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DEPARTMENT OF MECHANICAL ENGINEERING

MSc THESIS

The Use of a Modified IQT<sup>TM</sup> Apparatus and Detailed Chemical Kinetic Model to Investigate the Atmospheric Autoignition Characteristics of Model Fuels

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May 19, 2009
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Nicholas Savage
Acknowledgements

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Executive Summary

Background

Certain combustible mixtures are capable of autoignition, this means that the mixture ignites without any external ignition source, such as a spark or a flame. Autoignition is required in compression ignition engines to initiate combustion and must be avoided in spark ignition engines due to the damage it can cause.

Hydrocarbon fuels will autoignite if the rate of heat released from the exothermic oxidation reactions exceeds the rate of heat dissipation to the surroundings. The delay between the exposure of the combustible mixture to a hot environment and autoignition is referred to as ignition delay.

Objectives

Relationships can be found between the length of this delay and the initial temperature, initial pressure, and air/fuel ratio. This report communicates the results and findings of a project involving an investigation into the ignition delay characteristics of various hydrocarbon fuels at atmospheric pressure. This data is required to complement autoignition data obtained at high pressures from a Rapid Compression Machine (RCM). The characterisation of jet fuels is also desired to assist investigation into the possible effect of ignition delay on gas turbine start up and high altitude relight.
Conclusions

A significant finding of the project was that heat transfer can have a significant effect on ignition delay in the NTC region and in certain circumstances extinguish autoignition entirely.

The modified apparatus was capable of characterising the ignition delay characteristics of complex commercial fuels at atmospheric pressure. The results showed a good qualitative measurement of octane rating.
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List of Acronyms

AIT - Autoignition Temperature
ASTM - American Society for Testing and Materials
EtOH - Ethanol
FPGA - Field Programmable Gate Array
iC8 - iso-octane
IQT™- Ignition Quality Tester
NTC - Negative Temperature Coefficient
nC7 - n-heptane
PRF - Primary Reference Fuel
RON - Research Octane Number
SI - Spark Ignition
ULP - Unleaded Petrol
Glossary of Terms

**Arrhenius Expression** - A formula for the temperature dependence of a chemical reaction rate of the form: \( k = Ae^{-\frac{E_a}{RT}} \)

**Autoignition** - Ignition of a combustible mixture that occurs without spark or flame.

**CHEM@IN™** - A chemical kinetics modelling software package.

**Compression Ratio** - In an engine, the ratio of the total volume of a cylinder to the clearance volume.

**End-Gas** - The portion of the combustible mixture, in a SI engine, that has yet to be ignited by the flame front.

**Ignition Delay** - The time elapsed between the introduction of the fuel and combustion.

**Isomers** - are compounds with the same molecular formula but different structural formulae.

**Knock** - A common term for autoignition of the end-gas in a SI engine, so named due to the ‘pinging’ noise which can be heard.

**Oxidation Reaction** - An exothermic reaction during which a material loses electrons, whilst combining with oxygen.

**Run-on** - A phenomenon associated with SI Engines whereby autoignition causes the engine to continue running after the ignition has been switched off.

**Stoichiometric Mixture** - A mixture of fuel and air that will produce the most complete combustion.
Chapter 1

Introduction

1.1 Background

The autoignition characteristics of automotive fuels are of primary concern in modern internal combustion engine design. Autoignition behaviour is responsible for compression ignition in diesel engines and autoignition of the end-gas or 'knock' in spark ignition engines. Autoignition has also been shown to be responsible for the phenomenon of run-on in spark ignition engines [4, 5].

Autoignition occurs when a combustible mixture ignites without an external ignition source, in other words, autoignition occurs when the rate of heat dissipated from the exothermic oxidation reactions exceeds the rate of heat released to the surroundings and causes ignition [6]. The control of autoignition is essential to improving fuel efficiency and reducing emissions.

A long term goal of the Sasol Advanced Fuels Laboratory (SAFL) at the University of Cape Town (UCT) is to develop an empirical ignition delay model that provides a complete autoignition map of singular fuel components and complex commercial fuels. In order to achieve this goal experimental data is required across a wide range of temperature and pressures. A rapid compression machine (RCM) has been constructed and is currently being commissioned which will provide the majority of ignition delay data. The RCM however is incapable of operating at low pressures or in situations with long ignition delays. A low pressure device is required to provide information in these regions.
Another application of low pressure autoignition data is in the area of gas turbine combustion. Traditionally it is believed that chemical time scales are insignificant relative to evaporation and mixing times with regards to gas turbine combustion[7]. However this may not be the case in marginal combustion situations such as start up and high altitude relight. Reliable autoignition data at relevant temperatures and pressures is essential for further investigation into this matter.

1.2 Project Aim and Scope

The primary aim of the project is to provide atmospheric ignition delay data for specific reference and complex commercial fuels. The following aspects of the autoignition characteristics will also be investigated:

- To what extent is NTC behaviour still valid at low pressures.
- To what extent are the air/fuel ratio relationships still valid at low pressures.
- Can the low pressure information be used to reliably predict real fuel performance under engine conditions.

In order to achieve these aims, the following goals should be accomplished:

- Design and construct a new fuel system for the IQT™.
- Setup of a new electrical control system and associated software to increase the flexibility of test conditions.
- Numerical modelling of ignition delay at atmospheric conditions using detailed chemical kinetics.
- Validation and comparison of experimental results.
- Provide autoignition data for commercial jet fuels at atmospheric pressure.
1.3 Plan of Development

This report begins with a review on the current understanding of autoignition characteristics of hydrocarbon fuels. The review covers basic combustion kinetics, autoignition characteristics such as the Negative Temperature Coefficient (NTC) region, the cool flame phenomenon and resulting two-stage ignition. Topics such as Octane rating and autoignition temperature (AIT) are also covered. Following the literature review, are details of the chemical kinetic modeling performed, which provided a basis of comparison with experimental results and the majority of the theoretical component of the project.

The focus then shifts to the experiments, an overview of the experimental apparatus, including calibration and investigations into the reliability of the experimental data is presented. This is followed by the presentation of experimental results and relevant discussions. Finally conclusions are drawn on the basis of these findings, followed by recommendations for future research and study.
Chapter 2

Literature Review

The topics of combustion, autoignition and cool flames have been studied for over 100 years and even more so in the last few decades primarily to improve emissions and engine performance. There are such a wide range of operating conditions and fuels that the available literature is vast. Many conflicting statements and ideas exist and discrepancies between researchers results can be massive.

2.1 Common Devices used in the Study of Ignition Delay

There are many types of devices used by researchers to study ignition delays, a selection of the most common devices are discussed below. The majority of the apparatus are custom made and as a result have unique operating characteristics.

2.1.1 Rapid Compression Machines (RCM)

A rapid compression machine is, in effect, a single shot engine. A piston is rapidly accelerated in a cylinder and held at top dead centre (TDC) for the duration of combustion. The pressure and temperature for combustion is generated by the compression stroke, and controlled by adjusting the di-
2.1. COMMON DEVICES USED IN THE STUDY OF IGNITION DELAY

Lutents, initial temperature and compression ratio. RCMs typically operate over peak pressures of 10 - 40 Bar and peak temperatures of 600 - 1000 K at the end of compression. Advantages include, a homogeneous charge and operating ranges close to IC engines. Disadvantages include the complex design and operation, fuel handling and the influence of the compression stroke on the ignition delay history.

Rapid Compression Machines rely on compression to heat the air/fuel mixture and are thus not capable of operating at low final pressures. The high turbulence of the mixture during and after compression also introduces high amounts of heat transfer, that affect longer ignition delays.

2.1.2 Shock Tubes

A shock tube is essentially a long tube separated into two sections, a driver and driven section. High pressure gas is suddenly released from the driver section which forms a supersonic shock wave. This wave compresses the end gas in driven section producing a step change in pressure and temperature. Shock tubes can attain very high pressures and temperatures, in excess of 50 Bar and 2000K. Advantages of the shock tube are, homogeneous charge and the ability to investigate the very high temperature region of a fuel with very short ignition delays. Disadvantages of the shock tube include, a relatively long 'reload' time, the equipment is not compact and generally has limited operational range.

Shock tubes, like RCMs are also incapable of testing at low pressures and ignition delays longer than the order of 10ms are also difficult to achieve due to reflections of the driving shock wave.

2.1.3 Combustion Bombs

Combustion bombs used for the investigation of ignition delay consist of a high strength pressure vessel. The vessel is usually pre-heated and pre-filled to the desired pressure with the oxidiser. Fuel is then introduced to the hot environment in the form of an injected spray where evaporation, mixing and the autoignition occur. Advantages of combustion bombs are, rapid repetitive testing, ability to explore a wide range of initial conditions. Disadvantages, include instrumentation difficulties associated with permanently
2.1. COMMON DEVICES USED IN THE STUDY OF IGNITION DELAY

hot devices and poor homogeneity of mixture. Some variants of the combustion bomb use a pre-combustion of specific gas concentrations to reach the desired initial conditions allowing excess oxygen in the filling process to ensure adequate residual for the test combustion.

A combustion bomb removes a lot of the mechanical complexity associated with RCMs and shock tubes, enabling rapid automated repetitive testing and characterisation of fuels. With the correct auxiliary systems it is also capable to operate over a wide range of conditions, including atmospheric pressures with ignition delays in excess of 10 seconds. However heat transfer is still perceived to be a possible issue.

Evaporation

The physical process of evaporation can have a significant effect on fuel mixing and ignition delay. As the chemical time scales for autoignition become shorter, so the effect of evaporation times become more significant. In the case of the combustion bomb used, the air/fuel mixture was not premixed, thus at certain conditions evaporation timescales may have an effect on ignition delay. Figure 2.1 illustrates that, at the temperatures under consideration the evaporation times are in the order of 30 - 100ms, which should be relatively insignificant in respect of the expected ignition delays.

![Figure 2.1: Rate of Gasoline Droplet Evaporation in a Hot Environment][8]
2.2 General Combustion Kinetics

The combustion of hydrocarbons in air is not a simple oxidation process from reactants to products. There are thousands of intermediate species and reactions the full extent of which are not yet fully understood. The intricate chemistry involved during this process is beyond the scope of this project, however a basic understanding of the dominant features is essential.

The general oxidation reaction for hydrocarbons and oxygen:

\[ C_xH_yO_z + (x + \frac{1}{4}y - \frac{1}{2}z)O_2 \rightarrow xCO_2 + \frac{1}{2}yH_2O \]

The general stoichiometric oxidation reactions can be divided into three principal mechanisms, namely[9]:

- **Initiation - radicals are generated from fuel molecules.**

- **Propagation - the initial radicals formed during initiation react with other compounds in the mixture through straight chain or chain branching mechanisms.**
  - Straight chain - one radical reacts with a stable molecule to form a stable molecule and one other radical.
  - Chain Branching - two radicals are formed for each radical consumed.

- **Termination - radicals combine to form product molecules.**

Oxidation chemistry is dependent on pressure, temperature, and air/fuel ratio in the system. With respect to temperature there are three separate oxidation pathways[9]:

- **A low temperature regime, where peroxo oxidation chemistry occurs.**

- **An intermediate temperature regime, where HO2 and H2O2 chemistry dominates.**

- **A high temperature regime, where pyrolysis and small size radical chemistry occurs.**
2.2 General Combustion Kinetics

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- **Propagation** - the initial radicals formed during initiation react with other compounds in the mixture through straight chain or chain branching mechanisms.
  - Straight chain - one radical reacts with a stable molecule to form a stable molecule and one other radical.
  - Chain Branching - two radicals are formed for each radical consumed.
- **Termination** - radicals combine to form product molecules.

Oxidation chemistry is dependent on pressure, temperature, and air/fuel ratio in the system. With respect to temperature there are three separate oxidation pathways\[9\]:

- A low temperature regime, where peroxy oxidation chemistry occurs.
- An intermediate temperature regime, where \( HO_2 \) and \( H_2O_2 \) chemistry dominates.
- A high temperature regime, where pyrolysis and small size radical chemistry occurs.
2.3 Ignition Delay

Autoignition is caused by runaway chain-branching reactions leading to a highly exothermic reaction. The ignition delay is the time between the air/fuel mixture being introduced to a hot environment and the onset of the runaway exothermic reaction. There is a large amount of data in the literature regarding ignition delay characteristics of various fuels under different conditions. The majority of these investigations have been carried out at high temperature and pressure, using rapid compression machines and shock tubes. A search of the literature yielded little data for ignition delays of liquid fuels at constant volume conditions and atmospheric pressures. Literature data found for atmospheric and sub-atmospheric pressures was generally for gaseous fuels in constant flow reactors.

Figure 2.2 shows a typical ignition delay curve for a two-stage fuel across a range of pressures, the three distinct temperature regions are clearly visible. The logarithm of the ignition delay is plotted against the reciprocal of the initial temperature. The effect of pressure on ignition delay is different across the three temperature regions, but in general an increase in pressure decreases ignition delay.

- In the low temperature region, the effect of pressure on ignition delay is significant but not as remarkable as in the NTC region.
- An increase in pressure reduces the width of the NTC region and shifts it to higher temperatures.
- In the high temperature region, the effect of pressure is very small and the ignition delays tend towards the same value for a specific temperature.

2.3.1 Two-Stage Ignition and the Cool Flame

As has been noted the autoignition of some hydrocarbons is characterised by a two-stage ignition process involving a low temperature cycle followed by a high temperature cycle [5].

The low temperature stage is referred to as the cool flame and is characterised by a pale blue luminosity. As seen in Figure 2.3 the cool flame causes
Figure 2.2: Stoichiometric Constant Volume Ignition Delay Data for n-heptane for Several Pressures (Data Generated from [10])

an appreciable rise in temperature followed by a short period of stability, which is reflected as a plateau on the temperature vs delay plot. The cool flame is followed by a second stage violent explosion that causes a rapid rise in temperature and pressure, this is often referred to as hot flame combustion.

Cool flame is an important and complex ignition phenomenon. Its faint pale blue luminescence, is due to chemiluminescence of electronically excited formaldehyde, and occurs preferentially under fuel rich conditions during degenerate branching reactions in early combustion. [11]

The delays associated with the different regimes are usually defined as; \( \tau_1 \), the delay before the appearance of the cool flame, and \( \tau_2 \), the delay between the appearance of the cool flame and the second stage of combustion [12]. It should be noted that there is no specific chemical process that begins and ends during \( \tau_2 \), it is a convenient term that represents the difference between \( t_2 \) and \( t_1 \). It follows that \( t_1 \) and \( t_2 \) affect the overall ignition delay with varying strength depending on the region under consideration. If one considers Figure 2.2 again, it can be shown that \( t_1 \) has the dominant role in the low temperature region, whereas \( t_2 \) has a far greater effect in the high
2.3. IGNITION DELAY

temperature region. Both the delays play a varying role in determining the overall ignition delay in the intermediate or NTC region.

Figure 2.3: Idealised Two-Stage Ignition Delay for n-heptane at 1 Bar, Phi = 1.0

Figure 2.3 shows a typical two-stage ignition process assumed to have been initiated by a step increase in temperature to $T_i$. One can see the first abrupt temperature rise associated with the cool flame, a period of stability, then the large exponential temperature rise associated with hot flame ignition. The period of stability occurs when the forward and reverse oxidation reactions, of alkyl radicals and oxygen to alkyl peroxy species, are in equilibrium [10]. As the initial temperature of the mixture rises so the cool flame temperature rise decreases. Once $T_i$ is greater than $T_{cf}$ (the temperature after the cool flame) then the two stage ignition phenomenon disappears altogether as seen in the higher temperature trace in Figure 2.3. It also shows $\tau_1(\tau_{u1})$ and $\tau_2(\tau_{u2})$ as they are usually defined in the literature.

2.3.2 Cool Flame Temperature Rise

Figure 2.4 illustrates that the temperature rise due to the cool flame decreases as the initial temperature increases. Once the initial temperatures approach about 950K the cool flame falls away, this leads to an increase in the overall
2.3. IGNITION DELAY

ignition delay. The varying effect of the cool flame is the main contributor to NTC behaviour. The illustrated data was obtained using constant volume simulations at 20 Bar with stoichiometric mixtures of n-heptane [10].

![Diagram of temperature rise over time]

**Figure 2.4:** Cool Flame Temperature Rise for n-heptane at 20 Bar, Phi = 1.0[10]

Figure 2.5 illustrates the magnitude of the cool flame temperature rise based on initial temperature and pressure. It can be seen that as initial pressure decrease the magnitude of the cool flame temperature rise for a specific initial temperature decreases. The highest temperature at which a cool flame occurs also decreases with decreasing initial pressure. This results in a shifting of the NTC region to a lower temperature range as initial pressure is decreased.

**Comment** The experiments performed for this project were carried out within the temperature range where cool flames are experienced, an understanding of the cool flame and its varying effect was essential for the interpretation of the results. Due to the lower initial pressures, the cool flame temperature rise was expected to decrease. The maximum temperature where cool flames occur was also expected to decrease.
2.3. IGNITION DELAY

![Graph showing temperature rise for constant volume n-heptane simulations.](image)

Figure 2.5: Cool Flame Temperature Rise for Constant Volume n-heptane Simulations, Phi = 1.0[10]

**Ignition Scenarios Involving Cool Flames**

Several oxidation phenomena involving cool flames have been observed at low temperatures. Experiments conducted by Luckett et al. [13] show the wide range of ignition scenarios. The experiments were performed on mixtures of iso-butane and oxygen at temperatures from 300-410°C. The results are shown in Figure 2.6 with detailed captions below.

- (a) multiple cool flames
- (b) slow combustion
- (c) rapid single cool flame occurrence
- (d-f) two stage ignition
- (g) multi stage ignition

**Comment** Experiments were conducted over a wide range of temperatures and air/fuel ratios, it is expected that several of these ignition scenarios will occur. It is necessary to be able to detect and distinguish between the different scenarios.
2.3. IGNITION DELAY

![Graph showing different ignition scenarios involving cool flames](image)

Figure 2.6: Different Ignition Scenarios Involving Cool Flames[13]

2.3.3 The Negative Temperature Coefficient Region

The Negative Temperature Coefficient (NTC) region is a region of the ignition delay curve where the ignition delay increases as initial temperature increases. The NTC region is caused by a change in the relative reaction rates of the dominant reactions responsible for autoignition.

“This region represents a transition in the oxidation chemistry from the low temperature to intermediate temperature reaction regime, where the rate of the accelerating or branching mechanism of the low temperature regime begins to subside before that of the intermediate temperature regime becomes important; thus the overall reaction rate decreases” [14].

Figure 2.2 shows how the NTC region occurs over a narrower temperature range at higher pressures, as well as shifting to higher temperatures. As a result of this, a wide NTC region at relatively low temperatures is expected for atmospheric experiments. The NTC region has also been found to be
most prominent at stoichiometric operation, with richer and leaner mixtures exhibiting less NTC behaviour [10].

Non-Ignition in the NTC Region

When Westbrook et al. were performing experiments on isomers of n-heptane in rapid compression machine, they noted that at around 750K no ignition occurred, even though ignition had occurred either side of this temperature[15]. This peculiarity had also been noted in a previous study by Leeds University when testing iso-octane. The non-ignitions were put down to complex heat loss under certain circumstances, specifically when long ignition delays allowed for a great heat loss. The effects could not be reproduced in their computational model even with the inclusion of a distributed heat loss model. However no significant effort was made to fully explain the peculiarities. [15]. The effects are show in Figures 2.7 one can clearly see the greater variability of results in the NTC region as well as non-ignitions, where ignitions are predicted by the computational model.

Figure 2.8 shows results from RCM experiments performed by Griffiths et al [16]. Points of interest are the results for iso-octane (triangles) in Figure 2.8(a), which only autoignites over a very high temperature narrow range thought to be due to high post-compression heat loss. Another obvious anomaly is the erratic results of PRF60 (squares) in the NTC region. Note that the errant ignition delays are similar in magnitude to the maximum iso-octane delays. The results in Figure 2.8(b) are for higher octane components with longer ignition delay. The results are highly erratic throughout the NTC region and do not show the expected smooth curve. The researchers did not provide a suitable explanation for the unexpected behaviour, other than it was possibly apparatus specific. It is certainly plausible that it was related to greater heat loss in the NTC region, causing unreliability in results.

**Comment** There is clearly a significant effect of heat loss on the chemical kinetics in the NTC region which warrants further investigation. It is also clear that as octane number increases the effect is magnified. Heat loss is a feature in any real world situation and there is a definite need for a better understanding of the peculiarities in this region, both from a physical and computational perspective. The non-ignition phenomenon experienced by these researchers turned out to be a major feature of this project.
2.3. IGNITION DELAY

(a) n-heptane (upright triangles) n-Pentane (circles) PRF 60 (squares) iso-octane (downward triangles)

(b) 2,4 Dimethylpentane (upright triangles) neo-Pentane (circles) PRF 80 (squares) 3,3 Dimethylpentane (downward triangles)

Figure 2.8: Experimental Ignition Delays from RCM Data [16]
2.3.4 Effect of air/fuel Ratio on Ignition Delay

It has been demonstrated by Fish et al. [17] that the air/fuel ratio ($\lambda$) has a significant influence on the overall ignition delay [17].

![Diagram showing effect of stoichiometry on ignition delay](image)

Figure 2.9: Effect of Lambda on Ignition Delay[17]

In Figure 2.9 $\tau_1$ represents the ignition delay before the cool flame and $\tau_2$ represents the delay between the appearance of the cool flame and the second stage of combustion as defined in Figure 2.3. The overall ignition delay is thus $\tau_1 + \tau_2$.

It must also be noted that the definition of $\lambda$ used by Fish is not in line with current conventions. He defines $\lambda$ as “the ratio of the amount of fuel actually present to that required for stoichiometric reaction”[17]. This implies that $\lambda < 1$ represents a lean mixture whereas by the modern convention (see Appendix D.3) this would be a rich mixture. In this report the equivalence ratio (Phi or $\phi$) is used to indicate the ratio of air/fuel ratios to stoichiometric air/fuel ratio , where $\phi = \lambda_{fish}$.

The data shows that $\lambda$ has negligible effect on $\tau_1$, the delay associated
with the cool flame reactions, but has a significant effect on $\tau_2$, the delay associated with the reactions after the cool flame.

It has also been shown that although ignition delay decreases as equivalence ratio increases, once mixtures exceed $\phi = 1.25$ further reduction in ignition delay is very limited [18].

2.4 Chemical Kinetic Modeling

The continual improvement of computing technology has enabled the chemical kinetics of thousands of complex chemical reactions and species to be numerically simulated. The models are usually constructed from data from rapid sampling and gas chromatography of products at various stages of combustion. Critical reactants, intermediates and products are identified and representative reactions derived until a suitable model is constructed. The results of the models are validated by comparing them with exhaustive experiments where parameters such as equivalence ratio, temperature and pressure are varied. The reactions and species within the model are adjusted until a reliable fit is obtainable across the range of parameters [11]

2.4.1 Limitations

The accuracy and realism of detailed chemical kinetic mechanisms are always improving through ongoing experimentation and refinement. However large differences between experimental and computed data are still common, especially in the low and intermediate temperature region. Figure 2.10 shows the discrepancies between several different models and experimental data in predicting the autoignition limits of a propane-air mixture (up to 150°C variation).

"Hydrocarbons are a family of compounds for which reliable and detailed chemical kinetic models exist [19]. However, most of these mechanisms are only valid for high temperature combustion (1000K), while kinetic data and mechanisms for the low temperature region are still scarce [20]." [21]
Figure 2.10: Comparison of Autoignition Threshold for Propane as Calculated by Various Research Models [21]

**Comment** A detailed chemical kinetic model was used to provide theoretical data for comparison with experimental results. The limitations of chemical kinetic models indicate that caution should be taken when considering simulated results. The chemical kinetic simulations may be inaccurate, especially in certain temperature and pressure regions.
2.5 Autoignition Temperature

The Autoignition Temperature (AIT) is defined by ASTM E-659 as:

"the lowest temperature at which the substance will produce hot-flame ignition in air at atmospheric pressure without the aid of an external energy source such as a spark or flame. It is the lowest temperature to which a combustible mixture must be raised, so that the rate of heat evolved by the exothermic oxidation reaction will over-balance the rate at which heat is lost to the surroundings" [22].

The AIT is used to determine the fire risks and hazards of operating at elevated temperatures with combustible materials in industrial processes. Although the determination of AIT was not a primary aim of this project, it holds relevance in regards to expected ignition delays and propensity to autoignite.

There are several methods for determining the AIT of a substance and values quoted in the literature can vary by up to the order of 100°C, depending on the apparatus and methods used [23]. Some typical values for the AIT of fuels of interest to the present investigation are shown in Table 2.1. Note the large variation in the recorded AIT for both ethanol and toluene. The ASTM method determines the AIT by inserting a small test sample into a heated flask containing air. The mixture is observed in a dark room until a flame or sharp rise in temperature is observed. The AIT is taken as the lowest flask temperature where this occurs. As would be expected from a typical ignition delay relationship that the AIT is lowered by an increase in pressure [22].

Differences in AIT could be caused by many factors such as variations in air/fuel ratio, ambient conditions, the rather subjective nature of determining an autoignition event and even material of the test vessel [6].

The question of whether AIT is a reliable safety specification has been raised by several researchers, specifically the exclusion of cool flames from the definition is seen as a potential hazard. Cool flames can occur hundreds of degrees below a substance’s AIT.

"It is, for example, widely believed that a fuel-rich, flammable
mixture kept below its AIT in process apparatus cannot ignite and therefore cannot explode. Unfortunately this is not always true, since phenomena like cool flames may lead to unwanted side reactions and, in the worst case, to explosion."[9]

Table 2.1: Autoignition Temperature in °C from the literature

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>n-heptane</td>
<td>220</td>
<td>223</td>
<td>222</td>
</tr>
<tr>
<td>iso-octane</td>
<td>410</td>
<td>417</td>
<td></td>
</tr>
<tr>
<td>Ethanol</td>
<td>400</td>
<td></td>
<td>363</td>
</tr>
<tr>
<td>Toluene</td>
<td>535</td>
<td>422</td>
<td>480</td>
</tr>
</tbody>
</table>

**Comment** Although several disclaimers about variability are included in the ASTM method for AIT the discrepancies in the literature are too large to accept AIT as a reliable measure. If one recalls Figure 2.8(b) for 3,3 dimethylpentane, it is plausible that one could miss the lowest AIT when crossing the gap in the NTC region. This will be described more fully in the context of the experiments described in this thesis.
2.6 Octane

The most commonly used octane rating is the Research Octane Number (RON). It is measured in a Cooperative Fuels Research (CFR) engine at conditions specified in ASTM D2699. The method determines the value of the octane number by comparing the test fuel to a range of primary reference fuels. A fuel’s octane number is a measure of its resistance to autoignition. The octane rating of a fuel is generally a good indication of where it will appear relative to other fuels on an ignition delay plot. It is also a good indication of where a commercial fuel will appear relative to the reference fuels.

2.6.1 Effect of Octane Number on Ignition Delay

It is common cause that at a specific temperature and pressure, an increase in octane number will also increase ignition delay. It can be seen from Figure 2.11(a) that there is indeed an increase in ignition delay with an increase in octane number but that this relationship is not linear. In the ASTM method for determining octane number, the ignition delay is kept virtually constant and the pressure and temperature are varied by changing the compression ratio. One can see that the compression ratio must also be varied by a similar non-linear relationship (see Figure 2.11(b)). Indicating the interaction between octane number and ignition delay.

2.6.2 PRF Blends

Primary Reference Fuel blends (PRF) are made by mixing n-heptane and iso-octane on a liquid volume percentage basis in order to attain the required octane rating. eg PRF 75 has a RON of 75 and consists of 75% iso-octane and 25% n-heptane by volume. The boiling points of n-heptane and iso-octane are very similar (372K after rounding) and thus the boiling point of any PRF is essentially constant.

Comment An understanding of autoignition characteristics is essential for investigation of fuel performance and octane. One of the goals of the project is to be able to provide autoignition data for complex fuels, thus enabling further studies of the relationships between RON and autoignition per-
formance. The relative positions on an ignition delay map of fuels with different RONS were also considered in Chapter 6.5.

(a) Ignition Delay vs RON - Specifically the PRF Curve[5]  
(b) ASTM Compression Ratios for RON Test[27]

Figure 2.11: Relationship Between Octane and Ignition Delay
Chapter 3

Theory

The primary aim of the project was to investigate the autoignition characteristics of fuels at atmospheric pressure and ascertain whether high pressure trends were still applicable. Owing to the lack of reliable literature data for the pressure and temperature regions considered, detailed chemical kinetic modeling was used to provide a baseline for comparison of results. Details of the fuels selected and mechanisms used are described below.

3.1 Classes of Fuels

The following four single component fuels were selected for investigation based on their autoignition performance, relevance to commercial fuels and the availability of chemical kinetic mechanisms:

- n-heptane - Paraffinic fuel exhibiting NTC behaviour with high propensity for autoignition.
- iso-octane - Paraffinic fuel exhibiting NTC behaviour with high resistance to autoignition.
- Ethanol - Alcohol fuel exhibiting single stage behaviour with high temperature autoignition similar to n-heptane and iso-octane.
- Toluene - Aromatic fuel exhibiting single stage behaviour with long ignition delays.
Table 3.1: Properties of Selected Reference Fuels

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Boiling Point °C</th>
<th>RON</th>
<th>MON</th>
<th>Latent Heat of Evaporation kJ/kg [28]</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-heptane</td>
<td>100</td>
<td>0</td>
<td>0</td>
<td>365.7</td>
</tr>
<tr>
<td>iso-octane</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>307.5</td>
</tr>
<tr>
<td>Toluene</td>
<td>125</td>
<td>120</td>
<td>105</td>
<td>412.3</td>
</tr>
<tr>
<td>Ethanol</td>
<td>77.8</td>
<td>108.6</td>
<td>89.7</td>
<td>1103</td>
</tr>
</tbody>
</table>

3.2 Chemkin

Detailed chemical kinetic simulations were performed using Chemkin and the PRF mechanism developed by Westbrook et al. [1, 2]. This mechanism consists of 1034 species in 4238 reactions and has been extensively validated against jet-stirred reactors, flow reactors, shock tubes and rapid compression machines.

The physical model that was specified for the simulations was that of a constant volume closed adiabatic system, containing the required fuel and air concentrations in a perfectly mixed homogeneous system. Although this physical model represented a situation that was more idealised in comparison to the conditions within the bomb, it allowed separation of the chemical and physical effects on ignition delay. These simulations provided the theoretical data for n-heptane, iso-octane and ethanol. Further details of the mechanism are available in Appendix D.

Results for n-heptane and iso-octane at different equivalence ratios are shown in Figure 3.1. The results show, as expected, that in general ignition delay decreases as equivalence ratio increases. The ignition delay curves for n-heptane demonstrate the relatively small effect of equivalence ratio on the low temperature region, a greater effect is clearly evident in the NTC and high temperature region where \( \tau_2 \) has a greater effect on overall ignition delay as discussed earlier in Chapter 2.3.4. The results for iso-octane show similar effects, however the lower temperatures are not low enough to extend fully past the start of the NTC region.

No direct simulations of toluene were performed owing to a lack of chemical mechanism data, but previous research at high pressures using the Djuristic mechanism [29] for toluene provided an indication of the expected relative position of toluene as shown in Figure 3.2.
3.2. CHEMKIN

Figure 3.1: Results for Chemical Kinetic Simulations of n-heptane and iso-octane with Varying Equivalence Ratio at 1 Bar

Figure 3.2: Chemical Kinetic Predictions for the Four Reference Fuels at 5 Bar and \( \Phi = 1.0 \)[30]
3.2. CHEMKIN

Figure 3.3: Pressure Traces from Chemical Kinetic Simulations of n-heptane at 700K, 1 Bar and Phi = 1.5 with Varying Heat Transfer

3.2.1 Heat Transfer

In order to gauge the effect of heat loss on ignition delay during the cool flame, non-adiabatic simulations were also performed using the simple heat loss model incorporated into Chemkin. The model incorporates convective heat loss at the wall of the reactor in the form:

\[ Q_{loss} = h \cdot A \cdot (T - T_{wall}) \]

Where \( h \) represents a global convective heat transfer coefficient. Values were selected by comparison with preliminary experimental results in order to approximately match the pressure traces. \( A \) represents the internal surface area of the reactor. \( T_{wall} \) was kept constant at the initial temperature of the reactor.

Figure 3.3 shows three simulated traces with varying degrees of heat loss for n-heptane at 700K. The results demonstrate how even a small amount of heat loss can have a large effect on the simulated ignition delay and how a
Figure 3.4: Results for Chemical Kinetic Simulations at 1 Bar Showing the Effect of Heat Transfer

further marginal increase in heat transfer can completely extinguish the hot flame ignition. [15].

Figure 3.4 shows the effects of adding slight heat transfer to a range of temperatures for n-heptane, iso-octane and Ethanol. The heat transfer coefficient was kept constant for all simulations shown. The results for n-heptane show a significant increase in the ignition delay throughout the NTC region, the area expected to be most affected by heat loss. They also show a point at 725K where the heat transfer was sufficient to extinguish hot flame ignition entirely. The results for iso-octane show the effect of heat loss increasing as temperature decreases towards the NTC region, with no ignition occurring below 750K. These results are qualitatively similar to the experimental peculiarities discussed in Chapter 2.3.3 and reinforce the hypothesis that heat loss has a significant effect on ignition delay in the NTC region. Ethanol exhibits single stage behaviour and thus exhibits no NTC behaviour, this results in a relatively small effect of heat loss on ignition delay.
3.2.2 Theoretical Peak Pressure

The pressure vs time information was extracted from the Chemkin output files providing an adiabatic peak pressure after combustion. This value can be compared with experimental results to quantify the extent of heat loss, illustrated by the pressure difference, as will be discussed in Chapter 6.3.3.
Chapter 4

Experimental Apparatus

The following chapter is a summary of the experimental apparatus used to perform the experiments, for a detailed explanation refer to the relevant Appendix. The primary apparatus used for the experiments was a modified version of the IQT™ combustion bomb. The IQT was originally designed to perform ASTM 6890-08 [31] under specified test conditions. The device was modified extensively to enable a much more flexible testing regime illustrated in Table 4.1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Original</th>
<th>New</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Temperature (K)</td>
<td>≈ 820</td>
<td>300 - 950</td>
</tr>
<tr>
<td>Initial Pressure (Bar Gauge)</td>
<td>21.34</td>
<td>0 - 21</td>
</tr>
<tr>
<td>Equivalence Ratio</td>
<td>≈ 0.7</td>
<td>0.2 - 4</td>
</tr>
</tbody>
</table>

In addition the tolerance of the apparatus to different classes of fuels was greatly improved. The modified system contained no moving parts except for the needle of the injector and is thus completely insensitive to fuel lubricity issues. This enabled the use of a wide range of liquid fuels including:

- Alcohols
- Aromatics
- Primary Reference Fuels (PRFs)
- Petrols
4.1 Combustion Chamber

A schematic diagram of the original combustion chamber is shown in Figure 4.1, the combustion chamber was essentially left unaltered except for external modifications to the injector housing and sealing mechanism on the left-hand side. The chamber had a fixed volume of 213cm$^3$ and was preheated by 9 circumferential cartridge heaters with a total heating capacity of 3150W. The chamber was also cooled at both ends to protect the fuel injector and combustion pressure sensor. Thermocouples are situated throughout the chamber for monitoring certain temperatures. The chamber surface thermocouple was used to control the set point temperature because it was embedded in the body of the bomb and not subject to lag from air heating. The chamber was filled, purged and sealed by two pneumatically actuated high temperature valves - Air In and Exhaust Out. For a more detailed explanation please see Appendix A.

4.2 Fuel System

The standard IQT$^\text{TM}$ used a pneumatically driven, fixed volume, single shot injection pump and a pintle type diesel injector. The system delivered a single fixed volume of fuel to the combustion bomb that resulted in a globally lean mixture at standard test conditions. The fuel system was extensively modified to enable testing at a wide range of equivalence ratios at different set points.

A schematic diagram of the new fuel system is shown in Figure 4.2. The modified fuel system used a solenoid-actuated injector from a Gasoline Direct Injection (GDI) engine. The system consisted of a high pressure section responsible for fuel injection into the combustion chamber and a low pressure section used for refilling. The high fuel pressure was achieved by using laboratory nitrogen gas at 200 Bar, which was regulated down to 2 - 110 Bar to pressurise the fuel tank and injection system. Once the fuel pressure was
4.2. FUEL SYSTEM

Figure 4.1: Schematic Diagram of the Combustion Chamber [3]

set, the amount of fuel injected could be controlled by varying the injection duration on the control software.

The control of the amount of fuel delivered was open loop and thus extensive calibration of the fuel system and injector was performed. The hazards of working with high pressure combustible liquids were considered and several safety features were installed on the system to minimise the relevant risks. Further details of the fuel system and its calibration are available in Appendix B, safety considerations are detailed in Appendix E.
Figure 4.2: Schematic Diagram Showing Primary Fuel System Components
4.3 Electrical System and Software

All hardware and software upstream of the sensors and actuators installed on the IQT™ was replaced for two reasons:

1. To allow complete control over test conditions
2. To leave the original control system intact, for possible return to service.

A schematic diagram of the new electrical control system is shown in Figure 4.3. The central component of the system is the National Instruments CompactRIO System. The CompactRIO system provided a robust interface between the software and the actuators and sensors of the apparatus as well as the platform for the software.

All analogue and digital connections were routed through the relevant IO Module where they underwent signal conditioning and conversion. This information was then passed on to the FPGA (Field Programmable Gate Array) where basic triggering and analysis functions were performed. The FPGA runs at 40MHz an adequate speed due to the customisation of gate configuration. The next layer is the real-time controller where higher level functions that require more memory are performed, without sacrificing the time-determinism of the results. Lastly information is relayed to the PC where the user interface is situated. Data flowed in all directions between the layers, however an important feature was that the real-time controller could run independently of the PC, ensuring safe operation in the event of a PC failure. Further details of the control system can be found in Appendix C

4.3.1 LabVIEW

National Instruments LabVIEW (Laboratory Virtual Instrumentation Engineering Workbench) software is run on all 3 layers of the control system. LabVIEW is a graphical based programming language that is specifically aimed at instrumentation and control. Further details of the software design and implementation can be found in Appendix C.3

In order to allow for an entirely automated fuel characterisation, the software was capable of the following:
4.3. ELECTRICAL SYSTEM AND SOFTWARE

- Accurate control of the combustion chamber temperature.
- Calculation of required fuel quantity based on initial conditions and the required injection duration as a result.
- Reliable, time-definite recording of combustion pressure traces.
- Automatic purging and filling of the combustion chamber.
- Processing and recording of all relevant data.
- Monitoring of certain parameters for safety purposes.
- Complete flexibility of test sequencing.
Figure 4.3: Schematic Diagram of I/O and Control System
Chapter 5

Experimental Method and Certainty

As is the case with all physical experiments, there were several factors that could affect the accuracy and reliability of the results. The more significant factors are discussed and addressed in this chapter.

5.1 Temperature Control and Stability

Stable control of the combustion chamber temperature was critical. Small variations in temperature can have a large effect on ignition delay, specifically at lower temperatures. Temperature control was performed in LabVIEW using PID (Proportional Integral Derivative) control. PID constants were obtained using the Ziegler-Nichols tuning method. Due to the wide range of temperatures used it was necessary to have a range of constants for different temperatures for details see Appendix C.3.3. The temperature was only deemed to be stable, and tests performed, after ten minutes of no variations greater than 0.5%.

Table 5.1 illustrates the stability of the control and combustion chamber (Air Back) temperature. Temperature values were recorded over 100 tests, the tests were performed at a set point temperature of 300°C.
5.2. IGNITION DELAY MEASUREMENT

Table 5.1: Temperature Stability of Combustion Chamber

<table>
<thead>
<tr>
<th>Thermocouple</th>
<th>Control</th>
<th>Air Back</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of samples</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Average Temperature (°C)</td>
<td>299.9</td>
<td>314.3</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>0.07</td>
<td>0.24</td>
</tr>
</tbody>
</table>

5.1.1 Combustion Chamber Temperature Profile

Previous research has shown that the combustion chamber of the IQT\textsuperscript{TM} does not display uniform temperature over its length. Computational Fluid Dynamic (CFD) modeling performed by Metcalf et al [32] shown in Figure 5.1 shows the extent of this temperature gradient. This temperature profile was also clearly evident from the difference in temperatures recorded between the front and back thermocouples in the chamber. The back thermocouple always showed a higher temperature, this temperature difference increases with increase in test temperature as illustrated in Figure 5.2.

Because of the NTC aspect of most hydrocarbon fuels, it was not a given that autoignition would occur at the hottest temperature in the combustion chamber. Within the NTC region, the ignition delay increases as temperature increases. This could result in a colder region of air/fuel mixture autoigniting before any other hotter regions, the resulting localised temperature and pressure increase could be expected to cause autoignition in the rest of the mixture. This would result in a shorter ignition delay than would normally be expected at the specific temperature. Therefore when plotting ignition delays the control thermocouple temperature was used as the test point as this was the most stable temperature and its value was in between the front and back thermocouples.

5.2 Ignition Delay Measurement

Possibly the most critical aspect of an ignition delay test is the accurate measurement of the start of ignition. There are three events that need to be identified namely: the start of injection, the hot flame ignition (autoignition) and in some cases the cool flame temperature rise. There are no clear cut definitions for any of these events and one can only be consistent in the measurement to minimise error and subjectiveness.
Figure 5.1: CFD Model of Combustion Chamber Heating[32]

Figure 5.2: Temperature Difference Between Front and Back Thermocouples in the Combustion Chamber
Also with consideration of Figure 2.6, there were thus five different scenarios for a test that needed to be identified and accurately recorded:

- No discernible combustion
- Cool flame only
- Hot flame only
- Cool flame followed by a long delay before the hot flame
- Cool flame followed shortly by hot flame

Figure 5.3 shows three common ignition scenarios in the three different temperature regions. Figure 5.3(a) shows autoignition in the low temperature region, where the cool flame temperature rise was large and causes hot flame ignition immediately after the cool flame. The events happened so close to one another than it was not possible to differentiate between the two. Figure 5.3(b) shows autoignition in the high temperature region, where no cool flame occurs and only a rapid pressure rise due to hot flame ignition is visible. Figure 5.3(c) shows an experiment where hot flame ignition did not occur and only the cool flame was detected. Where no discernible combustion occurred, it was generally identifiable by a lack of pressure rise, in such cases the only rise recorded was due to mild heat release or drift from the pressure transducer. In cases where a cool flame only occurred, it was identifiable by the significantly lower maximum pressure ($< 1\text{Bar}$).

The hot flame ignition event was taken as the point of maximum pressure rise rate, i.e. the maximum of the first derivative. The ignition delay was logged as the time between the start of injection and the hot flame ignition. Although this is a simplification of the ignition delay, the pressure rise rates are sufficiently high that the error is insignificant over the long time scales. An experimental pressure trace and the accompanying first derivative is shown in Figure 5.4 to demonstrate ignition delay measurement.

Figure 5.4 also shows a cool flame, the identification of the cool flame was significantly more challenging to locate. It can occur very close to the hot flame as well as being a slow pressure rise over a relatively long time scale. Post-processing using the second derivative was performed to identify the cool flame.
5.2. IGNITION DELAY MEASUREMENT

(a) Low Temperature Region 530K and Phi = 1.5

(b) High Temperature Region 870K and Phi = 1.5

(c) NTC Region 670K and Phi = 1.0

Figure 5.3: Experimental Pressure Traces for n-heptane at 1 Bar Showing Different Ignition Scenarios, t0 = Start of Injection
By comparison, the start of injection was more easily determined. The start of injection was measured by monitoring the voltage across a shunt resistor connected in series with the injector coil. The voltage was sampled at the same rate as the combustion pressure transducer i.e. generally 10kHz (one sample every 100\mu s). The start of injection was taken from the rising edge of this voltage signal, effectively the energising of the solenoid and thus the start of needle lift. Although this method only triggers off the electrical signal and not the physical response of the needle, the time difference between the two would be insignificant over the time scales under consideration. This error would also be effectively constant across every test.

Both the combustion pressure signal and injection signal were sampled continuously by the FPGA, they were sampled within the same timed loop and thus perfectly synchronised. The data however, was only sent to the real time controller and the PC after an injection had occurred.
5.3 Repeatability

The results from the apparatus were found to have good repeatability. As part of the commissioning experiments, a series of 100 tests were run on n-heptane at 300°C, the results are shown in Table 5.2. For all subsequent testing, each set point was repeated five times and averaged.

<table>
<thead>
<tr>
<th>Number of samples</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average Ignition Delay (ms)</td>
<td>1230</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>26</td>
</tr>
</tbody>
</table>

Furthermore, two identical tests were carried out several months apart to verify the repeatability over a period of time. From Figure 5.5 it can be seen that the second set of tests was marginally higher than the first, but that the fit between the two sets is very good.

![Graph showing ignition delay vs 1000K/T](image)

**Figure 5.5:** Results for Repeatability Tests Using n-heptane
5.4 Other Factors Affecting the Experiments

5.4.1 Residual Exhaust Gas

Any exhaust gases left in the combustion chamber would affect the next test. The low pressure conditions of the tests compounded the issue by reducing the pressure difference across the exhaust valve. Therefore following a combustion event the chamber was flushed with pressurised fresh air. Experiments were performed to verify that the combustion chamber was fully purged. Results for these experiments are shown in Table 5.3.

<table>
<thead>
<tr>
<th>Number of Purges</th>
<th>Ignition Delay (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>No Combustion</td>
</tr>
<tr>
<td>1</td>
<td>1.25</td>
</tr>
<tr>
<td>2</td>
<td>1.26</td>
</tr>
<tr>
<td>3</td>
<td>1.29</td>
</tr>
<tr>
<td>4</td>
<td>1.29</td>
</tr>
<tr>
<td>5</td>
<td>1.26</td>
</tr>
</tbody>
</table>

5.4.2 Drift

In order to obtain the most faithful pressure records over significant time scales, it was necessary to use the "long" function of the charge amplifier for the combustion pressure sensor. In this mode, drift of the output signal is unavoidable, drift is caused by the flow of a small fault current which can be exacerbated by poor insulation resistance. In practice this drift is small typically - 0.03pC/s or 0.002bar/s based on the sensitivity of the sensor [33]. The actual drift recorded was in the order of 0.005bar/s which although is higher than expected, is still relatively small even over a typical 30s time scale (TotalDrift = 0.15Bar). The effect of drift on measurements was minimised by utilising the remote control function of the charge amplifier to reset (zero) the output signal at the beginning of each test, just prior to injection.
5.4.3 Synthetic Air

The use of bottled air purchased from a laboratory gas supplier increased the reliability of the experimental results. As opposed to using ambient air, it reduced any possible effects of humidity and environmental hydrocarbons.

Air Specifications:

- Oxygen Concentration: $20.9 \pm 1.0\%$ by volume
- Hydrocarbon Concentration: $< 0.003\%$ by volume
- Water Concentration: $< 0.025\%$ by volume

5.4.4 Effect of Fuel Temperature

The fuel temperature for the experiments was assumed to be the same as the nozzle tip temperature which was recorded. The coolant flow through the injector housing was manually controlled. Therefore the nozzle tip temperature was not actively controlled, and was affected by the combustion chamber temperature. Theoretically the fuel temperature could have a slight effect on the air/fuel ratio by affecting the density of the fuel and also an effect on the evaporation time which could in turn affect ignition delay.

The effect of fuel temperature on ignition delay was therefore investigated. Tests were performed at two combustion chamber temperatures and the flow rate of coolant, and thus the nozzle tip temperature, was adjusted to vary the tip temperature between a high and low extreme. The results are shown in Table 5.4 and it is clear that for even a large change in fuel temperature, there is minimal change in ignition delay. Each set point is an average of five tests at that point.

<table>
<thead>
<tr>
<th>Set point °C</th>
<th>Fuel Temperature °C</th>
<th>Average Ignition Delay (ms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>35.1</td>
<td>1222.4</td>
</tr>
<tr>
<td>300</td>
<td>84.3</td>
<td>1218.0</td>
</tr>
<tr>
<td>600</td>
<td>47.6</td>
<td>319.5</td>
</tr>
<tr>
<td>600</td>
<td>89.8</td>
<td>326.7</td>
</tr>
</tbody>
</table>

Table 5.4: Effect of Fuel Temperature on Ignition Delay
5.4.5 Noise and Calibration

In all cases, shielded and earthed cables were used to reduce the amount of electrical noise from the sensors. Gas pressure and temperature signals were further averaged to provide a stable reading. All sensors were calibrated using the appropriate laboratory equipment.
Chapter 6

Discussion of Results

The following chapter presents the most significant and relevant results from the many tests conducted. Unless otherwise stated all experimental results are for constant volume (CV) situations with atmospheric initial pressure (1 Bar).

6.1 Equivalence Ratio Effects

Figure 6.1 shows a comparison between two full range tests of n-heptane at $\phi = 1.0$ and $\phi = 1.5$. The curves show the generally expected trend that richer mixtures have shorter ignition delays. However the most striking feature is the amount of failed ignition events in the NTC region for $\phi = 1.0$.

As explained in Chapter 2.3.3 other researchers have noted similar regions of non-ignition for isomers of n-heptane and iso-octane specifically in the NTC region at temperatures around 750K. The research in question was conducted using an RCM, and it was speculated that these non-ignitions were caused by the influence of heat loss and its effect on the very sensitive chemical kinetics in the NTC region, this matter is discussed in more detail later in this chapter. The unreliability of stoichiometric mixtures to autoignite in the NTC region is the reason for the majority of the remaining results being presented for rich mixtures with $\phi = 1.5$.

The effect of equivalence ratio on ignition delay was investigated at three temperature points and the results are shown in Figure 6.2. The points
6.1. EQUIVALENCE RATIO EFFECTS

Figure 6.1: Improved Reliability with Richer Mixtures - n-heptane Experimental Results for Phi = 1.0 and Phi = 1.5

Figure 6.2: Equivalence Ratio Effects - n-heptane in the 3 Temperature Regimes
were selected to fall within the low temperature, high temperature and NTC region to gauge the relative effects. The first significant finding was that lean operation was only possible in the high temperature regime. This is most likely due to a heat loss effect.

The data generally agrees with the literature presented in Chapter 2.3.4 in that equivalence ratio has a minimal effect in the low temperature and NTC regions, with an inverse relationship in the high temperature region. It must be noted that the majority of equivalence ratio effects in the literature were measured below $\phi = 1.25$ [18] therefore the lack of reliable lean experimental data prevents an illustration of the full effect. The straight lines support the approximate underlying relationship where $\tau \propto \phi^\beta$.

6.2 Fuel Pressure Effects

Figure 6.3 shows the effect of altering the fuel injection pressure on the ignition delay. These experiments were carried out using n-heptane at high temperatures, to avoid any inconsistencies in the NTC region. A higher fuel pressure will result in a shorter injection pulse, and would be expected to form a more finely atomised spray with improved evaporation and mixing. Thus one would reasonably expect an increase in fuel pressure to shorten the ignition delay, but the experimental results show the opposite trend. The ignition delays at higher fuel pressures were found to be $\approx 20\%$ greater than those at low fuel pressure.

Analysis of the pressure traces and specifically the pressure drop due to evaporation provides a possible explanation for the unexpected results. The evaporative pressure drop at a fuel pressure of 10 Bar was $\approx 50\%$ less than the drop at 100 Bar. From the ideal gas law it is clear that the pressure drop is directly related to the temperature drop of the air mixture. At lower pressures the fuel droplet size will be larger and more fuel is likely to hit the walls directly. This will result in the energy required for evaporation coming from the walls rather than the air in the combustion chamber. At higher pressures more of the energy for evaporation is extracted from the combustion chamber air, resulting in a greater temperature drop. The magnitude of this difference in the initial temperature could theoretically account for the difference in ignition delay.
6.3. EXPERIMENTAL AND THEORETICAL COMPARISONS OF PRFS

Figure 6.3: Fuel Injection Pressure Effects on Ignition Delay of n-heptane

6.3 Experimental and Theoretical Comparisons of PRFs

Figure 6.4 shows the full range results for n-heptane and iso-octane and their corresponding Chemkin simulations. The simulations were conducted for both fuels including and excluding heat loss. It is clear that there are several inconsistencies between the theoretical and experimental data. These inconsistencies were investigated at length and can be suitably explained by several physical factors.

- Heat loss during combustion.
- The temperature gradient within the combustion chamber.
- Peak combustion pressures.
6.3.1 Heat Loss Effects

For a two-stage ignition, the chemical reaction associated with the ultimate hot exothermic reaction is significantly accelerated by the temperature increase that is associated with the initial cool flame phenomenon. After the cool flame reaction, the temperature of the gas mixture rises significantly above the temperature of the chamber walls. If the cool flame was not quickly followed by a hot flame autoignition, heat would be rapidly lost to the chamber walls. Under certain circumstances the heat loss is sufficient to disable hot ignition completely. The time delay between the cool flame and second stage ignition increases as equivalence ratio decreases, therefore allowing more time for energy loss to the chamber walls. Thus leaner mixtures are more affected by heat loss.

Figure 6.5 shows a comparison between an experimental pressure trace and a Chemkin simulation with heat transfer. The heat transfer coefficient was chosen to match the ignition delay. It was found that the cool flame delays did not correlate well and this was most likely due to the evaporation and mixing of the fuel inside the combustion chamber. Evaporation time scales at this temperature would be of the order of 50ms, which explains the majority of the discrepancy. It must also be noted that the heat loss model in Chemkin is a simplified version of the real situation and has been shown to be an oversimplification in heat loss modeling previously studied[15].

The Chemkin simulations demonstrated that in cases of non-ignition, where only a cool flame was observed, products such as $H_2O$ continued to be formed. This indicates that, after the cool flame fuel is consumed continuously, in an effort to maintain the cool flame equilibrium temperature. Richer mixtures are less susceptible to extinction because they have excess fuel to feed the energy loss and because there is a shorter delay between cool flame and hot flame for richer mixtures. If there was sufficient fuel to survive until the hot-flame ignition occurred then it is presumed that autoignition would occur, if not the temperature falls back to the initial temperature.

In the case of the iso-octane experiments, as the temperature was reduced towards the NTC region, ignition ceased to occur. The point of extinction of ignition corresponded well with the numerical predictions. The lowest AIT in the literature for iso-octane is 410 °C which corresponds to 1.46 on the 1000K/T scale and corresponds well with the transition into the NTC region. The adiabatic simulations showed ignition occurring well below this temperature right through the NTC region. Therefore as heat loss effects are
amplified in the NTC region, it is unlikely that the idealised adiabatic curve could be reproduced in reality.

Figure 6.4: PRF Fuels and Corresponding Chemkin Simulations - CV, 1 Bar
Phi = 1.5 at 1 Bar

6.3.2 Temperature Gradient

The suppression of the gradient in the NTC region for n-heptane, shown in Figure 6.4, is believed to be partially due to the temperature gradient within the combustion chamber. The negative dependence of ignition delay on temperature in this region means that colder spots in the combustion chamber could in fact be triggering autoignition earlier than it would normally occur at the set point temperature. This would have the effect of producing an overall ignition delay vs temperature profile that had a flattened NTC region as was discussed in Chapter 5.1.1. These cool regions will also exacerbate the heat loss discussed above.
Figure 6.5: Comparison of Pressure Traces for n-heptane at 700K - Phi = 1.5

6.3.3 Theoretical Peak Pressure

The difference between the theoretical peak pressure and experimental peak is a good indication of the overall amount of heat loss in the system. Assuming that there are minimal gas leaks, the only causes for a lower combustion pressure are heat loss and incomplete combustion. Table 6.1 shows the differences between the theoretical peak pressures after adiabatic combustion calculated during Chemkin simulations and the experimental peaks extracted from pressure traces. Once again data points were selected in the low temperature, NTC and high temperature regions to gauge the relative effects. It is clear that there is a more significant pressure loss at lower temperatures and in the NTC region than at higher temperatures, most likely due to the longer ignition delay and thus the extended time for heat loss.
6.4.1 Ethanol

Figure 6.7 shows experimental and simulated results for pure ethanol. It is interesting to note that even with a so-called single stage fuel such as ethanol, where there would not be a cool flame and the associated temperature rise, heat loss still increases the ignition delay in simulations. When heat transfer was included in the ethanol simulations ignition ceased to occur at 700K and below as illustrated in Figure 6.7. Figure 6.8 shows detailed results of the Chemkin output files with the inclusion heat transfer of species concentration. Figure 6.8(a) shows a typical single stage autoignition, the mixture experiences a long period of minimal activity, followed by a very slight temperature rise, followed by a rapid temperature increase and consumption of fuel. Figure 6.8(b) shows a similar situation, yet the amount of heat lost during the slight initial temperature rise is just enough to prevent autoignition. The fuel is slowly oxidised as heat is lost to the walls.

After much investigation it was still unclear why ethanol exhibited shorter ignition delays than predicted by Chemkin and appeared lower on the ignition delay map relative to the other reference fuels than expected.

Figure 6.7: Ethanol - Comparison of Experimental and Simulated Results - Phi = 1.5


### Table 6.1: Difference in Peak Pressures Showing Heat Loss

<table>
<thead>
<tr>
<th>Ti  (K)</th>
<th>1000K/T</th>
<th>Adiabatic</th>
<th>Experimental</th>
<th>ΔP</th>
<th>ΔP%</th>
</tr>
</thead>
<tbody>
<tr>
<td>575</td>
<td>1.74</td>
<td>5.4</td>
<td>4.4</td>
<td>1.0</td>
<td>18.5%</td>
</tr>
<tr>
<td>675</td>
<td>1.48</td>
<td>4.7</td>
<td>3.8</td>
<td>0.9</td>
<td>19.1%</td>
</tr>
<tr>
<td>900</td>
<td>1.11</td>
<td>3.7</td>
<td>3.2</td>
<td>0.5</td>
<td>13.5%</td>
</tr>
</tbody>
</table>

### 6.4 Reference Fuels

Experiments were conducted with the four reference fuels at stoichiometric and rich (ϕ = 1.5) conditions. Figure 6.6 shows the experimental results, there was a good qualitative agreement with Figure 3.2, the only exception being Ethanol, which has shorter ignition delays than expected.

![Figure 6.6: Experimental Results for the 4 Reference Fuels - Phi = 1.5 Showing Relative Pressures](image)

Figure 6.6: Experimental Results for the 4 Reference Fuels - Phi = 1.5 Showing Relative Pressures
6.4.1 Ethanol

Figure 6.7 shows experimental and simulated results for pure ethanol. It is interesting to note that even with a so called single stage fuel such as ethanol, where there would not be a cool flame and the associated temperature rise, heat loss still increases the ignition delay in simulations. When heat transfer was included in the ethanol simulations ignition ceased to occur at 700K and below as illustrated in Figure 6.7. Figure 6.8 shows detailed results of the Chemkin output files with the inclusion heat transfer of species concentration. Figure 6.8(a) shows a typical single stage autoignition, the mixture experiences a long period of minimal activity, followed by a very slight temperature rise, followed by a rapid temperature increase and consumption of fuel. Figure 6.8(b) shows a similar situation, yet the amount of heat lost during the slight initial temperature rise is just enough to prevent autoignition. The fuel is slowly oxidised as heat is lost to the walls.

After much investigation it was still unclear why ethanol exhibited shorter ignition delays than predicted by Chemkin and appeared lower on the ignition delay map relative to the other reference fuels than expected.

![Ethanol - Comparison of Experimental and Simulated Results - Phi = 1.5](Image)

Figure 6.7: Ethanol - Comparison of Experimental and Simulated Results - Phi = 1.5

58
6.4. REFERENCE FUELS

(a) Single Stage Ignition 725K and Phi = 1.5

(b) No Ignition - 700K and Phi = 1.5

Figure 6.8: Chemkin Results for Ethanol Including Heat Transfer at 1 Bar Showing Species Concentration
6.5 Commercial Fuels

95 Octane Unleaded Petrol (ULP95) was tested and appears on the ignition delay plot exactly where expected, just below iso-octane (Octane 100). The relationship between octane number and ignition delay is not linear, hence RON 95 will be further away from RON 100 than a linear interpolation would suggest. Jet A1 which has a cetane rating of 39 also appears as expected just above n-heptane with a cetane rating of 56.

![Ignition Delay Chart](chart.png)

Figure 6.9: Experimental Results for Commercial Fuels in Relation to Reference Fuels - Phi = 1.5
Chapter 7

Conclusions

7.1 Ignition Delay Characteristics

- The NTC region is still present at atmospheric pressures, however heat transfer limitations of the apparatus prevented full range operation at stoichiometric and lean operating points.

- Heat transfer can have a significant effect on autoignition time scales in the NTC region and can lead to extinction of autoignition entirely. The effect is not limited to the low pressure environments and has been observed at high pressures by other researchers.

- Heat transfer can affect even single stage fuels which exhibit no NTC behaviour.

- This effect could have significant implications for determining AIT of a substance. If one followed the test method and reached such an area of non-ignition, one could easily overlook the lower region where autoignition begins to occur again.

- The apparatus provides a good qualitative comparison of a fuel's autoignition characteristics and is capable of providing useful information about complex multi-component fuels. For the fuels tested the apparatus provided a good reflection of octane and cetane number.

- The apparatus was capable of characterising a commercial jet fuel, with the potential to provide insight into gas turbine relight situations.
• Very long ignition delays were not achievable, once again due to heat transfer from the combustion chamber during slow oxidation of the fuel.

7.2 Chemical Kinetic Modeling

• Although it was not possible to quantitatively match experimental data with a detailed chemical kinetic simulations, general trends were well predicted.

• The inclusion of heat loss in the modeling provided a reasonable explanation for the majority of the discrepancy between experimental and theoretical data. The simple heat loss model included with Chemkin proved insufficient to accurately reflect the complex heat loss within the apparatus, although it was qualitatively acceptable.
Chapter 8

Recommendations and Future Work

8.1 Experimental Apparatus

The temperature profile of the combustion chamber and inherent heat loss was perceived to have the largest effect on the experimental results. A new apparatus, purpose built for lower pressures could provide greater accuracy and confidence in experimental results, as well as increasing the range of achievable results.

The following should be considered during the design process of such an apparatus:

- Improved temperature uniformity across the combustion chamber, in practice this is often achieved by separating the combustion chamber and heating device. ie Using an oven.

- If possible heat loss to the walls of the combustion chamber should be minimised, through optimising surface area to volume ratio and perhaps material selection. Conceivably an almost adiabatic chamber could be created where a preheated mixture is introduced, rather than the chamber performing the heating.

- The internal volume of the combustion chamber should be increased to at least $1000cm^3$. Several studies have shown that an increase in
volume of the test chamber decreases the AIT [21, 24] and thus, would expand the range of results.

- The laboratory has recently purchased a very high speed camera, significant insight into the initiation location of autoignition and the modes of combustion could be realised by including optical access in the new device. The emission spectrum of light during combustion could be analysed to distinguish between cool and hot flames [9].

- Rapid development of gasoline direct injectors may have produced a more suitable injector that could deliver higher fuel flow rates for testing at higher pressure.

8.2 Numerical Modelling

The chemical kinetic mechanism used for the experiments was calibrated using RCM (Rapid Compression Machine) experiments, which operate at much higher pressures and temperatures than the input values used in this project. There are many chemical kinetic mechanisms available, especially for pure components such as n-heptane, an investigation should be conducted into the most applicable mechanism for the pressure and temperature range under consideration.

8.3 Further Testing

Experiments at higher pressures should be conducted to investigate the pressure effect between 1 and 5 bar. The increased pressures should also reduce the overall ignition delay dramatically which will reduce the time available for heat loss to the walls. Once reliable data is available from the laboratory's new RCM, experimental results should be compared using derived pressure dependencies. Further experiments should also be conducted to investigate the cause of ethanol's unpredicted behaviour.
References


REFERENCES


REFERENCES


REFERENCES


Appendices
Appendix A

Combustion Bomb

Contents

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A.2 Heating System .................. A-3
A.3 Cooling System .................. A-3
A.4 Pneumatic System ................. A-4

A constant volume combustion bomb was required to attain accurate initial conditions for the experiments as well as monitoring of the results. Accurate control of temperature, pressure and air/fuel ratio were required. The Ignition Quality Tester IQT™ is a pre-heated combustion bomb designed to perform ASTM 6890-04 under very rigid test conditions (listed in Table A.1). It was decided that modifications to IQT, which the laboratory was already in possession of, would provide a satisfactory solution.

<table>
<thead>
<tr>
<th>Table A.1: Standard Test Conditions for the IQT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Charge Air Temperature</td>
</tr>
<tr>
<td>Charge Air Pressure</td>
</tr>
<tr>
<td>Fuel Temperature</td>
</tr>
<tr>
<td>Nozzle Opening Pressure</td>
</tr>
<tr>
<td>Injected Fuel Quantity</td>
</tr>
<tr>
<td>Injection Cone Angle</td>
</tr>
<tr>
<td>Calibrated for n-heptane ID</td>
</tr>
</tbody>
</table>

The IQT system consists of the following sub-systems:
A.1. COMBUSTION CHAMBER

- Combustion Chamber
- Fuel Injection System
- Heating System
- Cooling System
- Electrical System
- Control and Data-Logging Software
- Pneumatic System

To meet the requirements of the experiments the fuel injection, electrical system and control software were redesigned, minor modifications were performed on the combustion chamber and pneumatic system.

A.1 Combustion Chamber

"A 0.213 l combustion chamber is the heart of the system. The chamber body is equipped with thermocouple ports, a pressure transducer port (for measuring combustion pressure), inlet and outlet port with associated servo-valves, and an end cap. The injector nozzle is located inside the end cap at one end of the chamber, with the combustion pressure transducer located at the other end. The end cap and two seals (highly insulating) act as a shield for the fuel nozzle against the high temperature conditions inside the chamber. The end cap is equipped with passages connected to the coolant system. The purpose of the coolant flow is to reduce the heat transfer from the chamber nozzle and maintain the nozzle at a constant temperature." [3]

The end cap of the combustion chamber was modified in order to house the new fuel injector, details of the modification can be found in Appendix B.4 and G. A schematic of the original layout can be seen in Figure A.1.
A.2 Heating System

The combustion chamber was heated by nine 350 watt electrical cartridge heaters inserted circumferentially into the walls of the chamber, as shown in Figure A.2. Temperature feedback is provided by a K-type thermocouple located in the combustion chamber wall. The original test temperature of the device was approximately 560°C, after modification temperatures from 200-680°C were used.

A.3 Cooling System

The combustion pressure transducer and injector nozzle are cooled by a circulating coolant system to protect them from the high combustion chamber temperatures. The system circulated a mixture of anti-freeze and water from a reservoir through a circulation pump. The coolant flowed through the chamber end cap and the pressure transducer housing, individual flow control
Figure A.2: Location of Combustion Chamber Electrical Heaters [3]

was provided on the respective return lines. Heat absorbed by the coolant was dumped to the ambient air using a forced air to water heat exchanger. A schematic of the cooling system is shown in Figure A.3.

An electrical backup system was installed to ensure the cooling system would run in the event of a power failure, for details see Appendix C.2.2.

A.4 Pneumatic System

A basic pneumatic system was incorporated in the original device to provide mechanical power for several components:

- The inlet and exhaust valves were pneumatically operated diaphragm valves, triggered by 240VAC solenoid valves.
- A pneumatically driven fuel pump, which was removed.

A schematic of the original pneumatic system can be seen in Figure A.4
A.4. PNEUMATIC SYSTEM

Figure A.3: Schematic Diagram of the Cooling System [3]

Figure A.4: Schematic Diagram of the Pneumatic System [3]
Appendix B

Fuel System

Contents

B.1 Selection and Design .................. B-1
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   B.1.2 Selection of the Injector .......... B-2
B.2 Final Implemented Fuel System .......... B-5
B.3 Injector Flow Characteristics .......... B-5
B.4 Mounting the injector .............. B-8
B.5 Test Fuels ....................... B-10

The standard IQT™ uses a pneumatically driven, fixed volume, single shot injection pump and a pintle type diesel injector. The system delivers a single fixed volume of fuel to the combustion bomb that results in a globally lean mixture at standard test conditions. The primary goal of designing and implementing a new fuel system was to increase the flexibility of the IQT™ test conditions.

B.1 Selection and Design

B.1.1 Requirements

- Easily variable injection volume
B.1. SELECTION AND DESIGN

- Allows for variable air/fuel ratio over a wide range of temperatures and pressures.

• Accurate delivery of small fuel quantities
  - Fuel volumes required at high temperatures and low pressures can be as low as \(2\mu l\).

• Insensitive to fuel type
  - Lubricity of fuels is a significant problem especially when using a pump where the fuel acts as a lubricant.
  - Alcohol fuels can be corrosive to both moving and stationary parts.
  - Certain fuels are incompatible with rubber seals and can cause swelling and leaking.

• Good atomisation
  - Better atomisation lowers evaporation time and improves homogeneity.
  - The better the evaporation and mixing, the shorter the ignition delays that can be measured.

• Operation at elevated temperatures
  - The injector, although housed in a water-cooled jacket is subjected to temperatures in excess of 50°C.

B.1.2 Selection of the Injector

There is a wide range of commercial automotive injectors available on the market, an extensive review was conducted of all the available options in order to find the best solution. Port fuel injectors were ruled out early on, due to their inability to inject directly into the combustion chamber. Primarily modern direct injectors are divided into 4 groups, diesel or petrol actuated and solenoid or piezo. Diesel injection systems operate at pressures of up to 2000 bar and petrol up to 200 bar.

Diesel injector pumps use the intrinsic lubricity of the diesel to provide lubrication for moving parts within the pump. Previous experience with
these pumps has shown that exposure to low lubricity fuels causes rapid wear and deterioration of performance, ultimately resulting in pump failure. Obviously such a pump is not suitable for the application as the suitable test fuels would be significantly limited. On the other hand petrol injector pumps have a separate lubrication system, this allows a greater flexibility of fuels, but limits the maximum pressure.

The primary difference between solenoid and piezo injectors is their actuation method. In a solenoid injector current is passed through an electromagnet which lifts a needle and allows the fuel to flow. Usually flow is directed through a swirl plate such as the one in B.1, this improves the atomisation of the fuel by introducing and accelerating a rotational velocity on the fuel. Modern petrol solenoid injectors are capable of injection times as short as 0.35ms resulting in small injection volumes. Fuel spray Sauter Mean Diameters less than 20 microns are also achievable. [34]

Piezo injectors make use of the piezo electric effect to actuate the needle, a high voltage applied over a stack of piezo crystals causes them to expand, acting directly on the needle. Piezo injectors generally perform better than solenoid injectors in all areas, but are significantly more expensive and complex to control. The benefits of the piezo injector did not outweigh the extra expense and a suitable solenoid injector that met the requirements of the fuel system was selected.

![Figure B.1: Close up of Disassembled Injector Showing Swirl Plate](image)

B-3
Figure B.2: Schematic Showing Primary Fuel System Components
B.2 Final Implemented Fuel System

The diagram in figure B.2 illustrates the main features of the implemented fuel system. The system used a solenoid actuated gasoline direct injector, with fuel pressure supplied by high pressure bottled nitrogen. The system was divided into two sections; the high pressure section which supplied the fuel to the combustion chamber and the low pressure section which was used for refilling. Switching between the two sections was controlled by two manually operated three-way valves.

Using high pressure nitrogen removed the necessity for a high pressure fuel pump and the complexity associated with it. It allows for complete fuel flexibility and minimises the amount of fuel used when changing fuels and flushing the system.

Figure B.3: Photograph of Implemented Fuel System

B.3 Injector Flow Characteristics

In order to ensure an accurate air/fuel ratio inside the combustion chamber, it was essential to know the exact amount of fuel injected. This required the
B.3. INJECTOR FLOW CHARACTERISTICS

measurement of the effects of fuel pressure and injection duration on the flow rate of the injector. A basic test rig was constructed to hold the injector and a measuring cylinder. The measuring cylinder was loosely sealed against the flask to prevent evaporation of the fuel but also prevent a pressure buildup within the flask.

The test procedure was as follows:

1. The fuel system was primed as detailed in F.
2. Desired fuel test pressure and pulse width were set.
3. The measuring cylinder was emptied and dried.
4. The cylinder was weighed on a scale accurate to 2mg and the start weight recorded.
5. The cylinder was placed on the test rig and the injector sealed against it.
6. Several thousand injections were performed, until approximately 100g of fuel had been delivered.
7. The cylinder was removed and weighed again, recording the final weight.

This procedure was performed on several fuels for fuel pressures of 10, 20, 40, 75 and 100 bar and for pulse widths from 0.5 - 6ms. The results for n-heptane are shown in B.4. Once the injector needle has fully lifted, which takes 0.3ms the area of the flow path remains constant until the needle is closed. Thus one would expect that for constant fuel pressure the injected fuel volume would have a linear relationship to injection duration. If one looks at a single contour for constant pressure, as in B.5, this linear relationship is clearly visible.

Using Bernoulli’s equation \( p + \frac{1}{2} \rho v^2 + \rho g z = k \) [35] and accounting for real world inefficiencies, one would expect that for constant injection duration the relationship between volume injected and fuel pressure would be of the form \( y = a x^b \) where \( b \approx 0.5 \). This expected relationship is obvious from looking at the constant injection duration contour plots for n-heptane in B.6. For example; the relationship for n-heptane with constant 4ms duration is \( y = 5.6241 \cdot x^{0.4672} \).
B.3. INJECTOR FLOW CHARACTERISTICS

Figure B.4: 3D Plot of Flow Calibration Test Results for n-heptane

Figure B.5: Constant Pressure Contour Plots for n-heptane
Figure B.6: Constant Injection Duration Contour Plots for n-heptane

Using the experimental results it was possible to obtain the required coefficients for the different conditions. After testing several fuels it was found that after correcting for fuel density, there was only a small difference (less than 2.5%) in the flow characteristics of the injector between fuels. This finding allowed us to use one set of coefficients for all fuels and save the time-consuming process of flow testing every fuel being investigated.

B.4 Mounting the injector

It was necessary to redesign the end plate of the IQI™ in order to house the new injector. The end plate incorporated a cooling water jacket for the injector and a thermocouple for measuring nozzle tip temperature. It was also the primary mounting point for the combustion chamber and the attachment point to the base stand. The original end cap utilised a complicated insulating double sealing mechanism to reduce heat transfer from the combustion chamber. Fortunately the new injector had a higher temperature tolerance and a single insulating seal was implemented. The new shape of the end cap also allowed for simplification of the cooling galleries and thus was easier to manufacture.

As seen in figure B.7 The injector is sealed from the combustion chamber using a soft copper washer. The rear of the injector is sealed using a rubber
o-ring to contain the water jacket. As seen in figure B.9 the injector is clamped into place from behind. The dimensions were carefully selected to ensure the force from the clamp is transferred to the front face to ensure sealing. Circumferential location was provided by a closely tolerated fit between the middle of the injector and the hole.

The injector was mounted 15° off centre to counter the effect of the offset spray nozzle (see figure B.8) and ensure the centre line of the injection cone and the bomb were aligned. Due to the wider cone angle of the new injector(90°), the distance between the nozzle and the combustion chamber had to be minimised to prevent wetting of the relatively cooler narrow passage. Wetting of this passage would affect both air/fuel ratio and evaporation times.

The spray is expected to hit the walls due to the lack of resistance from the low pressure air within the chamber. When the chamber is heated the walls are well above the boiling point of the fuels under test and will aid evaporation. The extent of the spray was examined using a borescope inserted through the hole for the combustion pressure sensor. The majority of the fuel spray was seen to clear the passage with a large portion ending up on the combustion chamber walls.

Figure B.7: Cross Section of End Plate Showing Injector Location
B.5 Test Fuels

Important data for the test fuels:

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Stoich AF Ratio</th>
<th>Density (kg.m⁻³)</th>
<th>AIT (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-heptane</td>
<td>15.14</td>
<td>683.74</td>
<td>220</td>
</tr>
<tr>
<td>iso-octane</td>
<td>15.09</td>
<td>691.91</td>
<td>415</td>
</tr>
<tr>
<td>Ethanol</td>
<td>8.98</td>
<td>789.3</td>
<td>400</td>
</tr>
<tr>
<td>Toluene</td>
<td>13.5</td>
<td>865.2</td>
<td>535</td>
</tr>
<tr>
<td>ULP 95</td>
<td>14.56</td>
<td>743.75</td>
<td></td>
</tr>
<tr>
<td>Jet A1</td>
<td>14.66</td>
<td>798.4</td>
<td></td>
</tr>
</tbody>
</table>

Figure B.8: Close up of Disassembled Injector Showing Offset Nozzle
Figure B.9: Photograph Showing Installed Injector
Appendix C

Electrical and Control System

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All hardware and software upstream of the sensors and actuators installed on the IQT™ was replaced for two reasons; to allow complete control over test conditions and to leave the original control system intact, for possible return to service.

C.1 National Instruments Hardware

After consideration of several products, including PLCs, microprocessors and direct PC control, the National Instruments CompactRIO system was se-
lected as the central component of the control system.

The benefits of the CompactRIO system include:

- Reliability and robustness
- Reconfigurable for future use
- Compatible with commercially available injector drivers
- Relatively simple software leading to rapid development and prototyping

"CompactRIO combines an embedded real-time processor, a high-performance FPGA, and hot-swappable I/O modules. Each I/O module is connected directly to the FPGA, providing low-level customization of timing and I/O signal processing. The FPGA is connected to the embedded real-time processor via a high-speed PCI bus. This represents a low-cost architecture with open access to low-level hardware resources. LabVIEW contains built-in data transfer mechanisms to pass data from the I/O modules to the FPGA and also from the FPGA to the embedded processor for real-time analysis, postprocessing, data logging, or communication to a networked host computer. [36]"

A diagram of the basic architecture for the CompactRIO can be seen in Figure C.1 and a specific overview of the data acquisition system implemented can be seen in Figure C.2

C.1.1 IO Modules

The IO modules that plug into the CompactRIO chassis provide the physical connections to the sensors and actuators, perform analogue to digital conversion and basic signal conditioning. The following modules were selected:

- NI 9215 - 4-Channel, 100 kS/s, 16-bit, 10 V Simultaneous Sampling Analog Input Module
C.2. OTHER HARDWARE

Figure C.1: CompactRIO Architecture [36]

- NI 9211 - 4-Channel, 14 S/s, 24-Bit, 80 mV Thermocouple Input Module
- NI 9205 - 32-Ch 200 mV to 10 V, 16-Bit, 250 kS/s Analog Input Module
- NI 9477 - 32 Ch, 8 μs, 5 to 60 V, Sinking Digital Output Module

C.2 Other Hardware

C.2.1 Drivven Injector Driver

The solenoid injector chosen required a very specific current trace to ensure reliable and accurate operation. The generation of this current trace is not a trivial matter and requires high voltage and current DC circuitry with very accurate timing, the design of such a circuit is not central to the project and thus a commercial system was purchased from Drivven. The injector driver consists of a module for a National Instruments CompactRIO system and the associated software (LabVIEW VIs).

Basic Features [37]:

- 3 Channel solenoid injector drivers
Figure C.2: Schematic of I/O and Control System
• 2 Channel piezo injector drivers
• Up to 150VDC internal boost power supply
• Up to 30A peak current/ 10A hold current
• Operates from a 6 - 32V Battery

Current Trace

It is notoriously difficult and time consuming to obtain data, such as current traces for injection equipment from manufacturers. Fortunately it was possible to obtain the current trace, by installing a hall effect current clamp on the injector circuit in a car equipped with the selected injector. The current trace obtained at idle is shown below in Figure C.3. Parameters extracted from the current trace (shown in Table C.1) were entered into the Drivven VI to reproduce injector function.

![Inject Current Trace at Idle](image)

**Figure C.3: Physically Measured Current Trace**

<table>
<thead>
<tr>
<th>Table C.1: Injector Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak Current</td>
</tr>
<tr>
<td>Hold Current</td>
</tr>
<tr>
<td>Boost Time</td>
</tr>
</tbody>
</table>

C-6
C.2.2 Backup System

The combustion chamber pressure transducer required constant cooling whilst the bomb was heated, cooling was supplied by a circulating water system. It was essential for the cooling system to run for at least 3 hours after the heaters were turned off, and in the event of a power cut. A self-contained time delay relay mechanism ensures that the cooling system remains on for 3 hours, even in the event of a control system failure. A simple backup system was designed using a battery charger, car battery and an inverter to provide AC power during power cuts. The backup system was switched in or out using an AC controlled double pole double throw (DPDT) relay which was actuated using the mains AC supply. As soon as the mains supply drops the relay switches over to the inverter supply and keeps the cooling system running.

![Schematic of Backup System](image)

Figure C.4: Schematic of Backup System

C.2.3 Shunt Resistor

During initial commissioning and prototyping a hall-effect current clamp was used to measure injector current. Once all systems were operational, the current clamp was replaced with a shunt resistor placed in series with the
injector coil. The voltage across the shunt resistor is sampled by the high speed analogue module, a threshold voltage is used as a trigger for the start of injection. After using the relevant conversion factors the current signal can be displayed on LabVIEW.

C.3 Software

C.3.1 Design Requirements

In order to allow for an entirely automated fuel characterisation, the software must be capable of doing the following:

- Control and vary combustion chamber temperature accurately.
- Create reliable injection pulses that vary in duration based on desired air/fuel ratio.
- Reliably record pressure traces from combustion.
- Automatically purge and fill the combustion chamber.
- Monitor certain parameters for safety purposes.
- Process and record all relevant data.

C.3.2 National Instruments LabVIEW

LabVIEW (Laboratory Virtual Instrumentation Engineering Workbench) is a graphical programming language that was used to control the National Instruments hardware. The diagram in Figure C.5 show an example of a simple LabVIEW VI (Virtual Instrument). The VI shown reads integer values from a thermocouple module and converts them to linearised temperature. The control software for the combustion bomb is made up of many VIs and sub-VIs which are controlled through an easy to use GUI (Graphical User Interface).
C.3. SOFTWARE

Figure C.5: LabVIEW VI for Basic Thermocouple Measurement

C.3.3 Layers

Functions of the software were separated into individual 'blocks' and placed on specific layers. Each layer has its own specific requirements and restrictions, for example only integer values may be used on the FPGA. The major blocks are listed in their respective locations below:

- On the FPGA:
  - Reading and writing of data to all analogue and digital modules
  - Driven injector driver and single shot injection latch
  - Current sensing trigger and combustion pressure capture
  - Calibration coefficients and offsets for analogue devices

- On the Real Time Controller:
  - Calibration parameters for the injector
  - PID temperature control and square wave generation
  - Linearisation of temperatures
  - Safety interlock and warning level settings
  - Communication between PC and FPGA

- On the PC:
  - Graphical User Interface and display of data
Appendix D

Chemical Modelling and Calculations

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<th>Title</th>
<th>Page</th>
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</thead>
<tbody>
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<td>Chemical Kinetics Package and Mechanism Description</td>
<td>D-1</td>
</tr>
<tr>
<td>D.1.1</td>
<td>Modifications</td>
<td>D-3</td>
</tr>
<tr>
<td>D.2</td>
<td>Hardware</td>
<td>D-3</td>
</tr>
<tr>
<td>D.3</td>
<td>Equivalence Ratio</td>
<td>D-4</td>
</tr>
</tbody>
</table>

Detailed chemical kinetic simulations were performed for the PRFs, blends thereof and Ethanol. Simulations were carried out at initial conditions similar to the physical experiments conducted in order to provide a basis for comparison and validation.

D.1 Chemical Kinetics Package and Mechanism Description

The chemical kinetics package (Chemkin) and the reaction mechanism (Westbrook et al.) had been set up and used by previous researchers in the laboratory, the details are included below.
Detailed kinetic mechanisms reflect the actual molecular collisions that are responsible for the autoignition reactions and these descriptions are therefore theoretically fundamental [39]. Many groups, such as those of Pitz, Westbrook and co-workers at LLNL and Battin-Leclerc and co-workers in Nancy, have been active in the development of detailed kinetic mechanisms that are suitable for describing the low-to-intermediate temperature chemistry that is of importance in autoignition. Because detailed kinetic models are based on fundamental chemical kinetic mechanisms, their development can rely on both measurements and theoretical analyses of elementary reaction rates [39]. A significant disadvantage posed by the use of detailed kinetic mechanisms relates to the computational demands of the large set of nonlinear equations used to simulate the reactions. For example, the mechanism for blends of n-heptane and iso-octane (PRFs) from LLNL that was used in this study, contains 1034 species in 4238 reactions [40]. This implies relatively long run times which can take several hours for a single simulation when running on a personal computer.

The Chemkin Collection (Version 3.7) software, which has been used for numerical simulations in this study, is a powerful software system for solving complex chemical kinetics problems. It was developed originally for gas phase combustion problems [41] and the Chemkin input data format has become the de facto standard in combustion modeling for describing all the chemical reactions, their rate parameters and the thermodynamic and transport properties of species [19].

The physical model that was selected for the majority of the simulations was that of a constant volume closed adiabatic system, containing the fuel molecules and a stoichiometric amount of air in a perfectly mixed homogeneous system. This was considered to be a reasonable representation of a Rapid Compression Machine (RCM) for ignition delay calculations using detailed kinetic mechanisms. Constant pressure simulations, approximating a shock tube experiment were also investigated. Both the initial temperature and the starting pressure of each simulation were specified. Thereafter the computer code solved the coupled conservation equations of energy and mass and those for each chemical species. After a time, the heat release due to the oxidation reactions causes an increase in the temperature of the system, and eventually the degenerate branching reactions and
resultant exponential growth of the pool of free radicals causes
the temperature runaway associated with autoignition." [42]

D.1.1 Modifications

The input files for Chemkin were modified to include heat transfer. A heat
transfer coefficient in units of cal/(cm².K.s) and a reference temperature are
used in conjunction with the surface area of the reactor to calculate a heat
transfer rate for a specific gas temperature. Thus there is no heat transfer
until the gas temperature rises above the wall temperature of the reactor.
This enabled investigation into the effect of the perceived heat loss on the
ignition delay. It was evident from early on, that even a relatively small
amount of heat transfer can have a dramatic effect on the ignition delay and
the extinction of ignition altogether.

D.2 Hardware

The numerical simulations were run on a dedicated PC with the following
specifications:

- HP Workstation xw4200
- Pentium 4 3.60 GHz Processor
- 4GB DDR2 RAM
- Windows XP Service Pack 2
- Chemkin Version 3.7

An individual simulation took approximately 20 minutes to run. The
simulations were batch processed for a range of conditions generated by a
Microsoft Excel spreadsheet. The number of saved data points and save
period per simulation was varied based on expected ignition delay. After
initial results the data was analysed and the saving parameters adjusted to
focus on the important ignition delay character, generally 3 iterations of
a simulation was sufficient to bracket the most important data. Save files
generated were of the order of 5MB per simulation.
D.3 Equivalence Ratio

The equivalence ratio ($\phi$) is equal to the actual fuel/air ratio over the stoichiometric fuel/air ratio [43]:

$$\phi = \frac{m_{\text{fuel(actual)}}}{m_{\text{fuel(stoich)}}} \frac{m_{\text{air(actual)}}}{m_{\text{air(stoich)}}}$$  \hspace{1cm} (D.1)

The air/fuel ratio ($\lambda$) is also used throughout the literature [43]:

$$\lambda = \frac{1}{\phi}$$  \hspace{1cm} (D.2)

In order to calculate the required amount of fuel, one must calculate the mass of air in the combustion chamber. From the ideal gas equation of state [44]:

$$PV = mRT$$

$$m_{\text{air}} = \frac{P_i.V_c}{R.T_i}$$  \hspace{1cm} (D.3)
Appendix E

Safety Considerations

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This chapter serves to highlight the risks associated with the various aspects of the test apparatus and how each of these was addressed.

E.1 High Gas Pressures

The fuel system configuration resulted in certain components being subjected to pressures of up to 200 Bar. Specifically all the components before the fuel pressure regulator would be subjected to pressures up to 200 Bar and those
after up to 110 Bar. An extensive review was conducted of the equipment already in place and careful consideration was taken when selecting new components to ensure they could handle the required pressures safely.

The majority of the equipment was purchased from Swagelok®, with working pressures well in excess of the requirements. Two pressure relief valves were installed to protect the equipment upstream and downstream of the regulator. Following assembly, joints were thoroughly checked for integrity and leaks[45, 46].

### E.1.1 Pressurised Fuel Vessel

A pressurised cylinder filled with an incompressible fluid represents a significant safety risk, should the temperature of the fluid rise and not have room to expand it would cause a significant rise in pressure, possibly bursting the cylinder. The cylinder used has multiple safety features to prevent bursting.

- The cylinder is rated to a working pressure of 124Bar and hydrostatically tested to 5/3 times this pressure.
- A relief valve after the fuel pressure regulator, should blow if the gas pressure exceeds 110 Bar.
- An outage tube was installed, this ensures there is always a vapour space above the fluid in the cylinder. This allows for expansion of the fluid and prevents over-filling of the cylinder.
- A rupture disc was installed, a last resort that would burst should the pressure exceed 196 Bar, and vent the pressure in a reasonably controlled manner. This rating follows Swagelok guidelines and is still within the tested pressure of the cylinder [47].

### E.1.2 Nitrogen Leaks

The increased pressure of the gas lines in the laboratory, increases the risk of nitrogen leaks, both slow and rapid. High concentrations of nitrogen can cause asphyxiation and death without warning. A simple calculation was done based on the volume of the room and the mass of gas stored in the
E.2 Fire and Explosions

The combustion chamber of the IQT™ is designed to withstand pressures in excess of 345 Bar. This far exceeds both the cylinder gas pressures and peak combustion pressures [3]. The fuel system is also designed to resist explosion as discussed above.

Whenever one is working with flammable fuels there is a risk of fire, by pressurising the fuel system with an inert gas such as nitrogen, one minimises the risk of fire by depriving the combustible fuel of oxygen. It was also ensured that no fuel lines pass over hot surfaces, thus even if the fuel leaks and is exposed to oxygen it won’t have an ignition source. Fires within the combustion chamber are limited by a lack of oxygen, when the valves are closed there is a fixed volume of air, once that air is consumed, any internal fire or combustion event will be extinguished.

E.3 Fuel Handling

Gloves and safety glasses should be worn during all fuel handling in line with laboratory policy. When handling raw fuel, reference should be made to the appropriate MSDS information with regards to the specific fuel being tested. All fuel preparation should take place at the appropriate fuel station, with the ventilation system switched ON.

E.3.1 Glassware

Suitable holders were provided for all glassware used, in order to minimise the risk of broken glass. The glass refilling cylinder is protected from the high pressure circuit by a check valve. This valve prevents high pressure fuel or
nitrogen from shattering the glass, should the operator make an error during refilling.

### E.3.2 Fuel Spills

The volume of fuel being handled is generally less than 0.5l, any spills could easily be handled with the fuel spill kits on hand. There were no drains in the vicinity that could be contaminated.

### E.4 Electric Shock

The equipment used utilises 220VAC and High Voltage DC both of which represent a significant risk of electric shock. The majority of electrical components are contained in a locked cabinet. All electrical cables are properly terminated and there are no bare connections within reach of the user. Both the electrical cabinet and the IQT are earthed. The electricity supply to the cabinet should be turned off before opening.

### E.5 Hot Surfaces

Certain surfaces on the IQT reach over 680°C, obviously a significant burn risk. A finger proof cage was installed over the device to prevent anyone touching the hot surfaces.

### E.6 Exhaust Gases

After passing through a silencer, all exhaust gases were extracted through the laboratory extraction system.
Appendix F

Operating Procedures

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F.1 Refueling

F.1.1 Emptying Excess Fuel

Refer to Figure B.2

1. Ensure that injector bleed line is firmly secured to the slops bottle.

2. Ensure that the throttling valve is fully closed.
3. Set the nitrogen pressure regulator to approximately 5 bar.

4. Turn valve A to Nitrogen supply and valve B towards the injector.

5. Slowly open injector bleed valve, fuel will flow into the slops bottle. (Note: The bleed valve has no packing so a small amount of fuel may leak from the stem.)

6. Once all the fuel has been drained open the bleed valve further to allow the Nitrogen to flush the system.

7. Close the bleed valve.

8. Run the injector with a long pulse width for at least 1000 injections to flush out the dead volume after the bleed valve.

9. Use the manual override and purge the cylinder with charge air to empty any fuel from the combustion chamber.

F.1.2 Refilling

1. Ensure throttling valve is fully closed.

2. Turn valve A towards throttling valve.

3. Slowly open throttling valve and relieve gas pressure to atmosphere.

4. Fill the LP fuel tank with the required amount of fuel.

5. Turn valve B towards the refilling tank.

6. The fuel will gravity feed into the HP fuel tank.

7. Once all the fuel has transferred, Close the throttling valve.

8. Switch valve B towards the injector, and valve A towards the Nitrogen.

9. Open bleed valve slowly and bleed any air from the system.

10. Run the injector with a long injection duration for at least 1000 injections to flush out the dead volume after the bleed valve.

11. Use the manual override and purge the cylinder with charge air to empty any fuel from the combustion chamber.

When changing fuels it is recommended to perform the procedures above twice in order to flush the system with the new fuel.
F.2  Bomb Operation

F.2.1  Start Up and Testing

1. Start the LabVIEW PC Application, it should automatically connect to the Real-Time Controller.

2. Start the cooling system, and verify that it is running by checking the flow indicator.

3. Start the ventilation system in the control room and place tag on the hook.

4. Verify that the pressure transducer is connected, then switch on the charger amplifier.

5. Open the valves on the Nitrogen and Synthetic Air gas bottles.

6. Switch the purge valves behind the combustion bomb for the Shop Air, Nitrogen and Synthetic Air.

7. Verify the gas pressure on the LabVIEW application, adjust regulators as necessary.

8. Enter the values for the stoichiometric air/fuel ratio and density of the fuel.

9. Enter the file path for results data to be saved, and the number of tests required per point (Default = 5).

10. Enter the required range of temperatures to be tested as well as step size, do the same for air/fuel ratio. Values can be entered in ascending or descending order.

11. Click the multiple test button and turn on the heaters, the bomb will heat up and perform the automated test sequence for all the set points.

F.2.2  Shut Down

1. After testing has finished, click the fill sequence button to purge the combustion chamber.
3. Set the nitrogen pressure regulator to approximately 5 bar.

4. Turn valve A to Nitrogen supply and valve B towards the injector.

5. Slowly open injector bleed valve, fuel will flow into the slops bottle. (Note: The bleed valve has no packing so a small amount of fuel may leak from the stem.)

6. Once all the fuel has been drained open the bleed valve further to allow the Nitrogen to flush the system.

7. Close the bleed valve.

8. Run the injector with a long pulse width for at least 1000 injections to flush out the dead volume after the bleed valve.

9. Use the manual override and purge the cylinder with charge air to empty any fuel from the combustion chamber.

F.1.2 Refilling

1. Ensure throttling valve is fully closed.

2. Turn valve A towards throttling valve.

3. Slowly open throttling valve and relieve gas pressure to atmosphere.

4. Fill the LP fuel tank with the required amount of fuel.

5. Turn valve B towards the refilling tank.

6. The fuel will gravity feed into the HP fuel tank.

7. Once all the fuel has transferred, Close the throttling valve.

8. Switch valve B towards the injector, and valve A towards the Nitrogen.

9. Open bleed valve slowly and bleed any air from the system.

10. Run the injector with a long injection duration for at least 1000 injections to flush out the dead volume after the bleed valve.

11. Use the manual override and purge the cylinder with charge air to empty any fuel from the combustion chamber.

When changing fuels it is recommended to perform the procedures above twice in order to flush the system with the new fuel.
F.2 Bomb Operation

F.2.1 Start Up and Testing

1. Start the LabVIEW PC Application, it should automatically connect to the Real-Time Controller.

2. Start the cooling system, and verify that it is running by checking the flow indicator.

3. Start the ventilation system in the control room and place tag on the hook.

4. Verify that the pressure transducer is connected, then switch on the charger amplifier.

5. Open the valves on the Nitrogen and Synthetic Air gas bottles.

6. Switch the purge valves behind the combustion bomb for the Shop Air, Nitrogen and Synthetic Air.

7. Verify the gas pressure on the LabVIEW application, adjust regulators as necessary.

8. Enter the values for the stoichiometric air/fuel ratio and density of the fuel.

9. Enter the file path for results data to be saved, and the number of tests required per point (Default = 5).

10. Enter the required range of temperatures to be tested as well as step size, do the same for air/fuel ratio. Values can be entered in ascending or descending order.

11. Click the multiple test button and turn on the heaters, the bomb will heat up and perform the automated test sequence for all the set points.

F.2.2 Shut Down

1. After testing has finished, click the fill sequence button to purge the combustion chamber.
2. Turn off the heaters and cooling system on the PC application, the cooling system will continue to run for 3 hours.

3. Purge the gas lines by switching the purge valves on the wall behind the combustion bomb.

4. Close the valves on the gas bottles outside.

5. Switch off the ventilation system in the control room and remove tag.

6. Close the PC application and shut down the PC.

**F.2.3 Pressure Test**

From time to time a pressure test of the bomb must be performed to ensure that the seals and valves aren’t leaking and affecting experimental results.

1. Heat the bomb to at least 300°C.

2. Switch Valve control to manual and reset the charge amplifier.

3. Close the exhaust valve, and activate the charge air solenoid.

4. Once the bomb has filled to the syn air pressure, close the inlet valve and the charge air solenoid.

5. Monitor the pressure in the bomb, it should drop by less than 3.5 KPa/s. In practice the value was found to be much lower than this - \( \approx 0.1 \) KPa/s.

6. Open the exhaust valve and inlet valve and switch off manual control.

**F.3 Maintenance**

Maintenance procedures should be carried out according the to the IQT™ manual, as the majority of serviceable components are still in their original configuration [3].
Appendix G

Manufacturing Drawings

G.1  End Cap
Figure G.1: Manufacturing Drawing for New End Cap
Figure G.2: Manufacturing Drawing for New End Cap - Critical Angles
Figure G.3: Manufacturing Drawing for New End Cap - Cross-Section