THESIS

DUAL-FUEL COMBUSTION OF HYDROCARBON FUEL DROPLETS IN LEAN, PREMIXED METHANE/OXIDIZER MIXTURES IN A RAPID COMPRESSION MACHINE

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ABSTRACT

DUAL-FUEL COMBUSTION OF HYDROCARBON FUEL DROPLETS IN LEAN, PREMIXED METHANE/OXIDIZER MIXTURES A RAPID COMPRESSION MACHINE

The combustion of two fuels with disparate reactivity (dual-fuel) has been shown to be an effective method for increasing fuel efficiency and reducing both fuel costs and pollutant formation in internal combustion engines. Due to recent decreases in the price of natural gas, the incentive has grown to operate engines in dual-fuel mode, where some amount of diesel is substituted with natural gas. Since natural gas is expected to remain less expensive on a per-unit-energy basis than diesel fuel for the foreseeable future, it will continue to be economically advantageous to maximize the substitution percentage of natural gas in dual-fuel engines. However, at higher natural gas substitution percentages, uncontrolled fast combustion (i.e. engine knock) can occur, which limits the load of the engine and can shorten the lifetime of engine components. Emission of unburned methane has also been shown to increase with increasing natural gas substitution percentage. Previous detailed computational engine modeling at CSU with reduced chemical kinetics and simplified spray models has captured these effects but little data are available to validate chemistry and spray models at engine-relevant conditions. In this study, a rapid compression machine (RCM) was used as a platform to provide a high-temperature/high-pressure environment to better understand the thermodynamic, transport and chemical kinetic phenomena of dual-fuel combustion. The RCM was modified to perform evaporation and combustion experiments on single n-alkane fuel droplets in gaseous inert, O₂/inert and O₂/CH₄/inert environments. Droplet evaporation experiments were performed on C₅ to C₁₂ n-alkane droplets in inert gas to measure

droplet evaporation rates at near supercritical and supercritical conditions (18 bar < P < 35 bar; 450 K < T < 850 K). The Dual-fuel droplet evaporation and combustion experiments were studied using pressure data and images collected a Schlieren optical system. In the combustion experiments, ignition delay of heptane/O₂/inert was quantified at elevated pressure and temperature (27 bar < P < 38 bar; 844 K < T < 1251 K). In addition, the process of dual-fuel combustion was captured, showing two distinct ignition events.

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1 Introduction

1.1 <u>Motivation</u>

Internal combustion engines (ICE) are convenient and efficient ways to generate mechanical energy via the combustion of carbon-based fuels. Because of their durability, reliability, and high power to weight ratio, ICEs remain the standard source of power for on-road vehicles around the world. In addition, the high energy density of liquid hydrocarbons makes them ideal transportation fuels. Despite a tenfold increase in U.S. sales of electric light duty vehicles in the past decade, the Energy Information Administration (EIA) estimates that in the year 2040, greater than 99% of on-road highway transportation vehicles will still be powered using ICEs [1]. Thus, continued research and development of new engine technologies, focused on increasing efficiency and reducing harmful emissions, is critical.

Generally, ICEs can be broken up into two different types: spark-ignition (SI) and compression-ignition (CI) engines. The fundamental difference between the two types of engines is the means by which ignition of the fuel/air mixture occurs and the role of autoignition on that process. Autoignition is an ignition event that results purely from changing ambient conditions, with no concentrated energy addition (e.g., from a spark or laser). In a diesel engine, the compressing cylinder volume results in an increase in pressure and temperature. Because diesel is a high-reactivity fuel, the increased temperature and pressure is sufficient to quickly ignite the fuel mixture without the need of a spark. Ignition results in a rapid release of energy that is converted to mechanical shaft work via the cylinder and driveshaft mechanisms. In CI engines, because ignition is generally dictated by the timing of the fuel injection into the cylinder, a careful balance must be struck between the timing of the fuel injection and the position of the cylinder along its stroke. Because of the speed and time scales at which engines operate, the fuel must be injected into conditions that will rapidly burn as much of the fuel as possible to achieve optimum combustion efficiency. Autoignition is desirable in CI engines as it serves as the main ignition mechanism.

In SI engines, the ignition timing is almost entirely dictated by the timing of the spark. Gasoline or natural gas are the most common fuels used in SI engines. Both are considered lowreactivity fuels because their reaction times are much longer (compared to a high reactivity fuel such as diesel fuel) and therefore require a more concentrated form of energy, such as a spark, to create very high local temperatures to achieve ignition. Spark-ignition gives precise control over the combustion behavior as it relates to the position of the crankshaft. Autoignition can occur in SI engines but it is not desirable. In an SI engine, autoignition can occur in the unburned gases (i.e. end-gas) upstream of the spark-initiated flame and this end-gas autoignition can lead to engine knock, which can damage the engine.

Advanced combustion ignition schemes have been the focus of recent research and development and include natural gas/diesel combustion (dual-fuel), homogeneous charge compression ignition (HCCI), and reactivity-controlled compression ignition (RCCI). HCCI takes advantage of the lower emissions achieved by igniting a leaner fuel mixture that combusts at lower temperatures; however, HCCI engines can be difficult to operate. Since HCCI combustion is achieved through autoignition of the homogeneous mixture near top dead center as it is compressed via the piston, the start of combustion and the rate of heat release can be difficult to control over a wide range of engine operating conditions [2]. RCCI combustion utilizes a homogenous premixed low reactivity fuel (such as gasoline or natural gas) and stratification of a high reactivity fuel (such as diesel fuel) via early direct injection. By stratifying the high reactivity fuel, ignition proceeds

from areas of high mixture reactivity to areas of low reactivity, which lengthens the combustion duration, lowers the pressure rise rate and peak pressure, and allows high loads to be achieved [3].

In dual-fuel engine operation, fuels of disparate reactivity are combusted together, taking advantage of the combustion properties of both. Typically, because of economic reasons, the fuels utilized in dual fuel engines are diesel and natural gas. Specifically, it is economically advantageous to offset the demand for energy from diesel fuel using as much natural gas as possible because, on a per-unit-energy basis, natural gas is less expensive. There are also potential greenhouse gas benefits of substituting diesel with natural gas since as these engines have the potential to reduce CO_2 emissions by 25% in comparison to diesel engines (due to the higher carbon to hydrogen ratio and heating value of natural gas) [4]. However, substituting high levels of natural gas also has disadvantages: Engines operating in dual-fuel mode are limited at high loads and do not handle transients as well as diesel engines. It is therefore desirable to use a combustion strategy that captures the benefits of both fuels. In addition, when unburned methane escapes via the exhaust, it enters the atmosphere. Using CO_2 as the reference case, CH_4 has 28-36 times the global warming potential over 100 years.

In a dual-fuel engine, the cylinder is charged with premixed natural gas and air. Diesel is then injected in the traditional manner during the compression stroke near top dead center. The higher reactivity diesel fuel spray autoignites, which subsequently ignites the natural gas/air mixture in the vicinity of the burning liquid spray. A visual depiction is shown in Figure 1.1. A dual-fuel spray involves two distinct types of combustion. A non-premixed flame causes the relatively high-reactivity diesel spray to react with available oxygen. This diffusion flame ignites the lean natural gas-air mixture present in the ambient, which combusts in a premixed propagating flame. Compression ratios are in the range of 15-18 for dual fuel operation [3].



Figure 1.1: A comparison between the proportions of fuel used in traditional diesel

operation (a) vs. dual-fuel operation (b).

1.2 Validation Experiment Simplification

Some of the issues associated with dual-fuel combustion can only be studied either through direct experimentation on an engine or through computer simulations. Because of the high cost of developing, manufacturing, and testing a physical engine, computational models are preferred to predict the behavior of an engine prior to it being manufactured. These models can also provide insight into the physical phenomena that govern behavior; diagnostic experiments on engines are difficult and expensive.

Computational fluid dynamics (CFD) models are used to simulate the behavior of a full engine. Various submodels are employed to simulate the in-cylinder environment, intake and exhaust manifolds, and any other areas in the engine where fluids are interacting. These models combine to form a full computational model that can be very accurate once each of the individual sub-models have been validated. If any of the sub-models are inaccurate, the manufactured engine will perform differently than expected, often in a way that can be detrimental to both engine efficiency and the intensity of the emissions produced. An improper understanding of the subtleties of dual-fuel combustion can also lead to uncontrolled rates of heat release, or knock. It is particularly important to confirm the sub-models that dictate the combustion chemistry. The heat release, which correlates to the pressure rise rate inside of the cylinder, is dictated by a series of high- and low-temperature chemical reactions.

Chemical kinetic models are a collection of chemical species (10 to 5000) that participate in a collection of chemical reactions (20 to 20,000), each with a reaction rate constant that varies exponentially with temperature. The chemical kinetic model governs the process and rate by which the fuel and oxidizer react and proceed through intermediate species (radicals and stable intermediate species) to final products. [5]. Because full CFD simulations with large chemical

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reaction mechanisms are very computationally demanding, it is advantageous to make simulations more efficient where possible. To do this, the number of species and possible reactions in a chemical kinetic mechanism must be minimized while maintaining a certain degree of accuracy relative to a larger, more comprehensive mechanism.

Andrew Hockett [6] recently studied the behavior of dual fuel natural gas/diesel combustion and developed a reduced chemical kinetic mechanism for this purpose. Hockett compared multidimensional CFD simulations against an injection timing performed in a 1.9 L diesel engine modified to operate on port-injected natural gas [6]. Using comparisons between experimental and computational data, Hockett et al. developed the CSU141 reduced dual-fuel chemical kinetic mechanism, which can be used in simulations modelling the interaction of chemical species associated with natural gas/diesel combustion. CSU141 contains 141 species and 709 reactions for mixtures of methane, ethane, propane, and n-heptane.

Additional steps can be taken to refine and validate the mechanism developed by Hockett et al. for diesel/natural gas combustion. To confirm the chemical kinetic sub-model, a method is needed that will reflect the chemical kinetics at temperatures and pressures typical of internal combustion engines. However, using entire engines or even individual engine cylinders for experimental chemical kinetic model validation is confounded by the complex geometry and myriad of physical phenomena present in an internal combustion engine. For example, turbulent mixing inside the cylinder strongly interacts with the combustion chemistry, making it difficult to isolate the purely chemical kinetic effects on the heat release rate and autoignition behavior. Thus, a simpler experiment is needed that can more effectively isolate the chemical kinetics effects by minimizing the effects of turbulence, complex geometry, and the droplet/fluid interactions present in fuel sprays. As stated by Marchese et al. [7], "a well-defined, uni-dimensional, time-dependent, laminar, non-premixed combustion problem is critical to developing, testing and validating submodels for diffusive burning processes."

As mentioned before, a dual-fuel diesel spray forms two distinct flames: a premixed flame, which propagates through the ambient and consumes the lower reactivity natural gas, and a stationary, non-premixed flame along the perimeter of the spray profile, which consumes the diesel fuel as it flows out of the injector. An experiment that allows the fuels to combust in a similar manner but in a more simplified geometrical configuration is desirable. Combustion of single droplets as a means to elucidate the underlying physics of sprays has been studied for over half a century with the first studies investigating droplet combustion occurring in the 1950s [8]. Despite the long history research on the combustion of liquid fuel droplets, little or no work has been done to date on the combustion of a highly reactive liquid hydrocarbon droplet in less reactive gaseous fuel/oxidizer mixture engine-relevant temperatures and pressures. As described herein, vaporization, ignition and combustion of suspended hydrocarbon droplets in methane/oxygen/inert environments at elevated temperatures and pressures was accomplished by means of a rapid compression machine as a simple but powerful analog for the dual-fuel combustion environment.

1.3 Droplet Theory

In this section, the classical theory of combustion of a liquid droplet in an oxidizing environment will be briefly reviewed. Then, the classical theory will be modified conceptually to predict the behavior of a combusting droplet surrounded by a methane-air mixture. For both theoretical droplet combustion scenarios, we examine a cool (\sim 300 K) single-component fuel droplet suspended inside a quiescent, infinite, ambient environment that is at a hot temperature (\sim 1000 K). We assume the absence of a gravitational field so that buoyancy effects can be ignored

and the droplet can be assumed to be spherically symmetric. This allows the assumption to be made that all mass and energy transport will be purely in the radial direction. All quantities and derivatives will only have a radial component.

For the classical case, the ambient is composed of an arbitrary concentration of inert and oxidizer. Figure 1.2 shows the radial profiles of fuel mass fraction, oxidizer mass fraction, and temperature sometime after the droplet has been suspended in the ambient environment. The grey circle located at the origin represents the liquid droplet. The horizontal axis represents the radius (measured from the center of the droplet), and the vertical axis represents the magnitude of species mass fraction or temperature. The plot shows the concentration of fuel at a given finite time after the droplet has been introduced, and a fraction of the droplet fuel has evaporated and has mixed with the oxygen some distance away from the droplet surface. The mass fraction of fuel at a given distance away from the droplet surface is determined using the assumption of vapor-liquid equilibrium at the droplet surface, which states that the concentration of vapor species will be determined by the composition of the liquid phase, including species concentration and temperature. The temperature profile approaches uniformity as $r \rightarrow \infty$ and approaches the cold droplet surface temperature as $r \rightarrow r_s$. Because heat transports from higher to lower temperatures, it can be assumed that heat is being transferred into the droplet surface. For the purposes of this theoretical section, we will assume this to be the initial state (t = 0).



Figure 1.2: Radial profiles of fuel, oxidizer, and temperature for a droplet in a hot ambient

and t = 0





Figure 1.3A depicts the onset of ignition, which will occur at some distance from the droplet surface after a finite delay period during which is governed by energy and mass transport times and a chemical kinetic induction period. For a large (\approx 1 mm) high-reactivity fuel droplet such as n-heptane in a moderately high temperature air (\approx 1000 K) at 1 atm, the ignition delay

period (as conceptualized by the time period between Fig. 1.2 and 1.3A) is approximately 250 ms [7]. Beginning at the initial state and up to this point, thermal energy is transported to the droplet surface. This is made clear by the slower temperature rise in the ambient environment immediately adjacent to the droplet surface. Part of this thermal energy is balanced by evaporating the liquid fuel and the remainder of the heat is transferred into the liquid interior. Fuel evaporated by this heat addition diffuses radially outwards and mixes with the oxidizer present in the ambient. Diffusion of fuel from the droplet surface is apparent from comparing the Y_{fuel} curves at the initial (Figure 1.2) state and in Figure 1.3A. One key feature of this temporal snapshot is the local increase in temperature and associated depletion in Y₀₂ in the far field. These phenomena are the result of temperature-sensitive exothermic reactions occurring in the far field. Although the Y_{fuel} curve does not appear to be much above zero at this point, there exists enough fuel that has spent sufficient time in the hot, oxygen-rich environment, that a certain energy threshold has been met. Once this energy requirement has been met, the exothermic reactions dominate the endothermic ones. In the earlier stages of the ignition process, these reactions produce a local region of heating. This local heating increases the reaction rate, causing more heat to be released, in turn speeding up the reaction rate. This repetitive process is called thermal runaway and is the mechanism that drives spontaneous ignition, or autoignition [9]. For a large (≈ 1 mm) high-reactivity fuel droplet such as n-heptane in a moderately high temperature air (≈ 1000 K) at 1 atm, the ignition delay period is approximately 250 ms [7].

Not long after the state described in Figure 1.3A, on the time-scale of perhaps a few hundred microseconds, the state shown in Figure 1.3B occurs. Thermal runaway leads to higher temperatures that create faster and faster chemical reactions. The peak of the resulting temperature profile is well above the ambient temperature and corresponds to the location of the non-premixed

flame front. Also worth noting is the change in the position of this peak temperature. As the fuel is depleted, the rate at which fuel is consumed at the flame front exceeds the rate at which fuel diffuses from the droplet surface. The flame front will move towards regions of higher fuel concentration. Because both the Y_{fuel} and Y_{O2} curves are non-zero at this point, the flame can be thought of as a premixed propagating flame. Because flame propagation happens very quickly, the state described in Figure 1.3C occurs a very short time after preceding state in 1.3B.

In 1.3C, the Y_{02} curve is very near zero. Since the flame front travelled from a fuel-rich environment, the fall of oxygen to near zero suggests that it is at this point that the maximum amount of fuel is being consumed from a maximized rate of reaction. This also correlates to the position where maximum flame temperature that will occur.

In Figure 1.3D, the premixed fuel and air mixture has been exhausted and the flame transitions to a non-premixed, transport-limited flame. From the droplet side, the flame consumes fuel vapor that is evaporating from the droplet surface, and oxidizer diffusing in from the ambient. Peak flame temperatures are slightly lower then the initial peak because the evaporated fuel has spent less time in the premixed hot environment. This state will exist until the combustion process has evaporated and consumed all of the liquid fuel.

It is worth noting that, in all of the states depicted, the far-field values asymptote to a fixed value as $r \rightarrow \infty$. This results is a mathematical characteristic of all spherically-symmetric domains due to the divergence of the flow field. Through all stages of ignition and burning, the far-field values remain the same as described in the initial state. These boundary conditions are also useful for computer simulation of droplet ignition and combustion.

Once the initial autoignition event has occurred, combustion of the gas-phase proceeds in a quasi-steady manner, meaning that the rate of fuel consumption due to combustion is balanced by evaporation from the droplet surface ($\dot{m}_{f,vap} = \dot{m}_{f,comb}$). Along with this requirement, the radial profiles of temperature (T), fuel mass fraction (Y_F), and oxygen mass fraction (Y_O) remain roughly constant when the radial coordinate is normalized by the time-dependent droplet radius, $r/r_{\rm s}(t)$. This phase of combustion is termed quasi-steady because recession of the droplet surface due to evaporation is sufficiently slow compared to the flux of gas-phase species, so gas-phase transport is assumed to be steady. A diagram depicting quasi-steady liquid fuel droplet combustion is presented in Figure 1.4. The liquid fuel contained in the droplet evaporates from the surface and diffuses outwards towards the flame front (shown as the dotted circle). The mass fraction of fuel is denoted by the thick line. Oxidizer diffuses from the far field and reacts with the combustible fuel at the flame front. The mass fraction of oxidizer is denoted by the dark dashed line. Combustion products (NO_x, CO₂, H₂O, etc) diffuse radially outwards away from the droplet surface. Useful results can be obtained if one assumes that the activation energy approaches infinity. This assumption is called the reaction sheet limit and is the foundation upon which classical droplet theory is built. When activation energy is very high, the region over which the chemical reactions take place becomes infinitely thin, which is referred to as a reaction sheet.



Figure 1.4: Quasi-steady reaction sheet diagram with profiles for temperature, reactant mass fraction profiles, and product fluxes [9].

The following section will summarize the derivation of the d² law as presented in Law [10]. The mass rate of consumption of reactants during a combustion process is described by Equation 1.1:

$$m_c = 4\pi \left(\frac{\lambda}{c_p}\right) r_s \cdot \ln\left[1 + \frac{c_p(T_\infty - T_s) + \left(\frac{Y_{O,\infty}}{\sigma_O}\right)q_c}{q_v}\right]$$
(1.1)

where λ is thermal conductivity, c_p is the specific heat at constant pressure, m_c is rate at which fuel mass is being consumed via combustion, r_s is the radius of the droplet surface, T_{∞} and T_s are the ambient and surface temperatures, respectively, q_v and q_c are the heat generation rates for the vaporization and combustion processes, and $Y_{O,\infty}$ is the ambient oxygen concentration.

The time rate of change of droplet mass is described by Equation 1.2:

$$m_{\nu} = -\frac{d}{dt} \left(\frac{4}{3}\pi r_s^3\right) \rho_l \tag{1.2}$$

where ρ_l is the density of the fuel in liquid form. If we assume a steady-state burning process, this inherently also assumes that all fuel that evaporates from the droplet surface also gets consumed by the flame, meaning we can equate the two above equations.

$$4\pi \left(\frac{\lambda}{c_p}\right) r_s \cdot \ln\left[1 + \frac{c_p(T_{\infty} - T_s) + \left(\frac{Y_{O,\infty}}{\sigma_O}\right)q_c}{q_v}\right] = -\frac{d}{dt} \left(\frac{4}{3}\pi r_s^3\right)\rho_l$$
(1.3)

With some manipulation, the above equation can be simplified to the following:

$$\frac{dr_s^2}{dt} = -K_c \tag{1.4}$$

where K_c is referred to as the burning rate constant for the droplet as follows:

$$K_{c} = 2 \frac{\left(\frac{\lambda}{c_{p}}\right)}{\rho_{l}} \ln\left(1 + \frac{c_{p}(T_{\infty} - T_{s}) + \left(\frac{Y_{O,\infty}}{\sigma_{O}}\right)q_{c}}{q_{v}}\right)$$
(1.5)

Using the initial condition $r_s(t = 0) = r_{s,0}$, the following is obtained:

$$r_s^2 = r_{s,0}^2 - K_c t \tag{1.6}$$

The equation is made in terms of droplet diameter by substituting $r^2 = d^2/4$ to yield:

$$d^2 = d_0^2 - 4K_c t \tag{1.7}$$

This result is the classic d-squared law, stating that the square of the droplet diameter will decrease linearly with time, which is consistent with experimental results for the combustion of a single component liquid droplet.

This classical model for droplet combustion is limited to a single fuel combustion scheme, with only inert and oxidizer species present. To accommodate dual-fuel droplet combustion behavior, the classical model must be conceptually modified. The following profiles (Figure 1.5 through Figure 1.8) correspond to those contained in Figure 1.2 and Figure 1.3 (A-D), with modifications made to adjust the behavior for the presence of a low reactivity fuel (LRF) in the ambient. This term "low reactivity fuel" is used because dual-fuel combustion typically requires that the fuel in the far-field not ignite easily on its own due to ambient temperature and pressure conditions. In the case of the experiments and simulations described herein and elsewhere, the LRF was methane gas. Liquid n-heptane served as the diesel surrogate, which was considered as the high reactivity fuel (HRF) for these experiments.

In Figure 1.5, similar to the classical model, an initial state has been established at t = 0. Note the addition of the Y_{LRF} profile, showing the concentration of methane in the ambient.



Figure 1.5: High reactivity fuel has begun to evaporate [Original figure by M. Baumgardner. Reproduced with permission]

Similar to the classical model, a portion of the HRF has been allowed to evaporate into the hot, lean fuel/air ambient and thus a concentration gradient has been established some distance into the far-field. This snapshot corresponds to Figure 1.2. At some point far enough away from the droplet surface to achieve sufficiently high reaction rates, thermal runaway begins due to the presence of the HRF. Some of the LRF is consumed in this process, shown by the dip in Y_{LRF} shown in Figure 1.6. At the "Point of Ignition" labeled in Figure 1.6, two flame fronts are established, and will move away from each other. The release of thermal energy from the chemical reactions associated with the burning of the HRF are such that the threshold to sustain a propagating flame through the lean fuel/oxidizer mixture in the ambient is met. It is important to note that although the flame appears to be a 2D travelling plane, it should thought of as a spherical shell growing or shrinking in diameter.



Figure 1.6: Thermal runaway begins near the limit of diffusion for the high reactivity fuel. [Baumgardner]

The first flame front shown in Figure 1.7, labeled " $T_{F,1}$ ", is similar to the classical nonpremixed flame, located at the intersection of the oxidizer and the evaporating HRF. If the lean LRF/oxidizer mixture is above the lean flammability limit, then a second, propagating pre-mixed flame will develop, travel outward away from the droplet surface, and consume the LRF.



Figure 1.7: Two flames develop. The first is a non-premixed diffusion flame which is held near the droplet surface. The second is a premixed flame which propagates through the

premixed fuel/air. [rendering courtesy of Marc Baumgardner]

Since the ambient fuel/air mixture is lean, as the propagating flame travels outward, it consumes some portion of the ambient oxidizer, with the remainder being left behind to be consumed by the non-premixed flame. This is shown in Figure 1.7. At the pre-mixed propagating flame front labeled " $T_{F,2}$ ", the profile for Y₀ increases to the right, as oxidizer levels approach ambient concentrations. To the left of $T_{F,2}$, the Y₀ continues to decrease as it is consumed by the semi-stationary diffusion flame. In theory the oxidizer concentration will reach zero as it is consumed by the diffusion flame. The position of the diffusion flame front will adjust to a point on the Y_{HRF} curve where stoichiometric conditions exist. In other words, depending on how much oxygen remains after being consumed by the propagating flame, the flame front will position itself to burn as much fuel as is possible.

The propagating flame will continue to move outwards into the ambient infinitely, by definition of the spherically symmetric domains. In reality, the flame will continue until it reaches the wall of a combustion chamber bound by the harsh reality of quenching at the walls. The cool

wall that the flame will inevitably come into contact with will cause the reaction rates to slow and the flame to extinguish. As shown in Figure 1.8, the non-premixed diffusion flame remains at a point where stoichiometric conditions exist, and will extinguish as the local reaction time becomes of the same order as the flame residence time, or once the all of the liquid fuel contained within the droplet has evaporated.



Figure 1.8: Once the premixed fuel/air is consumed the second flame extinguishes leaving only the non-premixed flame near the droplet. [Baumgardner]

1.4 <u>Rapid Compression Machines</u>

Because the evaporation and combustion of the injected fuel is so crucial to the efficiency of combustion inside of an engine cylinder, it is advantageous to study the evaporation behavior of the fuel under conditions similar to the in-cylinder environment. The conditions at TDC in an IC engine are near the critical/supercritical boundary for liquid hydrocarbons where droplet combustion theory breaks down and many spray models are based on simplified droplet evaporation theory. Extensive droplet testing has been performed in hot furnace environments at low to moderate pressure and elevated temperatures. In these experiments, a droplet is suspended, and very quickly a furnace is lowered over the droplet, effectively raising the temperature instantaneously; however, the experiments are typically conducted at roughly 1 atm. In order to achieve dual-fuel droplet combustion, you need and RCM, otherwise the gaseous fuel-air mixture would want to react as well.

Typically, rapid compression machines (RCMs) are used to test the reactive properties of fuels at engine-like pressures. A RCM simulates a single compression stroke of an internal combustion engine without the complex bowl geometry, cycle-to-cycle variation, and other complications associated with engine operating conditions [11]. A RCM combustion chamber is filled with a pre-determined mixture, and one or two pistons compress the volume when the RCM is fired. Piston compression causes a sharp rise in pressure inside of the chamber. This pressure rise also leads to a sharp rise in temperature, similar to the behavior of an engine cylinder. RCMs allow combustion researchers to study low-to-intermediate autoignition chemistry in engine-like conditions by quantifying changes in ignition delay as a function of temperature, pressure, and fuel/oxygen/diluent ratio. In addition, they can be equipped with optical setups that allow a wide range of combustion analytical methods to be applied to RCM experiments. Because of the ability to achieve high consistency between test results, RCMs are good tools for comparing and confirming chemical kinetic mechanisms.

Ignition delay is a widely used parameter to define the ignition characteristics of a fuel. Various instruments can be used to quantify ignition delay depending on the time scale of the expected delay. Shock tubes are widely used to quantify ignition delay times with high accuracy in the range of microseconds to approximately 10ms. The reliability of the test conditions deteriorates after residence times of greater value. For certain fuels and combustion conditions, 10 ms is not enough time for the mixture to autoignite. RCM's can measure ignition delays in the range of roughly one to hundreds of milliseconds. Thus, RCMs can be used to study autoignition characteristics over a wide range of fuels with slower reactivity than shock tubes would allow.

Particularly in temperature ranges of 600 to 1100K, the RCM is a very effective tool for carrying out these studies. The typical measuring ranges of shock tubes and RCMs are compared in Figure 1.9.



Figure 1.9: Ignition delay plot showing the range of measureable ignition delays for RCMs and shocktubes, compiled by the National University of Ireland-Galway.

Example pressure traces, recorded during compression of different inert species in an RCM, can be seen in Figure 1.10. The compression process is assumed to be adiabatic. This assumption is possible due to an assumed "adiabatic core region", which allows heat loss from the hot gasses to the relatively cold chamber walls to be neglected. Past research [12] [13] [14] has shown that the gas region shown in Figure 1.11 can be considered to compress in an isentropic manner. This assumption allows for a useful simplification when estimating the compressed temperature from the pressure trace. The adiabatic core assumption may only be made during a short period of time after the compression event. After that time elapses, the heat transfer between the hot gas core and the cool metal walls of the chamber becomes too great to ignore.



Figure 1.10: A sample pressure trace of 100% Ar and 100% N2 Inert Mixtures [15]



Figure 1.11: Cylindrical slice of RCM combustion chamber at TDC. The approximate

adiabatic core region is highlighted.

The adiabatic core, which can only be assumed in the absence of fluid motion effects, is also beneficial to droplet combustion inside of the RCM. The success of droplet experiments is heavily influenced by the effect of fluid mechanics on the body of the droplet itself. In a violent and turbulent test setting, a droplet hanging in the center of the chamber may be dislodged. In the absence of fluid effects, a droplet hanging in the center would, in theory, remain stable. In addition, the spherically-symmetric nature of the radial profiles for species concentration and temperature depend on a theoretical homogeneous far-field. The domain of RCM experiments is limited by the walls of the RCM combustion chamber; however, if these profiles can stay consistent out to a certain distance from the droplet surface, test conditions may be adequate.

The validity of the adiabatic core assumption depends on the configuration of the RCM pistons. Despite there not being many in use, RCMs have a wide range of designs. A majority employ only a single-piston that compresses the chamber against a static opposite end (see Figure 1.12 bottom). The CSU RCM consists of a dual-piston design, in which two pistons, fired from opposite sides of the combustion chamber, symmetrically compress the volume around a centerline (see Figure 1.12 top). The adiabatic core is made possible because of the relatively calm nature of the center of the chamber during perfectly symmetrical compression.



Figure 1.12: Approximate speeds at various points in the chamber during compression for two RCM designs.

If the piston were a flat profile with the outer edge flush with the walls of the chamber, the compressive motion would cause the stagnant boundary layer to form rollup vortices and disturb the center region, invalidating the adiabatic core assumption. Rollup vortices can be minimized using a creviced piston design (see Figure 1.13). As the pistons compress, the thermal boundary
layer along the sleeve wall is absorbed into the crevice instead of rolling up and forming vortices in the main part of the chamber.



Figure 1.13: Cross section of flat piston compared to a creviced piston. (Note: Radial clearance between piston and sleeve not to scale) [Original figure by Marc Baumgardner. Reproduced with permission.]

A study [11] was conducted using planar laser-induced fluorescence (PLIF) to observe disturbances in the flow field. The original flat piston design was compared to the new creviced piston design. The differences in the behavior of those fluids fields are shown below. The study showed a much more uniform temperature field for the creviced piston case, which can be used to assume that fluid disturbances are at a minimum.



Figure 1.14: Comparison of the flow field disturbances with creviced and non-creviced pistons [11].

A CFD analysis was conducted by Siddhesh Bhoite to explore the sensitivity of the crevice width to the disturbances in the adiabatic core region [16]. It was expected that, as crevice volume decreased, the boundary layer rollup effect would become more pronounced. The simulation results are shown in Figure 1.15. The results showed that as the crevice width is increased, the vortices formed on the face of the pistons become smaller.



Figure 1.15: Simulation of the turbulent effects of varying the crevice volume width. (a) 3mm. (b) 4mm. (c) 5mm.

In the past 10 years, several studies have been conducted on the behavior of fuel droplets inside of an RCM or in RCM-like conditions. Kim et al. used an RCM to study the evaporation of a single n-heptane droplet [17]. They found that evaporation effects on the droplet due to temperature and pressure were offset, confirming the classical d² law of droplet evaporation. In addition, Kim found that for a given compression ratio, the evaporation rate increased nearly linearly for a consistent decrease in droplet diameter. This result can be explained by the mathematical phenomena in spherical geometry where the ratio of the surface area to volume is inversely proportional to the radius. Kim et al. also found that, although the compression time affects the speed at which the droplet temperature reaches its maximum, the overall droplet evaporation rate remained constant as compression time varied, all other variables kept equal. It was inferred that this discovery showed that the time after TDC was much more important than the time previous regarding influence on the evaporation rates. Kim et al. since expanded on this work and looked at the combustion of binary fuel droplets in an RCM [18]. By examining the

combustion behavior of droplets of n-heptane mixed with iso-octane or n-decane suspended in an ambient oxidizing environment, it was discovered that the evaporation of the individual species, along with their chemistry behavior, factored heavily into trends in ignition delay for these droplets. The Kim studies did not explore the behavior of n-heptane droplets suspended in an ambient lean gaseous fuel/oxidizer environment. This gap in the literature has been explored during the work presented in this thesis. Included in this gap is the lack of optical observation of dual-fuel combustion in an engine. This work aims to fill these gaps in the literature.

Previous work on the RCM at CSU has explored the effects of fuel additives on the combustion behavior during spark ignition and laser ignition of methane/air mixtures [19]. A sample image, showing the initial stages of the propagating methane flame, can be seen in Figure 1.16. These images were taken during a laser-ignition campaign carried out at CSU in our RCM. Because methane is a low reactivity fuel, a concentrated burst of energy in the form of a laser spark was required to ignite the fuel.



Figure 1.16: A lean methane/air mixture is combusted via laser ignition in the CSU RCM

[19].

1.5 <u>Thesis Overview</u>

This thesis presents work directed toward modifying the CSU RCM to accommodate droplets and observe their evaporation and combustion under various conditions. The research was motivated by the need to further understand the phenomena associated with dual-fuel combustion. Along with the computational modelling carried out at the Powerhouse, this research will help to inform future generations of combustion scientists as the boundaries of advanced engine operation and combustion physics are pushed. A combination of experimental and computational methods was employed to explore the behavior of a liquid fuel droplet in a dual-fuel environment. Experimental work was carried out in the CSU Rapid Compression Machine (RCM) and the computational work was carried out by Siddhesh Bhoite [16], building on the preliminary work done by Andrew Hockett [3]. All simulations were carried out using the CONVERGE numerical modelling software.

The premise of the work focuses on the idea that the chemical kinetics of a diesel engine operating under "dual-fuel conditions" can be focused on and studied in simpler experimental and computational conditions while maintaining the accuracy of the chemical kinetic model. With additional understanding of these in-cylinder dynamics, engines running under these conditions can be designed to operate more efficiently and with lower emissions.

Chapter 2 will cover all details of the experimental setup including RCM operation, modification, and issues associated with each. Since the RCM is typically used to study the autoignition characteristics of gaseous fuels, a modification was required to accommodate the suspension and combustion of liquid droplets. The experimental plan will also be outlined. Chapter 3 will cover the results of both the computational simulations performed by Siddhesh Bhoite and

the experimental work performed by Colin Gould. Chapter 4 will summarize the findings from the project and provide recommendations for future work.

2 Experimental Methods

2.1 <u>RCM Overview</u>

The CSU Rapid Compression Machine (RCM) was designed and manufactured by Marine Technologies Ltd. in Galway, Ireland, and delivered to CSU in 2012. The CSU RCM follows a dual-piston design that was adapted from an older RCM designed by Shell and installed at the National University of Ireland – Galway.



Figure 2.1: Overview of CSU RCM.

The compression ratio of the CSU RCM can be changed by either varying the geometry of the piston head or removing metal compression spacers that change the initial position of the entire piston assembly. For all of the experiments presented in this thesis, the compression ratio was held constant at approximately 11.6:1 as shown in Figure 2.3. The exterior of the RCM combustion chamber and sleeves can be seen in the figure.



Figure 2.2: External View of RCM Combustion Chamber



Figure 2.3: TDC and BDC positions of the RCM pistons in the combustion chamber and sleeves. 1: Chamber Body Diameter: 4.3in 2: Combustion Chamber Diameter: 0.75in

This compression ratio was determined by using Chemkin to develop a volume trace that reproduced the measured pressure curves from RCM experiments. Depending on how heat loss

is accounted for in the calculation, the actual physical compression ratio may be slightly different. When measuring the volumes of the TDC and BDC positions of the CSU RCM, the CR was found to be 12.5, compared to the 11.6 calculated in the Chemkin simulations. Additional specifications of the CSU RCM can be seen below in Table 2.1.

Table 2.1: Specifications of CSU RCM.

Parameters	Values
Reaction chamber piston diameter	38.05 mm
Driving chamber pressure range	100 - 250 psi
TDC piston spacing	20 mm
BDC piston spacing	335 mm
Compression ratio	~11.6
-	

Each piston is driven using pressurized air which moves the piston assembly during the compression stroke. Hydraulic fluid is used to keep the pistons locked back until the machine is ready and has been given the command to fire. The layout of the hydraulic and pneumatic chambers can be seen in Figure 2.4.



Figure 2.4: The internal chambers of the RCM.



Figure 2.5: Top View of RCM Hydraulic and Pneumatic Chambers

The RCM combustion chamber, made of Super Duplex stainless steel, is located at the centerline of the machine, as shown in Figure 2.6. Most ports for optics or instrumentation were located adjacent to the TDC volume. The chamber has an outer diameter of 4.5 inches and an inner (chamber) diameter of 1.5 inches, as shown below in Figure 2.7.



Figure 2.6 Position of RCM Combustion Chamber



Figure 2.7: Cross Section of Droplet RCM Combustion Chamber. 1) 4.5 inches. 2) 1.5 inches.

Creviced pistons are used to minimize vortices caused by the boundary layer fluid build-up during compression. A crevice with a width of 4mm is machined into the piston head ~4mm behind the front piston surface. A taper is also machined between the crevice and the main volume of the

combustion chamber. The combination of the taper and the crevice serve a vital role in maintaining the stability of the adiabatic core region.

2.2 <u>Modification of the RCM for Droplet Experiments</u>

2.2.1 Experiment Requirement

Typically, RCMs are not used to ignite liquid fuels. If a liquid fuel needs to be tested in the RCM, mixing tanks are typically used to vaporize the fuel prior to charging the combustion chamber. A modification to the RCM combustion chamber setup was needed to allow for the suspension of liquid droplets. In addition to the primary combustion chamber, which was used for previous experiments in the lab (including methane autoignition, fuel additive characterization [15] and laser spark ignition [19]), CSU had a backup combustion chamber with minimal machining performed to the body. This secondary chamber was modified and used for droplet suspension as needed by this project.

The modification could not allow any leakage from the combustion chamber. In addition, the modification could not include any protrusion into the chamber that would damage the pistons as they compressed the gas phase. Because the modification had to remain leak free, the method used to deposit the droplet in the chamber could not have any pathway to the outside of the chamber at the moment of piston firing. For example, if a syringe was used to deposit the droplet, the syringe had to be removed from the chamber, prior to firing, while maintaining a negligible mass loss.

Because of the turbulent nature of the inside of the chamber during firing, the suspension mechanism needed to keep the droplet from falling or being blown sideways. In past research, a variety of methods and materials have been used to accomplish these goals. Thermocouples,

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silicon carbide fibers, and formed quartz rods have all been used in a variety of applications to hold up a droplet.

2.2.2 Original Setup of Secondary RCM Combustion Chamber.

The combustion chamber attaches to the main body sections of the RCM on each side by six bolts that attach the chamber to identical flanged sleeves. Because of the depth of the bolt holes, there is only space to machine ports in the six positions between the bolts. These six positions are labeled in Figure 2.8. The secondary chamber included machined access ports as part of its original configuration. The first (position 1) is a gas insertion valve. Any gaseous species that go into the chamber will be put in through this valve; filling and vacuuming operations occur through this valve. Located in position 4 on the bottom of the chamber is the port for the high-speed pressure transducer. Both of these ports and corresponding hardware are essential to basic RCM operation. Unless a specific need arises for the ports to be moved, they will stay as originally machined. Ports 2 and 5 were used to accommodate the requirements of the Schlieren imaging that will be discussed in Section 2.3. In the original chamber, there is also a stepped hole at position 6 that could be modified slightly to allow the installation of additional hardware or ports. Ports 3 and 6 were available for modification to enable hanging of droplets inside of the chamber, as seen in Figure 2.9.



Figure 2.8: Port Positions Labeled



Figure 2.9: Cross-section of RCM combustion chamber, with the space available for droplet suspension modification highlighted in red.

2.2.3 **Droplet Hanging Mechanism**

Modifying the RCM to accommodate droplets required studying the literature to learn from the methods used in previous work as well as a bit of creativity to fit the specific needs of our experiment given the unique design of our RCM. Because most RCMs are of the single-piston design, much of the literature on RCM droplet experiments details droplet suspension inside of a chamber that is very different from ours. In a dual-piston RCM, the pistons compress the volume in a symmetric manner as shown previously in Figure 1.12, with a theoretical stagnation point at the center line of the volume. Because of operational issues associated with the RCM which will be detailed in section **Error! Reference source not found.**, this geometrically symmetric dualiston design led to issues that affected our ability to reliably keep the droplet on the suspension device. In single-piston RCMs, the droplet is suspended close to the static wall, as shown in Figure 2.10. As shown previously in Figure 1.12. This feature of single-piston RCMs has multiple effects. Since the droplet is close to the wall, there very little flow past it, since the volume is compressed from the opposite end of the chamber. In addition, since there is no second piston, piston offset is no longer an issue.

Regardless of the suspension mechanism design, it must not impede normal RCM firing. While testing gaseous fuels (mixtures with no droplet), the following procedure is used (and repeated):

- 1. The combustion chamber is vacuumed to clear any products from previous tests. $(P_{chamber} \leq 10 \ mBar)$
- 2. The components of the desired mixture are added individually by partial pressures (P_i) until the final mixture pressure (P) has been reached and all *i* species are present. $\sum_{i=1}^{n} \frac{P_i}{P} = 1.0$

- 3. The charging sequence begins: hydraulic locking, pneumatic charging.
- 4. The RCM is fired and the mixture reacts.
- 5. Return to step 1.

It is unavoidable that upon placement inside the chamber, some portion of the liquid droplet volume will evaporate and mix with the surrounding gases. Thus, it is crucial to minimize the amount of time between droplet placement and firing of the RCM. Compounded with this; if a droplet is placed in the chamber during the vacuuming process, the droplet will evaporate and vacuum out of the chamber very quickly. The droplet must be placed while the pressure inside the chamber is at roughly atmospheric to minimize undesired evaporation (occasionally droplets are allowed to evaporate to establish a radial concentration of the high reactivity fuel). This requirement means that the droplet must be placed in the chamber once the final chamber mixture is set. Because the composition of this mixture is very important to the accuracy and repeatability of the RCM tests, gas cannot be allowed to escape to the outside or exchange with the outside ambient. Lower than expected compressed pressures could occur if gases are allowed to equalize between the ambient pressure outside of the chamber (~840 mBar) and the pressurized section inside (1000 mBar). The result could be a mixture that, given a proper initial pressure and composition, might have reacted, but because of leakage, did not. This is not desirable.

Because of the limited space inside of the RCM chamber, the droplet must be deposited from a source that lies external to the combustion chamber itself. Syringes are a widely used method for depositing a droplet inside of combustion zones and were an early front runner for use in our RCM droplet experiment [20]. If a syringe is used, the chamber should remain sealed during the syringe insertion, droplet deposition, and syringe removal processes. The syringe must be removed from the chamber prior to the firing of the RCM. If the syringe needle is present in

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the chamber during compression, the pressure rise will make its way through the needle and into the body of the syringe, potentially causing the glass to explode.

Previous studies investigating the behavior of droplets have used a variety of suspension methods. In numerous microgravity and zero gravity experiments, the droplets are held up using retractable devices such as the electrodes used to induce ignition [20] or needles. Kim et al [18] used a thin-wire thermocouple to hold an n-heptane droplet in place close to the optical viewing port at the end of their single-piston RCM, seen below.



Figure 2.10: Single-piston droplet suspension setup by Kim et al [17].

Thermocouples have demonstrated the ability to suspend droplets with great effectiveness in other studies as well **[21]**. They are extremely flexible and can be shaped to hold a droplet in a specific place. In addition, if the thermocouple is located inside of the droplet, acquiring accurate temperature data will be feasible. Previous work by Thomas Falloon explored the use of a thinwire thermocouple as the deposition location for a droplet. An example of his work can be seen in Figure 2.11. A K-type, un-insulated thermocouple with a wire diameter of 0.005" was mocked up inside the secondary combustion chamber. A syringe was used to inject a liquid droplet onto the thermocouple in-situ. The work was limited to the relationship between the thermocouple and the droplet at rest in the chamber. No work was done to study how a thermocouple would work inside of a sealed RCM chamber where there must also be a transfer of the droplet to the suspension device without the transfer of gasses between the sealed chamber and the ambient in the room. Depending on the conditions inside of the chamber, the thermocouple may change positions, making it a hard target if a syringe is used to insert the droplet. In addition, the thermocouple was not tested to study the effects of being immersed in a turbulent reaction zone similar to the RCM. Because of these combined factors, thermocouples were temporarily set aside as a possibility for droplet suspension.



Figure 2.11: Droplet suspended from a thin-wire thermocouple inside RCM combustion chamber.

Formed quartz rods have also been used to suspend droplets inside of combustion chambers. These rods have the advantage of low propensity for conduction through the body of the holder. It is very important that as much of the available heat around droplet be transferred directly to the liquid, allowing the maximum amount of evaporation to occur. Compared to metal thermocouples, the droplet temperature will drop negligibly due to the high conduction resistance that is inherent in ceramics. Quartz rods are also relatively easy to form. This becomes useful when needing to adapt the material to the confined space of a combustion chamber. In our case, the suspension mechanism must fit inside of a horizontally oriented cylinder that is 1.5 inches (38.1mm) in diameter and a height/length of 0.787 inches (20mm). In the case of droplet combustion inside of such a confined space, it is particularly advantageous to have a suspension device that is easily shaped to fit the dimensions of the chamber and also strong enough to withstand the heat in the chamber.

In previous studies, silicon carbide (SiC) fibers have been used to suspend droplets in test chambers. Avedisian et. all used two crossed fibers to suspend a droplet in a drop tower microgravity test chamber [20]. This general design is shown below in Figure 2.12, however there are more than two fibers used to suspend the droplet. There is no reason given in the referenced paper as to why multiple fibers might be an advantage. SiC fibers are good insulators, therefore heat transfer from the droplet into the fiber can be considered negligible. In addition, at 10 μ m, the fiber does little to interrupt the flame from consuming the fuel around the fiber. If it were larger, there might be some issues with the flame hugging the body of the suspension mechanism.



Figure 2.12: An n-Butanol droplet suspended via a web of SiC fibers [20].



Figure 2.13: An early test of crossed wire suspension. Wires are made of stainless steel.

Droplet diameter is ~2mm.

Building on this concept, a fiber suspension mechanism was designed that incorporates an epoxy bead placed in the middle of a single SiC fiber that spans the expected combustion zone.



Figure 2.14: Original plug and glass rod mechanism. A SiC fiber is glued to each glass rod at a position along its length which will place it in the center of the chamber.



Figure 2.15: Original epoxy and SiC fiber mechanism, rotated 90 degrees.

Due to sealing issues with the original plug design, the glass rod/SiC fiber suspension mechanism was modified to accommodate the new plug design (see Figure 2.16).



Figure 2.16: Modified droplet plug and hanger. 1) Section view in place in chamber. 2) Isomoetric view.

This design fixed a few of the fundamental issues associated with the original hanger design. The original plug was not self-sealing. In the original plug design, a plate was mounted to the outside of the chamber with an aramid gasket to hold pressure. Unfortunately, while this system did well to hold vacuum pressure, it did not perform as well when the chamber was subjected to high positive pressure. This led to large mass losses and an inability for the chamber to reach its highest potential compressed pressure. This original design is shown below in Figure 2.17.



Figure 2.17: Droplet combustion chamber with the original droplet suspension plug in place, with the sealing plate visible.

A cross-section can be found in Figure 2.18. The plug serves two functions: maintaining the sealing integrity of the chamber and holding the droplet suspension mechanism inside the chamber during droplet insertion and RCM firing.



Figure 2.18: Cross Section of droplet suspension plug with copper crush washers at the sealing surface.

In addition, because the glass rods that the fiber attached to were fixed relative to each other, it was very common for the fiber to break off of one side. These two issues were addressed by designing a new plug and modifying the chamber to seal properly. Instead of a traditional gasket design, copper crush washers were designed to hold the pressures experienced during RCM testing. A cross piece was also added to the glass rod assembly to prevent any relative movement between the two rods. This lowered the chance that the fiber would break due to anything other than the epoxy bead catching fire.

Because the SiC and epoxy combination was breaking constantly, and the epoxy bead itself combustible, a more durable material was chosen for use as the suspension mechanism; glass. Glass, or quartz more specifically is an excellent insulator and thus would remove very little heat from the droplet volume compared to the effect a thermocouple might have. Although the SiC was held up using a frame made of the same material, the entire assembly would be made of glass in the newer iteration. This would lower the chance that any part of the hanging assembly would be damaged by high heat or fluid dynamic effects. Early experimentation with glass blowing showed our ability to craft a mechanism that would hold up a droplet. One of those early iterations is shown in Figure 2.19.



Figure 2.19: An early iteration of a glass droplet holder with a droplet suspended from tip.

This technique was improved upon and a permanent hanging mechanism was attached to the existing droplet plug. This plug and droplet holder iteration can be seen below in Figure 2.20.



Figure 2.20: Final droplet suspension mechanism shown attached to the chamber plug.

2.3 Piston Offset Considerations

Due to the design of the hydraulic locking mechanism on the CSU RCM, it is very hard to precisely control the timing of the start of motion of each piston. When the firing command has been given to the RCM control system, the hydraulic pressure on the high-pressure chamber side releases the locking force on the rear end-stop, imposing a positive net force on each plunger assembly which points towards the centerline of the machine. Once this locking pressure has been released, there is a small delay as the static friction forces caused by the interference between the plunger and the various radial seals located along its length are overcome. After these forces have been overcome and the piston assembly begins to move, the friction between the seals and plunger assembly switches from a static to a dynamic friction force. The position profile for each piston once in motion is identical when the offset is accounted for, meaning that the net force on each plunger assembly, including the dynamic friction force on the seals, is very similar in magnitude. A force diagram on the drive plunger assembly is shown in Figure 2.21. Depending on the difference between the static friction forces on the plunger assemblies on the opposite ends of the RCM,



Figure 2.21: Representative Static Force Diagram on the RCM Drive Plunger assembly

there will be a corresponding time delay or offset between the position profiles of the piston as they begin their motion at different times. If the piston offset is greater than ~5 ms, there is a strong likelihood that the resulting asymmetry in the fluid field will cause the droplet to become dislodged from the fiber as was pictured in Figure 2.24. As that figure shows, even very small offsets (1.46 ms) can cause the droplet to become dislodged from the suspension mechanism. This issue can be addressed by making small adjustments to a set of needle valves, each placed adjacent to the inlet to the locking hydraulic chambers on each side. In theory, opening or constricting the flow path would alter the transit time of a pressure wave propagating through, slightly altering the start-of-motion timing for each piston assembly. The effectiveness of this method is difficult to quantify and a lot of guesswork is involved with adjustments.



Figure 2.22: Close up of the needle valve body that sits just above each hydraulic chamber on the RCM.

In addition to the obvious issue of an unsuccessful test when the droplet falls off of the fiber, more issues can arise. If the droplet remains on the fiber after firing, the liquid surrounding the epoxy bead inside of the droplet volume keeps the epoxy bead cool, keeping the bead intact. Even as the droplet burns and the fuel expended, the chamber has become cool enough by that time to not have an effect on the integrity of the bead. However, if the droplet is immediately dislodged, the temperature inside of the chamber in those first moments after TDC can be such that the epoxy bead will autoignite, as shown in Figure 2.23. This is due the relatively low temperature resistance of the epoxy used.



Figure 2.23: Epoxy deposition bead burning after the droplet has fallen off.

While troubleshooting the issue of the droplet falling off of the fiber, the issue of piston speed was considered. At the end of the compression stroke, the pistons are stopped with a metal-tometal contact point inside of the hydraulic fluid chamber of the RCM. The magnitude of the resulting vibrations from this impact is thought to be large enough that they might travel into the combustion chamber and dislodge the droplet from the fiber, as seen in Figure 2.24.



Figure 2.24: Schlieren Image of a piston offset of 1.46ms

2.4 Fuels

In this experiment, n-heptane is used as a surrogate for diesel fuel and methane for natural gas. It is widely accepted that n-heptane has similar ignition delay properties to diesel fuel [22]. For the purposes of this study, methane is considered a low reactivity fuel (LRF) and n-heptane a high reactivity fuel (HRF). In the ambient, methane was used as the fuel in a premixed combustible mixture through which a propagating flame traveled. Equivalence ratios in the far field were varied from $\Phi = 0.5 - 1.0$. In the dual-fuel droplet tests, n-heptane (C₇) was the primary droplet fuel. In the supercritical droplet tests, pentane (C₅), n-heptane (C₇), decane (C₁₀), and dodecane (C₁₂) fuels were used.

n-Heptane is a straight-chain alkane with the chemical formula C_7H_{16} . In anti-knock test engines, n-heptane is defined as the zero-point on the octane rating scale (and iso-octane is defined as having an octane rating of 100). Methane has an octane rating of 120. Heptane was chosen as the zero point on the octane rating scale because of the availability of very high purity n-heptane at the time. Originally distilled either from the resin of Jeffrey pine or from the fruit of Pittosporum resiniferum, plenty was available [23].

Heptane is an explosive fuel that is denser than air when in vapor form with a relative vapor density of 3.5 (Air = 1). At 20°C, the density of liquid n-heptane is 0.68 g/cm³, compared to 1 g/cm³ for water. The vapor pressure at 20°C of n-heptane is 4.6 kPa, or 46 mBar.

2.5 Data Aquisition

2.5.1 **Pressure and Piston Data Logging**

Chamber pressures are recorded at 2.0 MHz using a high-speed pressure transducer (Kistler 603B). To track the piston positions during the firing cycle, two linear transducers are used. The position profiles of each piston, in addition to the pressure data, make up the data output from the

RCM. Picotech's PicoScope PC oscilloscope was used to process test data for logging. An example of the two sets of data super-imposed onto each other can be seen in Figure 2.25. Worth noting is the relationship between the piston position and pressure curves as the pistons both approach top dead center (TDC). As both pistons approach their final position, the chamber volume compresses, causing a rapid increase in pressure, which peaks when the pistons have stopped, and immediately begins to decrease due to heat loss.



Figure 2.25: Piston position and compressed pressure for 100% N2 inside RCM

Because of the relatively slow speed of available temperature measurement methods, temperature is estimated via the following relationship:

$$\ln(\frac{P_{comp}}{P_0}) = \int_{T_0}^{T_{comp}} \frac{\gamma}{\gamma - 1} \frac{dT}{T}$$
(2.1)

Which assumes isentropic relations. P_{comp} and T_{comp} are the compressed chamber pressure and temperature, respectively and P_0 and T_0 are the initial chamber pressure and temperature, respectively. Gamma (γ) is the time-varying, temperature-dependent specific heat value. This value is calculated based on the bulk gas temperature.

2.5.2 Schlieren Imaging

To visualize the droplet combustion process inside the RCM, a high-speed schlieren imaging setup was implemented. Schleiren imaging is a widely used technique in combustion and fluid diagnostics [10]. Pressure traces provide insight into the thermodynamics of the mixture, but often this information does not tell the whole story. Optical imaging of combustion events can provide a window into the process that would not be possible otherwise. Images captured will be useful in providing information regarding the timing of droplet ignition and evaporation data based off the changing diameter of the droplet.

Schlieren works by using a series of lenses and mirrors to send light through a gaseous medium, past a crisp knife edge, and onto the image sensor of a camera. The schlieren image is comprised of two optical phenomena combined into one. Firstly, it acts as a shadowgraph, backlighting any solid or liquid object in the imaging path. Secondly, it exposes areas in the gas with high gradients in density. In the case of a combustion event, this can be very useful, especially if the flame burns relatively cleanly. The flame front passes through a medium, consuming the relatively cool fuel air mixture, leaving behind hot product gases. This is shown below in an example schlieren image from work done by Andrew Zdanowicz and Jeff Mohr.



Figure 2.26: Laser-ignited methane flame imaged using the schlieren system at CSU. Crisp black lines border the areas of products and reactants.

Schlieren images are captured though a 20 mm port bored into the wall of the chamber. At TDC, the clearance between the two piston faces is 25 mm. With a TDC chamber volume of 28.5 cm³ and an imaged volume of 11.96 cm³, 58% of the chamber volume will not be imaged. This makes it especially critical to image the process with as high a frame rate as possible. Lean conditions were tested, therefore the flame speed was slightly inhibited, which assisted the camera in capturing the travelling pre-mixed flame.

The optical setup and hardware were designed by Ciprian Dumitrache and detailed in [19]. Dumitrache et al. used the system to visualize the laser-induced ignition of lean methane-air mixtures. A narrow-band ($\lambda = 400 - 405$ nm) LED (LZ1-10UA00-00U7, LED Engin) provides the source of light that will be focused, collimated, passed through the combustion chamber and refocused onto the image sensor of a high-speed camera (PCO 1200s). A schematic of this system is shown in Figure 2.27.



Figure 2.27: Schlieren system used to image the evaporation and combustion of droplets inside the RCM combustion chamber. a) Narrow band LED. b) 50 mm focusing lens. c)
Iris. d) 50 mm objective lens. e) Mirror. f) RCM Combustion Chamber. g) Mirror. h) 300 mm focusing lens. i) Razor Blade. j) Mirror. k) 50 mm objective lens. l) Narrow-band mirror. m) High-Speed Camera.

Because of the intensity of the flame and the light being produced by it, there were concerns that the camera sensor might be adversely affected by the high amount of light. To combat this, a narrow-pass mirror (400 - 410 nm) was used at the last point before the light was reflected into the camera. In addition to balancing out the intensities of the LED and the luminescence off of

the flame, the narrow pass mirror also eliminated most of the broadband blackbody radiation emitted from the soot during the combustion of the n-heptane vapor.



Figure 2.28: Detail of the Schlieren Setup

The mirror also allows for very accurate and crisp imaging during the combustion process. For droplets in particular, having a sharp image of the droplet surface is important.

The scale of the images is arbitrary, therefore it is very important to get an accurate dimensional calibration. This is done by inserting a glass rod with a very precise diameter into the chamber and capturing an image. With the known dimension, a scale factor can be determined.



Figure 2.29: Glass calibration rod shown placed next to the droplet hanger. The red box is a square with side lengths of 87 pixels, or 1.00 mm.

Measurements of the glass rod were taken in ImageJ (https://imagej.nih.gov/ij/). A square was overlaid onto the rod as seen in Figure 2.29. The area of the square was calculated in square pixels (px^2) and converted to 1.00 mm^2 , since the rod is 1.00 mm in diameter. The calculated area was 7,569 px^2 , resulting in a side length of 87 pixels, giving us our scale factor. 87 pixels is equivalent to 1.00 mm, assuming the dimensions of the schlieren system are kept the same and no magnification occurs due to the change of a lens position along the beam path. Any time a droplet diameter is stated for a CSU RCM experiment in the rest of this thesis, this is the scale factor that was used.

To sync up the images with the pressure trace data, a relation was needed between the two data inputs. The camera is triggered via a voltage signal that is generated when the chamber pressure crosses a certain threshold. This voltage step function is tied into a channel on the
picoscope interface. The timestamp of this voltage spike will correspond to the time stamp on the first image recorded by the camera. This will allow us to relate the timing of any image we see to a point on the pressure trace. When calculating ignition delay, this information will be critical. The relation between the two data streams can be seen below in Figure 2.30.



Figure 2.30: Timing relation between data collection streams.

Where t_0 is some arbitrary start-of-collection time for Picoscope. t_{v_cam} is the timestamp of the camera voltage. This time is the same for the camera and Picoscope, therefore it is used as the syncing timestamp. t_{pp} is the time of peak compressed pressure, as read by Picoscope. t_{comb} is the timestamp of the image in which the first illumination from combustion is observed. To calculate ignition delay, the follow equation is used:

$$\tau_{ID} = \left(t_{comb} - t_{v_{cam}}\right)_{Camera} - \left(t_{PP} - t_{v_{cam}}\right)_{Pico} \tag{1.1}$$

2.6 Experimental Plan

2.6.1 **RCM Droplet Combustion**

The original objectives of the project as stated by the NSF proposal written by Dr. Marc Baumgardner were:

- Task 1: Demonstrate the ability to ignite a stationary droplet in a stagnant flow field under rapidly increasing temperature and pressure in a RCM.

- Task 2: Examine optically the entire process of RCM compression leading to droplet evaporation, ignition of the premixed fuel/air vapor in the vicinity of the liquid droplet, ignition of the premixed natural gas/air mixture, propagation of a premixed natural gas/air flame away from the liquid droplet, and non-premixed combustion of the liquid droplet.
- Task 3: Quantify relevant combustion phenomena such as ignition conditions, ignition delays, flame spread rates, and minimum flammability limits of the lean ambient mixture as they relate to droplet ignition. Perform experiments with various liquid fuels (n-heptane, n-hexadecane, ultra-low sulfur diesel) and gaseous fuels with various reactivity (methane, methane/ethane/propane, natural gas).
- Task 4: Develop a computational model of droplet combustion capable of incorporating the relevant physics with a sufficiently large chemical-kinetic mechanism to accurately predict ignition and flame spread phenomena.
- Task 5: Create an accurate reduced chemical mechanism capable of describing the initial dual fuel case of *n*-heptane droplets in lean methane/air environments

These goals describe a step by step process towards the development of a dual-fuel reduced chemical kinetic mechanism that is validated via the comparison of experimental and computational results. The purpose of this thesis project, coupled with the modelling done by Siddhesh Bhoite [16], was to pursue these goals as far as is feasible. Once the RCM was modified for droplet experiments, an experimental plan was crafted, following the framework described in Tasks 1-3 above.

To accomplish Task 1, the steps that are required are to successfully modify the RCM combustion chamber to suspend droplets, then achieve a sufficiently small offset such that the droplet doesn't become dislodged and the adiabatic core is contained to meet the requirement of

"stagnant flow field." If these conditions are achieved and the droplet is ignited, Task 1 will be complete.

Task 2 expands on the ability to ignite a droplet by adding requirements for observation of certain combustion phenomena including droplet evaporation, n-heptane vapor combustion, and distinct ignition and propagation events of the low reactivity fuel in the ambient environment around the droplet.

To this, we picked a parameter that was relatively easy to measure; ignition delay. For our testing, we followed the testing plan in Table 2.2. It is expected that as the proportion of argon goes up, and thus the compressed temperature, the ignition delay would go down, as the combustion reactions will speed up with the increased temperature.

	Mole Fractions			
Case				Est. Comp. T
#	N_2	Ar	O_2	(K)
1	0.8	0.0	0.2	844.53
2	0.6	0.2	0.2	961.22
3	0.4	0.4	0.2	1096.71
4	0.2	0.6	0.2	1251.29

 Table 2.2: Testing Matrix for n-Heptane Inert Combo Sweep

The goal was to collect as many data points at each testing point and develop a trend in ignition delay versus that compressed temperature estimation.

In parallel with this, n-heptane droplets will be suspended in a range of methane equivalence ratios to test the ignition behavior of that lower reactivity fuel. It is expected that the methane will not ignite at certain conditions, however the goal of Task 2 is to observe the two distinct ignition events.

2.6.2 Supercritical Droplet Evaporation Testing

An important step in the droplet combustion process is the phase change of fuel from a liquid on the droplet surface to a combustible vapor that diffuses radially into the ambient. To understand the dynamics behind the speed of the combustion of the droplet, it is important to understand the factors that affect it. Evaporation rates off of a liquid surface are functions of the relative densities between the liquid and the gas surrounding it, as well as the difference between the concentration of the fuel vapor present at the surface of the liquid and in the ambient. This is shown in equation 1.7 in section 1.3. Because the RCM operates at relatively high pressures and temperatures, there are operating conditions in which the droplet will exist in the "supercritical" region. This region exists above the critical point for a given fuel for both pressure and temperature. In this region, a given fuel exists as neither a vapor nor a liquid. This fact can have a large effect on a droplet's ability to fully evaporate and be consumed by the flame front. It is advantageous to study this phenomena. In collaboration with Jeff Mohr, droplet evaporation experiments were run in the RCM at subcritical and supercritical test points in an attempt to quantify the behavior of various alkanes at those temperatures and pressures. An interesting fact to note about alkanes is that as you move up in the number of carbons present in each fuel molecule, there is a direct correlation between that C# and the critical temperature and an inverse correlation between C# and the critical pressure. In the RCM, there is no way to provide an inverse relationship between pressure and temperature. This leaves only a handful of fuels for which supercritical conditions can be reached in the RCM. The values for P_{crit} and T_{crit} for each of the fuels considered.

Fuel	Pcritical (bar)	Tcritical (K)
n-pentane	33.6	469.8
n-heptane	27.4	540.0
n-decane	21.1	617.8
n-dodecane	18.0	658.2

 Table 2.3: Critical Temperature and Pressures for the fuels tested.

An issue with carrying out this type of testing inside of the RCM is that the conditions that would considered supercritical are not able to exist inside of the RCM chamber for very long. Heat transfer to the cool chamber walls causes the chamber to drop below supercritical conditions very quickly, leaving very little time for supercritical droplet behavior to be observed. Regardless, observations were made about the droplet behavior during the brief moment of supercritical conditions.

During the process of compression, the conditions inside of the RCM chamber follow the path shown in Figure 2.31.



Figure 2.31: Supercritical regions for various alkanes superimposed over the operational path typically measured inside of the RCM.

Worth noting is the length of time it takes to transition through the three time points. The isentropic compression stroke compresses from BDC to TDC, at a compression ratio of ~11.6, in 0.021 seconds. Immediately following this, isochoric heat loss causes the chamber pressure and temperature to drop quickly and asymptote out between 10 and 20 bar. The path from t_2 to t_3 takes 12.849 seconds, but much of the decreases in temperature and pressure occurs in the early stages of heat loss. In other words, it does not take very long for the chamber conditions to drop outside the bounds of the supercritical region for all fuels tested. This leaves only a small observation window in which to gather information related to supercritical evaporation. During the process, schlieren images were recorded to provide data about the droplet diameter as the fuel is vaporized into the ambient. Time and the droplet diameter squared were normalized by the original droplet diameter squared and plotted for each of the fuels tested. Chamber conditions for all fuels tested were as follows.

Y _{N2}	1.000	
Pi	1.25	bar
Ti	313	Κ
T _{comp}	840	Κ
P _{comp}	35	bar

Figure 2.32: RCM test conditions for supercritical evaporation tests.

3 <u>Computational Methods</u>

A transient, three-dimensional analysis was carried out for dual-fuel droplet combustion using the CONVERGETM CFD tool. CONVERGETM includes evaporation models only for spray simulations and hence it was difficult to model a single droplet evaporating and then subject the droplet to combustion. To solve this issue, an initial condition was established using theoretical droplet evaporation theory, parts of which were described in Section 1.3. This droplet theory included the following assumptions:

- The droplet evaporation process is quasi-steady and takes place in a quiescent, infinite medium.
- 2. The fuel is a single-component liquid with zero solubility for gases.
- 3. Gases follow the ideal gas law.
- 4. Thermal diffusivity and mass diffusivity are of the same order. (Lewis Number = 1.0)
- 5. All heat transfer to the droplet surface is used for evaporation of the liquid fuel at the droplet surface.

$$T_{s,i} = T_{boil,i} \tag{3.1}$$

6. Assuming a vapor liquid equilibrium at the surface along the gas phase.

$$P_{A,i} = P_{SAT,A(T_s)} \tag{3.2}$$

The heat transfer number of vaporization was derived by solving the energy equation which is defined as follows:

$$B_{h,v} = \frac{C_p(T - T_s)}{q_v} \tag{3.3}$$

where C_p is specific heat of the evaporating liquid fuel, T_s is the surface temperature of droplet, T defines the changing temperature value around the droplet, and q_v is the latent heat of vaporization of the liquid. The mass transfer number derived from the mass conservation equation is defined as follows:

$$B_{m,\nu} = \frac{Y_{F,s} - Y_{F,\infty}}{1 - Y_{F,s}}$$
(3.4)

where $Y_{F,s}$ is the mass fraction of gaseous fuel at the surface of the droplet, $Y_{F,\infty}$ is the mass fraction of the evaporating species in the far field. As mentioned in the droplet theory section, for the purpose of these experiments, that value is assumed to asymptote to zero as $r \to \infty$.



Figure 3.1 Initial Species and Temperature Distribution at time t = 0 sec

To consider the vapor released from the droplet surface, the droplet surface was modelled as a source term emitting vapor from the boundary at a velocity that was obtained using the proceeding equations. The mass flow rate from the droplet surface was found using the equation shown below,

$$\dot{m} = \frac{4\pi k_g r_s}{C_p} \ln(1 + B_{m,v})$$
(3.5)

where k_g is the thermal conductivity of the gases present, r_s is the radius of the droplet. The thermal conductivity is found by using Wilke's approach to mixing gases which takes into consideration the effect of all the gases surrounding the evaporating droplet. Finally, the velocity of the droplet vapors is found out using the equation shown below,

$$\dot{m} = 4\pi r_s^2 \rho V_r \tag{3.6}$$

where ρ is the density of the gas phase evaporating species and V_r is the radial velocity. Once these conceptual assumptions have been made, the data obtained was exported to the CONVERGE preprocessor to develop a model for droplet burning. CONVERGETM is only able to use a Cartesian coordinate system, therefore a mathematical analysis was necessary to convert the spherical coordinates to Cartesian coordinates before exporting the species and temperature distribution, which were defined in spherical coordinates. A mapping variable technique was used to map the data into the domain as shown in Figure 3.2.



Figure 3.2 (a) Initial n-heptane concentration (b) Initial methane concentration (c) Initial temperature distribution

In addition, an adiabatic core was approximated, making the flow field around the droplet uniform with minimal disturbances. This allowed us to model droplet ignition in a high temperature, high pressure, and low-flow environment. This initial condition was established at TDC, saving on computational time, as the compression stroke did not need to be modelled.

Boundary conditions for the chamber walls were set with law of wall as the heat transfer model. Adaptive mesh refinement was used to capture the temperature and velocity gradients coupled with the spherical embedding along the droplet source term to resolve the species distribution with a high degree of accuracy. For all tests, the initial compressed temperature of the domain was set to 765 K with a pressure of 27 bar, similar to the conditions found in the RCM after a typical compression event of a mixture containing CH₄, C₇H₁₆, and air. The first simulation examines the droplet behavior in an ambient containing a lean mixture of CH₄ and air. The temporal and spatial changes in temperature and species concentration were examined. In addition, CFD simulations were performed to give a visual representation of the flame development as the droplet evaporates and burns. Proceeding this, a sweep of equivalence ratios in the ambient was performed, tracking changes in flame speed, ignition delay, and steady-state position of the diffusion flame.

4 <u>Results</u>

4.1 <u>Computational Modeling</u>

The first case was carried out with an equivalence ratio of 0.5 in the far-field. As discussed in the development theory of dual fuel droplet combustion, a gradient of heptane concentration is established around the droplet surface. These vapors are heated up, resulting in an autoignition of the droplet resulting from a series of thermal runaway reactions taking place at some distance from the droplet surface as shown in Figure 4.1.



Figure 4.1 Species and Temperature Distribution at time of auto ignition

This autoignition event causes enough energy to be introduced to the system for the ambient methane (LRF) to ignite. As a result, the first flame observed during the initial autoignition splits into two flames. This first flame is a premixed propagation flame travelling away from the droplet surface through the low reactivity fuel/air mixture close to the droplet surface as shown in the Figure 4.2 and Figure 4.3. In the case of an infinite ambient, this propagating flame will travel

indefinitely. In the case of the RCM experiments and bounded CONVERGE simulations, the flame extinguishes at the wall of the chamber.





Since the mixture is lean, enough oxygen will be left in the domain for the standing diffusion flame. After some specific time period, the lean premixed flame completely disappears leaving only one diffusion flame in the system as shown in Figure 4.3.



Figure 4.3 Species and temperature distribution showing the diffusion flame peak temperature with no premixed flame

The initial propagation flame will continue to travel towards the droplet surface in the form of a premixed diffusion flame. This flame will initiate in a fuel-lean region and begin to move closer to the droplet surface, seeking a stoichiometric ratio of fuel to air. Close to the droplet surface it reaches a fuel rich region and the propagation ceases. At this time, the premixed flame transitions into a classical non-premixed diffusion flame front which is semi-stationary. At this flame position, the concentrations of fuel and oxidizer go to a theoretical value of zero as the flame establishes itself at stoichiometric conditions. The non-premixed diffusion flame receives oxidizer from the surrounding far field which remains after the low reactivity fuel has passed through the lean ambient and consumed parts of the oxygen present. Sufficient oxygen is left in the system to sustain the diffusion flame and the fuel is provided by the evaporating droplet due to heat transfer to the droplet surface as shown in Figure 4.3. When the steady diffusion flame is established, the temperature near the droplet surface becomes very high. As a result of this, the gaseous heptane evaporating off of the droplet surface undergoes thermal decomposition reactions, producing various smaller hydrocarbons such as methane, ethane, propane, and others as shown in Figure

4.4.





Figure 4.4 shows the progression as the longer chain hydrocarbons break down into methyl radicals near the flame front and get consumed, which sustains the flame front, allowing a diffusion flame to establish. Figure 4.5 shows the results of a simulation where a 1 mm liquid n-heptane droplet was ignited in a lean premixed CH₄/air mixture at $\Phi = 0.5$. The figure shows a series of heat release contours at various times after TDC wherein the ambient temperature and pressure of the mixture is 765 K and 27 bar, respectively. As the droplet surface vaporizes, the vapors are heated up and react with the ambient oxygen, causing autoignition of the droplet as shown in Figure 4.5(b). The ignition event results in a narrow temperature peak and local depletion of fuel and oxidizer approximately six diameters away from the droplet surface. This autoignition event

adds enough energy to the system for the lower reactivity fuel, CH₄, to ignite. As shown in Figure 4.5(c-d), the localized autoignition event then bifurcates into two separate flames – an outwardly propagating premixed CH₄/O₂ flame and an inwardly propagating CH₄/C₇H₁₆/O₂ flame. The inwardly propagating flame then transitions into a stationary, non-premixed C₇H₁₆/O₂ flame as shown in Figure 4.5(e-f). These results are simply a different way to visualize the results presented a few pages earlier.



Figure 4.5 Heat release contours in the gas phase surrounding a 1 mm n-heptane droplet in a $\phi = 0.5$ CH4/air mixture at 0.002 < t < 0.057 seconds after compression to To = 765 K, Po

= 27 bar



Figure 4.6 Temperature profiles in the gas phase surrounding a 1 mm heptane droplet in a $\phi = 0.5$ CH4/air mixture at 0.002 < t < 0.056 seconds after compression to To = 765 K, Po = 27 bar.

Figure 4.6 contains a plot of the gas phase temperature profiles at multiple times, which further illustrates the evolution of the position of the two flames. The figure reveals the initial inward movement of the diffusion flame and the outwardly propagating flame front of the premixed CH_4/O_2 flame as indicated by the sharp discontinuity in temperature across the flame front.



Figure 4.7 Parameter study of variation in flame speed, diffusion flame position and ignition delay with respect to equivalence ratios in far-field

As seen the Figure 4.7, simulations were run to examine the sensitivity of the flame speed, position of the diffusion flame, and the change in the ignition delays of the high reactivity fuel to the ambient methane equivalence ratio. As the equivalence ratio in the farfield is increased, the speed of the non-premixed CH₄ flame through the ambient increases. In addition, the resting position of the diffusion flame front increases. This agrees with theory. As the concentration of methane is increased in the ambient, less oxygen will be left over after the travelling flame passes through. Because of the lower ambient oxygen levels, the diffusion flame will need to travel farther from the droplet surface to a position of lower HRF concentration to reach stoichiometric conditions. The change in the equivalence ratio in the far field also effects the ignition delay time of the high reactivity fuel droplet. As shown in Figure 4.7, as the equivalence ratio was increased we find an increase in the ignition delay of the HRF.

4.2 <u>RCM Droplet Testing</u>

Originally built in the 1960's, rapid compression machines were designed to test the autoignition properties of gaseous fuel mixtures inside of a small test volume. At the time, the ability to compress a volume in a consistent way that provided high-temperature and high-pressure conditions was novel and very useful for characterizing the ignition properties of gaseous fuel mixtures. There are certain limitations that arise when physical objects such as a liquid-state fuel droplet are inserted into the chamber. In the case of the dual-piston RCM, asymmetries in the start-of-motion timing led to an imbalance in the fluid dynamic forces exerted on the droplet, causing the droplet to dislodge on occasion. The dislodging of a droplet during the compression stroke provides no useful information as the fuel has not yet had time to ignite, therefore it invalidates that test and leads to wasted time. The original SiC fiber droplet suspension configuration was very fragile and broke often, leading to lots of down time as the chamber had to be opened up and the fiber replaced. As the methods for suspending the droplet became more effective and robust, the success rate went up, allowing more data to be collected in a smaller amount of time. In the process of outfitting the new chamber to combust droplets and the subsequent testing, we discovered a few interesting phenomena that occurred in regard to the operation of the machine, odd fluid effects, as well as the combustion phenomena being investigated. This section will detail those findings as they relate to the original proposed objectives of the project and how they fit in with the limitations of the machine as we discovered them.

4.2.1 Supercritical Droplet Evaporation Results

Once the tests were completed for all fuels and the data separated for sub- and supercritical fuels, the evaporation rates were compared. Below are the results.



Figure 4.8: Evaporation plots for various alkane fuels.

The rates of change in droplet diameter decrease as the number of carbons in the fuel increases, suggesting the volatility of shorter hydrocarbons is higher, which is true. Building on this, the same data was compared between decane and dodecane, showing the regions during which the chamber was at subcritical or supercritical conditions. The plots for those two fuels are shown in Figure 4.9.



Figure 4.9: Droplet diameter histories of dodecane droplets at supercritical and subcritical

conditions.



Figure 4.10: Droplet diameter histories of decane droplets at supercritical and subcritical

conditions.

As would be expected during a droplet evaporation test, there is an initial period of thermal expansion where the droplet diameter expands and then begins to evaporate. This is usually the first step in the evaporation process before any evaporation rates are recorded. Unfortunately, the time interval where supercritical conditions are present happens even before this thermal expansion has begun. This makes it very difficult to make any specific observations about the nature of supercritical droplet evaporation or combustion in the RCM chamber.

4.2.2 **Droplet Combustion Results**

Early in the development of the droplet suspension mechanism, it was clear that it was possible to achieve conditions that would allow for the combustion of the vaporized droplet fuel. Before we were able to keep a droplet on the holder and observe combustion, dislodged droplets would often ignite. Though this provided no useful data, it was a good confirmation that ignition of the fuel vapor was possible. The sequence leading to this burning can be found in Figure 4.11. The droplet can be seen suspended prior to compression via the SiC fiber and epoxy assembly (top right). Upon compression, the piston offset is large enough that when the left piston arrives first, the droplet flies to the right (top left). When the delayed piston comes in violently from the right, it breaks the droplet into many smaller droplets (bottom left). As these fly back across the hot pressurized gasses in the center of the chamber, the vapor surrounding the flying droplets ignites and leaves behind it a trail of soot (bottom right), which absorbs some of the schlieren LED light transmitting through the cloud.



Figure 4.11: Sequence of images showing a droplet becoming dislodged during the compression stroke breaking into smaller droplets, and combusting. No methane is present in the mixture.

In Figure 4.12, the final image in Figure 4.11 is expanded to give the reader a closer look at the trailing soot cloud. Because heptane is combusting in the form of a non-premixed diffusion flame, lots of soot will be produced in the burned gases left behind by a flame front. An orange line denotes the border of the soot trail for one of these flying drops.



Figure 4.12: As an example, the soot cloud formed from the burning of an n-heptane droplet produced from the splintering of a fully-sized droplet is highlighted.

During the development of the SiC suspension mechanism, most of the tests were unsuccessful in that a droplet did not remain on the fiber and then combust with a clear, measureable ignition delay. There were a few exceptions to this fact, including the one detailed below in Figure 4.13. In this case, there was lean CH_4 present in the ambient chamber volume at ϕ =0.5, however it did not ignite. With an inert ratio of one third argon and two thirds nitrogen, ignition of the methane was not expected, as the expected compressed temperature has not historically been high enough to ignite such a lean mixture. Time zero represents the start of motion of the pistons. After 18ms, initial puffs of vapor propagate towards the center of the chamber, signifying the stop-of-motion for the pistons. In the case of these droplet experiments, ignition delay (τ_{ID}) is defined as the elapsed time between peak compressed chamber pressure and ignition of the fuel, as shown in equation 3.1 below.

$$\tau_{ID} = t_{ignition} - t_{peak\ pressure} \tag{3.7}$$

Image 5 in Figure 4.13 shows the ignition of the droplet. This gives an ignition delay of 78 ms. More insight into the expected ignition delays of n-heptane droplets will be discussed later in this section.



Figure 4.13: A droplet with an initial diameter of 1.195mm is burned inside the RCM.

After ignition, the droplet began to burn until all of the fuel was consumed 528 ms after the initial compression event. Image analysis was performed on the still images to determine a planar droplet area to then infer a diameter. The droplet in this case had an initial diameter of 1.195 mm, giving it an initial volume of 0.8935 mm³. The volume of the epoxy bead must be considered as well. The bead itself has a diameter of 0.84 mm and a volume of 0.311 mm³. When the differential volume between the two is calculated, it is shown that there is 0.583 mm³ of liquid fuel present at the start of the test. If we assume that a negligible amount has vaporized between TDC and the ignition event, an evaporation rate can be calculated. A volume of 0.583 mm³ is consumed in 438 ms. This yields an overall evaporation rate of 1.33 mm³/s. Despite the success of this test and the step-by-step droplet burning process shown in the images, another test of this quality never was achieved using the epoxy bead hanger design. As discussed in section 2.2.3, a quartz-only droplet suspension mechanism was developed. When this new system was introduced to the experiments, droplets began falling off less frequently and downtime as a result of plug maintenance was reduced to almost zero as there were no weak fiber attachment points to break. This allowed a larger number of tests to be performed in a shorter period of time. Chamber conditions were also more consistent because more tests could be run without needing any disassembly of the chamber body.

A sweep of tests was done with an n-heptane droplet suspended in a mixture of N₂/Ar/O₂. The ratios of Ar and N₂ were varied to reach certain compressed temperatures. In theory, as the temperature around the droplet increases, the rates of evaporation and chemical reaction should rise, leading to shorter ignition delays. This trend was confirmed after that round of testing was performed. Aside from the varying of the inert gases, the initial conditions of the tests were held steady at $P_i = 1000$ mBar and $T_i = 318$ K.



Compressed Pressure/Temperature [bar/K]

Figure 4.14: Trends in ignition delays for a sweep of compressed temperatures in the RCM chamber.

Part of Task 2, as stated in the proposal of this project, reads "Examine optically the entire process of RCM compression leading to droplet evaporation, ignition of the premixed fuel/air vapor in the vicinity of the liquid droplet, ignition of the premixed natural gas/air mixture, propagation of a premixed natural gas/air flame away from the liquid droplet, and non-premixed combustion of the liquid droplet." In other words, this task sets out the goal for observing a "dual-fuel" droplet combustion event, with the higher reactivity heptane igniting first, followed by the ignition of the lower reactivity methane some time later. Throughout the troubleshooting

process of the droplet combustion chamber modification, tests were run with methane composing some small part of the ambient, in an attempt to observe this very phenomenon.

For most of these tests, the droplet did not ignite in a clean fashion. The droplet would usually dislodge and ignite, which gave no clear information regarding ignition delay, nor a clear image of the droplet setting off the premixed propagating methane flame. The goal of that task was to observe a clear compression event, a clear ignition of the heptane droplet, followed by a delay period after which the flame from the heptane would ignite the lean methane mixture. Images, along with the corresponding times, are shown below in Figure 4.15.



Figure 4.15: Sequence showing the progression of a dual-fuel droplet combustion event.

The images show a distinct ignition event of the heptane vapor surrounding the liquid droplet. Because heptane vapor is denser than the gaseous medium in the chamber, it sinks towards the bottom of the chamber as it evaporates. The propagating flame front quickly consumes the heptane vapor and heads downwards. Somewhere towards the bottom of the viewing window, the hot gases produced from the burning of the heptane are at a high enough temperature that the ambient methane is able to ignite, quickly travelling upwards, consuming any fuel in its path. The pressure profile, with a non-dual fuel case superimposed, is shown below in Figure 4.16.



Figure 4.16: Pressure profiles for RCM droplet combustion of a single fuel and dual-fuel

case.

There were certain test cases that showed the expected pressure trace profile for a methane ignition, but no visual evidence of it. Below are frames from one such test, followed by the

pressure trace. The pressure trace shows a distinct ignition event of the premixed fuel, whereas the images do not.



Figure 4.17: Dual-fuel ignition case with no visible signs of methane ignition.

These result is slightly different than those from the simulations done by Siddhesh Bhoite. As mentioned in the section detailing the computational modelling, all simulations were carried out in a gravity free environment. This means that differences in the densities of gases will have no effect via buoyancy. This is useful when comparing the simulation results to expected droplet behavior based on theory, where gravity is also neglected. However, it bears no resemblance to what happens in the experiments. The addition of gravity causes the diffusing heptane vapor to travel generally in a radial direction, but sink as time passes. This creates a concentrated area of highly reactive fuel vapor below the hanging mechanism, leading to the downward travel of the flame after the initial heptane ignition. If we highlight certain frames from the CH₄ ignition process. Similarities can be drawn between the simulations and the experimental results.



Figure 4.18: Side by side comparison of dual fuel combustion cases between simulations and experiments.

In this figure, temporal snapshots can be seen from the RCM experiments (column ii) and from the CONVERGE simulations (column i) showing distinct non-premixed diffusion flames (row A) followed by a premixed propagation flame (row B).

5 <u>Conclusions and Future Work</u>

This project set out to observe and quantify the behavior of hydrocarbon droplets inside of a rapid compression machine. Published research on the behavior of fuel droplets in environments of rapidly increasing pressure and temperature was very sparse and usually only explored the evaporation characteristics of the droplet. The goal for this study was to continue this work and expand into the experimental combustion of the droplets along with a computational campaign to predict these behaviors. Modifications were made to allow the CSU RCM to carry out these experiments.

The simulations built on the work done by Andrew Hockett in exploring the subtleties of dual-fuel combustion. The simulation confirmed that the high temperature zone created by the ignited n-heptane vapor was high enough to split the semi-stationary diffusion flame into two flames; one, the same diffusion flame, and the other a propagating pre-mixed methane flame. Following this, combustion data were collected on the ignition of n-heptane droplets suspended in air. Trends in ignition delay data were found by varying the inert ratio to affect compressed temperature, which was swept from 850 K to 1250 K. For a number of reasons, direct comparisons were not made between this experimental sweep and an equivalent campaign in CONVERGE. The simulations were finished more than a year before the decision was made to do this regime of experiments. Images were also gathered of the n-heptane diffusion flame and methane ignition events using a schlieren imaging system. Comparing these results to the simulations done by Siddhesh Bhoite proved to be slightly difficult. Gravity was not turned on in the simulations, which changed the way vapor propagated prior to ignition.

Images were collected with two different techniques. In some cases, the standard schlieren technique was used, with the LED providing the backlighting. In addition, the camera gathered

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images of the pure luminescence off of the droplet. These techniques provided useful information, however they did not provide a clear way to determine the location of a propagating flame front. In the future, it could be beneficial to utilize techniques such as chemoluminescence or PLIF when possible. These methods provide a more direct way of imaging the flame front and leaving out the luminescence from the very bright soot that is present during the combustion of n-heptane.

The rapid compression machine at CSU presents many challenges related to the ignition of liquid fuel droplets. The dual-piston orientation introduces the potential for large fluid instabilities, making it difficult to keep testing conditions consistent and the droplets suspended. In the future, more work should be done to gain more control on the timing of the piston start-of-motion. This can be done potentially by having solenoid pressure dump valves located as close to the hydraulic chamber inlets as possible on either side of the RCM. In addition to this, more work can be done to improve the suspension mechanism. In most of our experiments, a formed glass holder was used. This design was a large improvement over the methods used before it. One issue with this design is related to the angle at which the glass comes down towards the end of the hanger. It lies angled to one side, causing the droplets surface tension to pull the droplet off to one side. This adds to the movement away from spherical symmetry that is started by the introduction of gravity. It is recommended that a new hanger be positioned such that the droplet hangs in line with the glass rod.

Through the course of troubleshooting the RCM and outfitting it for the combustion of liquid fuel droplets, a few conclusions were made about the usefulness of the RCM as a test medium for droplet combustion. As previously mentioned, when the travel profile of each piston is offset in time, there are a number of fluid dynamic effects that interrupt the sequence of events that should take place in droplet combustion. When the imbalance if sufficient that the droplet is dislodged, a

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test is immediately invalidated. Sometimes, the imbalance simply causes the droplet to be perturbed and deform as the pistons compress. This further removes the spherical symmetry assumed in the droplet theory section. In addition, heat transfer to the droplet surfaced is counteracted by the forced convection around the droplet surface as it is disturbed.

The RCM combustion chamber itself is small compared to how far a premixed CH₄ propagating flame might travel. The cool chamber walls may have an adverse effect on the residence time of a flame or effect the assumed adiabatic core region. Because of the limited size of the optical ports in the combustion chamber, the size of the overall chamber is not a huge issue. At TDC, the piston faces are ~25 mm apart, allowing a maximum imaging window diameter of the same value. Our windows are 20 mm, giving an effective imaged volume of 11.96 cm³ and a TDC chamber volume of 28.5 cm³, meaning that 58% of the chamber volume will not be imaged. This leaves some chance that a propagating CH₄ flame may ignite and escape the viewing window in the 2ms between camera captures. Or alternatively, only a single image may be caught of a CH₄, limiting the ability to make flame speed calculations.

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Appendices

Appendix A: RCM Operation Procedures

Start here if the RCM is completely powered off with all support systems also off.

- Turn on the exhaust fan located in the closet located in the back left of the combustion lab as viewed from the doors to the lab. The pump for the exhaust is powered through a power strip that must be flipped on. The exhaust must be on during all RCM operation.
- 2. Getting to "Holding State"
 - a. Turn the power strip above the mixing tanks <u>ON</u>
 - b. Flip breaker box switch to <u>ON</u> (Labeled "P2L2-32_34_36")
 - c. Turn the larger of the two black switches on the wall-mounted RCM control panel from <u>OFF</u> (270°) to <u>ON</u> (0°)
 - d. Turn the main air valve from <u>OFF</u> to <u>ON</u> (Located on the bottom left side of the RCM as seen from the gas manifold side.)
 - e. Turn the vacuum pump (VP) ON
 - f. Press the green "Reset ⁽ⁱ⁾" button located on the right side of the RCM control box.
 - g. After an elapsed time of ~20 seconds, there will be a noise and the first blue button on the RCM Control Box (Labeled "Retraction Vacuum") will light up. Push it.
 - h. Turn the green ball valve located on the bottom right section of the RCM-side gas manifold to "RCM Bellows", a vacuuming sound will begin. The piston assembly is now being vacuumed back
 - After an elapsed time, a valve will make a closing sound and the second blue light labeled "Locking Pressure" will light up. Push it. The RCM is now in a "Holding State" and can be left like this indefinitely

- 3. Prepping Data Logging
 - a. Right Click on the PicoScope icon in the dock. Click "Droplet_RCM.psdata". This will open PicoScope with the program setup for droplet testing.
 - b. Turn on the Pulse Delay Generator.
 - c. Turn on the power supply for the PCO 1200s camera.
 - d. Open CamWare. Ensure the following settings are correct: (Subject to change)
 - i. Under the menu item "Camera", open the "Camera Control" window.
 - ii. Timing Tab:
 - 1. Ensure the Exposure and Delay values are set as desired.
 - 2. Trigger Mode: "Auto Sequence"
 - iii. Recording Tab:
 - 1. Recorder Mode: Sequence
 - a. NOTE: If in Ring Buffer mode, the recording will continue to re-write the data until prompted to stop. This is not desirable due to the potentially short time-scale of droplet combustion.
 - 2. Time Stamp: ASCII
 - 3. Acquire Mode: Auto
 - 4. Sequence Trigger Mode: Off
- 4. Filling the Combustion Chamber
 - a.
- 5. Firing the RCM/Inserting Droplet

- a. On the wall-mounted RCM Control Box, flip the smaller black switch from the 2 o'clock position to the 10 o'clock position. The machine is now in manual mode.
- b. Dump the hydraulic pressure with the manual dump valve.
- c. Push the green button on the wall-mounted control box until the pressurization noise stops. The pressure gauge on the left hydraulic manifold should read 35 bar or higher.
- d. Flip the black switch back to the 2 o'clock position.

If firing with droplets in the chamber, attach the septum assembly to the syringe before beginning the charging process

- e. Press the 3rd blue button which should be lit at this point. The bellows will begin to pressurize to the value set on the RCM control box. (Standard is 160psi)
- f. During the charging process, insert syringe into chamber
- g. Deposit droplet on the epoxy bead
- h. Ensuring that the drop sticks to the fiber and stays there.
- i. When the bellows are charged, the red "control fuel charge" switch will light up.
- j. Flip this switch, and blue "initiate" button will light up.
- k. Push the "Go Start Capturing" button in PicoScope
- 1. Push the green "Meas" on the Kistler Charge Amplifier.
- m. Audibly say "FIRING", and push the button. There will be a loud noise, signifying the firing of the pistons.
- n. Flip the red switch back to its original position.
 - i. NOTE: At this point in the process, the combustion chamber is under very high pressure. It is very important that the chamber not be opened during

this period. If the high pressure is allowed through the gas insertion line, there is a potential for damage to the pressure transducers along that line. If pressure is dumped through the needle insertion valve, there is not much potential for damage to any components, however it may cause trouble during the piston retraction process. Without the help of the high pressure pushing on the piston face, the vacuum on the back side of the drive plunger may not be sufficient, or at the very least have more trouble, pulling back the piston assembly.

- o. After an elapsed time, the "Retraction Vacuum" button will light up blue. Push this button. Make sure the green vacuum diverter valve is switched to "RCM Bellows".
- p. The "Locking Pressure" button will light up. The chamber pressure has now reduced down to roughly the same magnitude as before compression. It is safe to open the chamber for vacuuming.
- q. Repeat back to Step j.

Appendix B: RCM Overhaul Procedure

The RCM is a precision research instrument that requires all of the parts to be functioning correctly in order to maintain confidence in the machine and the results it produces. To ensure this, periodic maintenance is required on the RCM. Every 9-12 months, the RCM must be completely overhauled to replace some of the harder-to-access seals. The following steps should be taken to complete the overhaul.

Tools required for RCM Disassembly:

- 9/16", 7/8", 1-1/16", 1-1/4" wrenches

- 1/2", 3/8", 5/16", 1/4", 3/16", 3/32" hex keys
- 15/16" socket wrench
- Set of strap wrenches
- Set of ratchet straps

Part 1: Center Section Disassembly

- 1. Ensure the pistons are in the retracted (BDC) position.
- 2. Disconnect the pressure transducer wire from the bottom of the RCM chamber.
- 3. Disconnect the gas insertion line that is attached to the needle valve at the top of the chamber using a 9/16" wrench.
- 4. Remove any heat wrap or insulation tape from the sleeves of the RCM
- 5. Using the 1/4" hex key, remove the 12 combustion chamber bolts from both sides of the chamber. First remove the bolts on the south side, where the free end is located.
 - a. If these are removed second, the entire combustion chamber and south side sleeve will be allowed to rotate freely, making it very difficult to remove the bolts.
 - b. It is recommended that the disassembler keep the bolts of a given size for a given side of the RCM in separate bags.
- 6. The south side (side closest to the window) sleeve should move freely along the axis of the RCM and allow you to push it towards the south end section. Keep your hand on the combustion chamber so that it does not fall off in this process.



- 7. Remove the combustion chamber.
- 8. Remove the south end sleeve by sliding it towards the centerline of the machine until it comes off of the south end piston assembly contained within.
- 9. Using the 3/16" hex key, remove the 3 sleeve bolts securing the north sleeve to the north end cooling collar, two of which are shown in the figure below.



- 10. Remove the north sleeve.
- 11. Fire the RCM to put the pistons in the TDC position in order to gain access to the piston securing assembly.



12. Once the pistons are in this position, loosen the set screws that hold the piston assembly in place using the 3/32" hex key.



- 13. Remove the piston/piston seals from the drive plunger.
- 14. Vacuum the piston assembly back to the retracted position.
- 15. Set aside all chamber bolts, sleeve bolts, sleeves, and combustion chamber in a safe place for the duration of the overhaul.

Part 2: Disassembly of the end sections.

This section will be repeated for each of the two end section assemblies. Before beginning this section, remove the gas manifold from the south side RCM cage. The Swagelok line leading to the wall-mounted gas manifold will need to be removed along with the vacuum hose leading to the RCM pneumatic manifold. Once these have been removed, the panel can be removed from the RCM and set aside until the overhaul is complete. Although the south and north end sections are identical, it is best to keep all respective components separated and re-assembled as they were originally.

The following figure will be used as a reference throughout the end section disassembly process:



 Using the 1/4" hex key, remove the 8 bolts that hold the cooling collar (14) in place. These bolts are located on the combustion chamber side of the Main Frame.



2. Remove the cooling collar, leaving the plastic fluid bottle attached. Set aside.

Place an oil pan underneath the drain port located on the bottom of the external oil chamber
 Using a 1-1/16" wrench, remove the drain plug. Oil should immediately begin to drain. Allow all of the oil to drain as you proceed to the next steps.



- 4. Using the 7/8" wrench, remove the Pneumatic Filling Pipe that is attached to the bottom side of the air chamber (4) outside of the RCM cage. Set aside.
 - a. It is important to do this step prior to removing the linear transducers in steps 5&6.If the filling pipe is not removed, a vacuum may still exist in the air chambers, making it very difficult to remove the transducers.



- 5. Using the 5/16" hex key, remove the 6 bolts that secure the linear transducer to the air chamber body.
 - a. Be careful while removing the transducer. There is a long magnetic rod on the end of it that should remain undamaged as the part is removed.





- 6. Using the 3/8" hex key, remove the 8 bolts that hold the air chamber onto the RCM. Set aside and bag 6 of the bolts and use the remaining 2 as pusher bolts. There are 2 threaded holes in the flange of the air chamber that can be used to push the chamber away from the RCM main frame, allowing for easier removal. Because of the weight of the air chamber and the tight tolerance between it and the RCM main frame, two people will be required for this step.
- 7. Set aside the air chamber.
- 8. After removing the air chamber, the drive side of the piston assembly should be exposed. To ensure that any remaining hydraulic fluid has been removed from the chambers, manually actuate the piston assembly by pushing on the back side of the drive plunger (9) until the assembly has reached the "fully compressed" position. Then, push on the compression plunger (16), moving it to the BDC position. Repeat this process as many times as appears necessary to empty any large excess of hydraulic fluid.

- a. Make sure to have the oil collection pan still in place during this step to avoid spillage.
- 9. Using the 5/16" hex key, remove the 8 bolts that secure the Drive Cylinder (5) to the Internal Oil Chamber (8). Remove the Drive Cylinder, making sure not to damage the drive plunger, which resides inside of the cylinder.
- 10. Using a 9/16" wrench, disconnect the secondary hydraulic line, attached near the top and back of the Internal Oil Chamber, and allow it to drain into a catch vessel. Once all of the oil has drained from the center hydraulic fluid overflow chamber, remove it, empty it of any extra fluid, and set aside.
- 11. Using the 15/16" socket wrench, remove the 8 nuts that secure the Internal Oil Chamber(8) to the External Oil Chamber (7)
- 12. Carefully remove the 3 Compression Spacers that sit between the rear flanges of the Internal and External Oil Chambers. (8&9)
- 13. Remove the internal oil and chamber and drive plunger assembly through the rear hole in the RCM main frame, pulling straight back along the axis of the RCM.
 - a. There may be some oil left inside of the Internal Oil Chamber, so make sure to keep the collection pan underneath as the assembly is removed.
 - b. Because of the weight and awkward shape of the assembly, as well as the chance of there being residual oil, two people are recommended for this section of the disassembly.
- 14. The drive plunger assembly is attached via threads in the middle. Use two strap wrenches to break apart the two plunger pieces; the Compression Plunger (16) and Drive Plunger (9).

- a. Prior to doing this, wipe off as much of the excess oil that is left on the assembly and inside the chamber as possible.
- b. This step can be very frustrating. Don't give up too quickly!
- 15. Using a 1-1/4" wrench, disconnect the main hydraulic line from the top of the external oil chamber and the T-fitting and set aside. Cover the open hydraulic line with a plastic bag and zip-tie to ensure oil does not drip out onto the optics below.
- 16. Using the 2.5" bars on the main frame as support, use a ratchet strap to cradle the underside of the External Oil Chamber in preparation for the next step.
- 17. Using the 1/2" hex key, remove the 8 bolts that attach the External Oil Chamber (7) and Neck Seal Housing (6) to the Main Frame of the RCM. Once they are all removed, all of the weight of the External Oil Chamber should be placed on the straps.
 - a. Note: The External Oil Chamber and Neck Seal Housing are attached and can be treated as a single unit until disassembly later.
- 18. Slowly slide the External Oil Chamber/Neck Seal Housing outwards axially until they can be removed through the back of the Main Frame.
 - a. Once this assembly has been removed from the machine, the two pieces should be removed so that seals between the two can be replaced.
 - b. When the Neck Seal Housing has been removed, it should resemble the image below.



- 19. Using a 3/16" hex keys, remove the 4 bolts securing the Neck Seal Retainer (17) in place.Once this has been removed, the Rear Neck Seal (k.) can be accessed and replaced.
- 20. Repeat this process for the opposite and identical End Section.
- 21. All parts should now be off of the RCM.
- 22. The Main Frame should look similar to the image below.



23. Once both sets of End Sections have been removed, the seals can then be replaced.

Part 3: Replacing the Seals.

The RCM has 15 different distinct seals located throughout the machine to prevent high-pressure gasses and fluids from escaping. Since Marine Technology Ltd. (MTL) manufactured the RCM, most of the seals come from distributors located in the United Kingdom. Due to complicated CSU purchasing policies, seal purchases were made through Patrick Meier at MTL. The one exception to this was the combustion chamber seals, which could be purchased through a domestic distributor. Table 0.1 lists the RCM's seals starting with those closest to the combustion chamber

and progressing out to the air chambers. The general seal position and relevant RCM parts are also listed.

	Seal Name	Description	Location*	Distributer/Part#
a.	Combustion Chamber Seal	Viton O-Ring	Between Combustion Chamber (23) and Combustion Chamber Sleeves (24)	McMaster-Carr / 9263K129 Abbey Seals / BS 225 V
b.	Piston Seals	PTFE U-Ring and Viton O-Ring	Between Piston Head (30) and Piston Body (28)	Claron / PD2850- 1795/V (U-Ring) Abbey Seals / BS 217 (O-Ring)
с.	Wiper Seals	Radial Lip Seal	Cooling Collar (14)	Walkersele / L6T-1 USA DS-1375 1.375 WR137175-018- 030M-P
d.	Neck Seals	PTFE U-Ring and Viton O-Ring	Neck Seal Housing (6)	Claron / PU175137/1V (U-Ring)
e.	Internal Cooling Collar Seal	Viton O-Ring	Cooling Collar (14)	Abbey Seals / BS 83370
f.	External Cooling Collar Seal	Viton O-Ring	Cooling Collar (14)	Abbey Seals / BS 24770
g.	Forward Hydraulic Oil chamber Seal	Viton O-Ring	Between Seal Housing (6) and Oil Chamber (7)	Abbey Seals / BS 25670
h.	Forward Taper Seal	Viton O-Ring	Between Taper Seal Holder (11) and Compression Plunger (16)	Abbey Seals / BS 21870

 Table 0.1: Rapid Compression Machine Seals.

i.	Rear Taper Seal	Viton O-Ring	Between Taper Seal Holder (11) and Drive Plunger (9)	Abbey Seals / BS 61770
j.	Rear Hydraulic Oil Chamber Seal	Viton O-Ring	Between External Oil Chamber (7) and Internal Oil Chamber (8)	Abbey Seals / BS 43370
k.	Rear Neck Seal	Poly U-Seal	Between Internal Oil Chamber (8) and Rear Neck Seal Retainer (12)	Hallite / 605-43461
1.	Drive Plunger Seal	Custom PTFD Seal	Between Drive Plunger (9) and the Drive Plunger Seal Retainer (10)	N/A
m	Air Chamber Seal	Viton O-Ring	Between Air Chamber (4) and Drive Cylinder (5)	Abbey Seals / BS 34770
n.	Linear Transducer Seal	Viton O-Ring	between Air Chamber (4) and Linear Transducer	Abbey Seals / BS 23070



Figure 0.1 Combustion Chamber Seals.



Figure 0.2 Piston Seals.



Figure 0.3 Wiper Seals.



Figure 0.4 Neck Seals.



Figure 0.5 Internal Cooling Collar Seals.



Figure 0.6 External Cooling Collar Seals.



Figure 0.7 Forward Hydraulic Oil Chamber Seals.



Figure 0.8 Forward Taper Seals.



Figure 0.9 Rear Taper Seals.



Figure 0.10 Rear Hydraulic Oil Chamber Seals.



Figure 0.11 Rear Neck Seals.



Figure 0.12 Drive Plunger Seals.



Figure 0.13 Air Chamber Seals.



Figure 0.14 Combustion Chamber valve Tip.



Figure 0.15 Linear Transducer Seals

Appendix C: "Quirky Things"

There were a few idiosyncrasies to the operation of the RCM that were slightly perplexing. This appendix is intended for the description of a few of those things.

As the pistons compress, there is a theoretical stagnation point at the center of the chamber. When the offset was close enough (i.e. approaching $\Delta t = 0$), a distinct line was observed running orthogonal to the travel of the pistons. An example is shown below.



Figure 0.16: Mystery line travels across the RCM chamber during compression.

It is worth noting that this line only appears when the n-heptane droplet, and consequently the cloud of n-heptane vapor, is introduced to the chamber. The line will appear in the absence of oxygen, with only inert gases present in the chamber, but not without the heptane present. It is unclear whether or not the line has an effect on the probability of the droplet to ignite. In addition to this line, plumes can be seen in the 3rd frame that come from the inwardly moving pistons. These did not always happen, but had an effect on the droplet when they did.

Occasionally during early testing, after the compression of the pistons, what appeared to be some kind of jet stream would blow down onto the top of the droplet, as seen below in Figure 0.17. The flow comes from small pockets of dead volume inside of the combustion chamber body. Dead volume refers to any volume that is pressurized but not part of the main reaction zone between the pistons or in the crevices. The two dead volumes that were found existed below the gas filling valve and the chamber and below the needle insertion valve. This issue was solved by machining specifically designed plugs to fill these spaces without interrupting the function of the port in question.



Figure 0.17: Jet stream coming from a pocket of dead volume inside the RCM combustion chamber body.

Droplet Hanging Mechanism Design Process and RCM Modification

RCM Droplet Chamber Modification

The modifications made to the droplet combustion chamber are shown below in Figure 0.18 and Figure 0.19. The modified chamber is labeled with number which correspond to the information in Table 0.2.

Port #	Description	
1	Gas Insertion Valve	
2	Optical Window 2	
	Droplet Suspension Plug	
3	Port	
4	Pressure Transducer Port	
5	Optical Window 1	
6	Syringe Valve Port	

 Table 0.2: RCM Droplet Combustion Chamber Pot Descriptions



Figure 0.18: Secondary "Droplet" chamber as originally machined.



Figure 0.19: Final machined design of Droplet Combustion Chamber

Copper Washer Considerations

As mentioned earlier, the optical window plugs incorporated copper crush washers as the primary sealing mechanism (97725A350, McMaster-Carr). These washers worked well from a sealing standpoint. Unfortunately, similar washers with the ID/OD dimensions needed for the new plug design, seen in Figure 2.20, could not be located. A custom set would have to be made. The radial clearance between the upper and lower sealing surfaces was very small, as shown in Figure 0.20. Cutting washers with custom dimensions could be achieved using a tap and die set. Since the dimensions of the washers would be custom, a custom tap and die set would need to be manufactured.



Figure 0.20: Cross section of the sealing area between the combustion chamber and the droplet suspension plug (copper washer not installed)

There is a waterjet cutter at the lab that is used to cut parts from sheet metal with relatively small tolerances. One issue associated with using a waterjet is the geometry of the profile of the cutting fluid as it passes through the sheet metal. As the cutting flow exits the nozzle of the waterjet cutter, the flow begins to diverge. When the flow hits the surface of the sheet metal where the cut is supposed to take place, the center of the cross-sectional flow profile begins to erode out the center of the projected cut area on the surface. As the cutter penetrates the thickness of the metal, the hole on the top surface of the sheet grows larger. As is shown in Figure 0.21, the profile of the jet constricts through the sheet, causing a taper to form along the edge of the cut length. With a sheet metal thickness of 0.032", this deviation from vertical causes the washer's outer diameter to increase from 1.126" on the top surface to 1.145" on the bottom, where the cutting jet exits from

the sheet metal. Given the radial clearance in which this washer must fit, this was not a small error.



Figure 0.21: Cross-section of waterjet cutting jet through copper sheet. *Figure not to scale.

In order for the copper to function well as a crush washer, the material must go through a process called annealing.

Piston Speed Considerations

An analysis was performed on the speed of the pistons to determine if the drive pressure had a significant effect on the piston travel speed. The piston has short acceleration and deceleration periods. These sections were ignored and the constant speed sections of the piston travel were analyzed. Drive pressure was swept from 160 psi down to 80 psi. This sweep was done with the piston sleeves ON and OFF. In the case of the sleeves ON, the pistons would not move at drive pressure below 120 psi.