂</td>
</tr>
<tr>
<td></td>
<td>CO₂</td>
</tr>
<tr>
<td></td>
<td>H₂O</td>
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</table>

<table>
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<tr>
<td>Ambient Density (kg/m³)</td>
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<tr>
<td>Ambient Gas Conc.</td>
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<td></td>
<td>N₂</td>
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<td></td>
<td>CO₂</td>
</tr>
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<td>H₂O</td>
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Table 5.2 Statistics of injection pressure in all tests

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<th>Injection Pressure Standard Deviation (psi)</th>
<th>Relative Error</th>
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<td>10023.85</td>
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Table 5.3 Statistics of ambient pressure

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<tr>
<th>Case #</th>
<th>Ambient Temperature (psi)</th>
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<th>Ambient Pressure Standard Deviation (psi)</th>
<th>Relative Error</th>
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<tr>
<td>1</td>
<td>1225</td>
<td>735.86</td>
<td>1.36</td>
<td>0.18%</td>
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<td>2</td>
<td>1125</td>
<td>673.86</td>
<td>3.73</td>
<td>0.55%</td>
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<td>3</td>
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<td>629.00</td>
<td>1.90</td>
<td>0.30%</td>
</tr>
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<td>4</td>
<td>1000</td>
<td>598.60</td>
<td>3.71</td>
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<td>5</td>
<td>900</td>
<td>544.68</td>
<td>15.16</td>
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Table 5.4 Comparison of experiment condition repeatability with different injection triggering strategies: a) without automatic adjustment; b) with automatic adjustment

<table>
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<tr>
<th>Case #</th>
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<th>Relative Error</th>
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<tr>
<td>6a</td>
<td>711.73</td>
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<tr>
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<td>716.46</td>
<td>2.36</td>
<td>0.330%</td>
</tr>
<tr>
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<td>2.84</td>
<td>0.477%</td>
</tr>
<tr>
<td>7b</td>
<td>603.38</td>
<td>6.27</td>
<td>1.039%</td>
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5.6 Figures

Figure 5.1 Spray images of ABE80 and D100 at 900K

Figure 5.2 Typical liquid penetration length history
Figure 5.3 Liquid penetration length history of ABE80 and pure diesel
Figure 5.4 Pressure trace and normalized heat release rate of ABE80 and pure diesel spray combustion
Figure 5.5 Ignition delay of ABE80 and pure diesel combustion

Figure 5.6 Combustion duration of ABE80 and pure diesel combustion
Figure 5.7 Natural flame luminosity of ABE80 combustion under 1100K and 900K
Figure 5.8 Spatial integrated natural luminosity of ABE80 under various conditions

Figure 5.9 Spatial integrated natural luminosity of pure diesel, ABE20 and ABE80 under 1100K, 21% oxygen concentration
Figure 5.10 Average and standard deviation of pressure traces at various ambient conditions

$T_{\text{amb}} = 1225K$

$T_{\text{amb}} = 1125K$

$T_{\text{amb}} = 1050K$

$T_{\text{amb}} = 1000K$

$T_{\text{amb}} = 900K$
Figure 5.11 Spray combustion pressure trace at 1200K and 1000K

Figure 5.12 Apparent heat release rate of spray combustion at 1200K and 1000K
Figure 5.13 Close-up view of pressure trace and the standard deviation at two different injection triggering mode
Chapter 6 Conclusions

The spray and combustion characteristics of high-percentage ABE-diesel blend (ABE80) was studied in a constant volume chamber under 1100K and 900K ambient temperatures and 21%, 16%, and 11% ambient oxygen concentrations. The main conclusions are as follows:

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In addition, the modified chamber has been tested and validated. Preliminary tests have shown that the performance and the consistency of the chamber system is within the acceptable range.

6.1 Recommended Future Studies

The upgraded chamber facility provides flexibility in injection strategy, fuel injection pressure, gas exchange control, thermocouple probe measurement, and more precise control of the injection quantity, ambient pressure/temperature conditions. Thus, some future works on this chamber are suggested as follows:

- Validate the in-cylinder pressure-temperature relationship using instantaneous temperature data acquired with fast-response thermocouple with radiative and convective heat transfer corrected.
- Perform forward-illumination light extinction (FILE) experiments in the upgraded chamber setup and measure the time-resolved soot generation at various ambient pressure/temperature and ambient composition conditions.
- Investigate the spray combustion characteristics at different fuel injection quantities.
- Investigate the spray combustion characteristics at different fuel rail pressures.
- Investigate the effect of pilot and/or post injection to the soot generation.
- Perform speciation experiments to investigate the completeness of premixed combustion, and study the effects of residual incomplete combustion species to the later spray combustion behaviors.
Based on the previous studies on ABE combustion, several undermined yet important topics of ABE research is needed:

- Validate the minor effect of ethanol in ABE-diesel mixture, in terms of both combustion characteristics and pollutant emissions.
- Construct guidelines for optimizing ABE-diesel blending ratios, including the identification of competing factors and numerically modelling of optimization problems.
- Validate the results using experimental results of ABE-diesel fueled diesel engines.

However, several challenges are faced in the area of research, which need to be considered for the future work.

- Due to the composition of ABE mixture, single-factorial design of experiment is not possible: changing concentration of one component will surely affect the other two. This issue makes the conclusions unconvincing, and obstructs the quantitative analysis of the problem.
- Incomplete reaction during premixed combustion of constant volume chamber can be expected. However, the minor species during this incomplete combustion process could act as precursors or introduce radicals for the following spray combustion process. Analysis of the degree of reaction and species after premixed combustion is important.
References


[55] Pickett, Lyle M., Sanghoon Kook, and Timothy C. Williams. "Visualization of diesel spray penetration, cool-flame, ignition, high-temperature combustion, and


