DESIGN, CONTROL, AND CHARACTERIZATION OF A CONTROLLED TRAJECTORY
RAPID COMPRESSION AND EXPANSION MACHINE (CT-RCEM)

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Dedicated to my parents Narendra Kumar Tripathi and Shalini Tripathi
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Abstract

This thesis presents the design, control and characterization of a novel experimental facility for fundamental and applied combustion investigations – a controlled trajectory rapid compression and expansion machine (CT-RCEM).

Rapid compression machine (RCM) has been a popular experimental facility used for the investigation of combustion characteristics of fuels in low to intermediate temperature ranges. The CT-RCEM, developed in this research, addresses a key limitation of the conventional RCM, i.e. an open-loop and calibration-based actuation philosophy. The CT-RCEM uses an electrohydraulic actuator driven by a precise motion controller to drive the piston in the combustion chamber. Any changes in the operating parameters can thus be made by electronically changing the piston trajectory sent to the controller, unlike the conventional RCM which requires hardware intervention. This allows the CT-RCEM to provide ultimate flexibility in the choice of operating parameters, a wider operating range with higher resolution, lower turnaround time, and exceptional run-to-run repeatability.

The key novelty of CT-RCEM, however, lies in the new paradigm of experimental investigation enabled by the ability to tailor the thermodynamic path inside the combustion chamber by suitable choice of piston trajectory. Specific examples include, the ability to investigate the effect of changing the thermodynamic path of compression on ignition delay, the ability to quench the chemical kinetics in the combustion chamber by extremely rapid expansion, and, the ability to produce isobaric conditions inside combustion chamber by slow creeping of the piston at a rate which offsets the rate of wall heat loss.

In this research, first, a control oriented dynamic model of the CT-RCEM is developed. The model serves three purposes for the development of the CT-RCEM – (i) to understand the impact of various design parameters of the CT-RCEM on its performance and tuning them to obtain a suitable mechanical design; (ii) to design a model based high
bandwidth controller that can provide precise tracking performance for the piston motion (iii) to guide the design of the various subsystems of the CT-RCEM.

Next, a model based, iterative learning control (ILC) scheme is implemented for the control of the actuation system of the CT-RCEM. Since the choice of the initial control signal for the first iteration has a significant impact on the number of iterations required for ILC convergence, the initial signal for the ILC is generated through simulation, from the dynamic model of the CT-RCEM, which uses a repetitive controller.

This is followed by the characterization of the CT-RCEM which essentially involves demonstrating that the facility can provide the desired functionality – fast compression and repeatable pressure history – over the designed operating range for both non-reactive and reactive mixtures. Also, the new capabilities of CT-RCEM enabled by the ability to tailor the thermodynamic path are demonstrated. Next, the utility of the CT-RCEM is demonstrated for applied engine research where a single combustion event of an engine can be recreated with well controlled initial and boundary conditions. It is demonstrated that the CT-RCEM can be used to perform a benchmarking study of the combustion characteristics of a realistic free piston engine operation and its effect on the piston trajectory by presenting a case study.

Finally, a multi-zone thermo-kinetic model is developed for computationally efficient analysis of the experimental data obtained from the CT-RCEM. A reaction path analysis performed using this model is used to explain a highly counterintuitive experimental observation made using the CT-RCEM – a faster compression does not necessarily lead to smaller pre-ignition reaction progress during compression and (consequently) a longer ignition delay. It is shown that the degree of pre-ignition reaction progress and consequently the radical pool at the end of compression can be quite sensitive to the thermodynamic path of compression, not just the end of compression thermodynamic state.
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CHAPTER 1  Introduction

1.1  Background and Motivation

Transportation sector is one of the key drivers of growth and prosperity around the globe. In the US alone, transportation sector accounted for 9% of the national GDP with the demand for transportation close to $1.5 trillion, 70% of which was personal consumption. Connecting small and large business together, ground transport moves more than $35 billion worth of goods daily. About one-fifth of the annual budget of an average US household is devoted to transportation related expenditure [1], [2]. However, the transportation sector currently suffers from two major concerns – addressing the growing energy demand and the environmental impact.

The pace of the national and global economy has renewed the push to address the growing energy demand for the transportation sector. In the US, transportation sector accounts for about 28% of the total energy consumption, 92% of which is powered by petroleum-based fuels. Furthermore, about 84% of the petroleum consumption by the transportation sector is attributed to highway transportation – passenger cars and light to heavy duty trucks – a segment significantly dominated by internal combustion engines (ICE) [1], [3].

Unsurprisingly, with such a heavy reliance on petroleum-based fuels, the environmental footprint of the transportation sector is also quite significant, contributing to over 27% of the total greenhouse emission in the US [1], [4]. The engine emissions – an
umbrella term used collectively for the several components of the engine exhaust such as NOx, CO, particulate matter, etc. – have been studied extensively for their adverse effects on the environment, driving stringent emissions regulations around the world.

The current efforts to address both, the energy security and emissions, for the transportation sector takes a two-pronged approach. On one hand, efforts are being made to develop advanced combustion technologies for the IC engine to provide higher fuel efficiency with lower emissions. Current downsized boosted SI engines offer substantially higher fuel economy with lower emissions compared to a similar power engine from just a decade ago. Additionally, significant research work is underway for developing engines operating on low temperature combustion modes which have shown the promise of significantly lower emissions and higher fuel economy.

On the other hand, renewable fuels are being developed with feedstock mainly coming from plant-based sources to minimize the net carbon footprint. The use of biofuels in the US has grown by over 900% from 2000 to 2016, majority of which is attributed to ethanol, derived mainly from corn starch [5]. The Federal Renewable Fuel Standard (RFS) in the US requires the introduction of increasing amounts of renewable energy into gasoline and diesel fuels each year, ultimately reaching 36 billion gallons by 2022 [6]. To put this in context, the total gasoline consumption in the US was 140 billion gallons in 2015 [1].

Efforts on both these fronts, however, require a deeper understanding of the physical and chemical processes of combustion, and, the chemical kinetics of the fuels.
1.1.1 Chemical Kinetics and Autoignition

A fundamental aspect of combustion research has been the development of comprehensive chemical kinetic models which can provide insight into the chemistry of combustion and enable predictive simulations that aid the development of advanced engines as well as new fuels and fuel additives. A deeper understanding of the chemistry of ignition and the subsequent heat release processes is the key to the optimization of the combustion process in conventional spark and compression ignition engines, as well as for the development of advanced engines operating in kinetically modulated combustion modes such as homogeneous charge compression ignition (HCCI), reactivity controlled compression ignition (RCCI), etc. [7]–[10].

A critical manifestation of the chemical kinetics of any fuel is its ignition delay characteristics over a wide range of temperature and pressures, which in turn depends on the autoignition chemistry. Understanding the autoignition chemistry is crucial to ensure a stable and knock free operation with low cycle to cycle variability for a conventional engine and achieving consistent combustion phasing in kinetically modulated combustion modes. Moreover, since the auto-ignition behavior is an inherent characteristic of the fuel chemistry, the ability of a chemical kinetic mechanism to predict the ignition delay of the fuel over a wide range of temperature and pressure conditions is a good indicator of the accuracy of the mechanism.

Various experimental apparatuses have been in use for obtaining chemical kinetic data, especially autoignition data, required for development, refinement and validation of
reaction mechanisms, such as combustion bombs, shock tubes, flow reactors, and rapid compression machines (RCM) [11]–[16]. The choice of the specific apparatus depends on the time scale of the ignition delay and the temperature and pressure conditions. RCM has been a popular and convenient tool for investigating the autoignition characteristics of fuels at low to intermediate temperature ranges, at engine relevant conditions.

1.1.2 Rapid Compression Machines

Rapid Compression Machines (RCM) [17]–[21] aim at studying combustion reactions at the time scales of typical internal combustion engines. Fuel-air mixture in the reaction chamber is compressed rapidly to the desired pressure and temperature, by moving the piston from bottom dead center (BDC) to the top dead center (TDC). Rapid compression ensures minimal progress of reactions in the air-fuel mixture during the compression phase. The subsequent combustion reactions following the rapid compression can be studied at constant volume conditions, in a well-defined and controlled environment without the complex fluid dynamics due to inlet, exhaust and mixing processes of a typical internal combustion engine, for a duration limited only by heat loss from the chamber (typically ~100 ms).

While the gas pressure inside the combustion chamber constitutes the primary data, RCMs allow the flexibility to accommodate a wide variety of measurement and diagnostic means such as gas sampling for intermediate species identification [22]–[24], optical diagnostics [25], [26], etc. This has led to the widespread use of RCM in combustion kinetic
investigations, especially the auto ignition investigations of transportation relevant fuels, at various temperature and pressure conditions for development, improvement or validation of chemical kinetic mechanisms [27]–[29].

The capability to perform an expansion stroke differentiates Rapid Compression and Expansion Machines (RCEM) from the RCM. In RCM, the piston in the compression chamber stays locked at the top dead center (TDC) after the completion of the compression stroke, but in RCEM, the piston can be retrieved after the compression stroke [21], [30].

As stated before, to minimize the reactions in the air-fuel mixture during compression process, the compression time must be small. The final compressed volume requirement at TDC determines the size of the combustion chamber and maximum compression ratio requirement dictates the stroke. This makes actuation of the piston in RCM and RCEM a challenging issue because fast compression over a long stroke would require high acceleration and high deceleration of the piston at the start and end of the stroke, respectively. The most popular actuation method is to use pressurized gas to provide high initial acceleration to the piston and use a stopping mechanism to deaccelerate the piston as it approaches TDC. Stopping techniques include the use of mechanical impact on a metal stopper [31], pneumatic cushion [17], or hydraulic cushion [19], [20], [32]. Use of a hydraulic cushion is currently the most popular stopping mechanism.
1.1.3 Limitations of The Current State-Of-The-Art RCM

The most profound limitation of the state-of-the-art RCM lies in the actuation philosophy which is inherently open loop and calibration based. This leads to the following fundamental limitations:

1) Current RCM are inherently rigid in terms of operating parameters. It is cumbersome to change parameters such as compression ratio, stroke, compression time, etc. as it generally involves manual replacement of parts such as adjustment washers, alteration of machine parameters such as driving pressure, etc. Such mechanical interventions often require subsequent re-calibration. This leads to repeatability issues, reduced accuracy, and long turnaround time.

2) Precise calibration of the stopping mechanism in the state-of-the-art RCM is a challenging and time-consuming task [32]. The effects such as piston bounce, piston trailing, and high-speed piston impact caused due to imprecise stopping force are a common nuisance and difficult to eliminate. Moreover, such calibration offers little robustness to variations in the approaching velocity.

3) The piston trajectory (i.e. compression profile) for the current RCMs is largely fixed by the geometry of the facility. This, in turn, implies that the thermodynamic path of compression, i.e. the pressure and temperature history to attain a certain end-of-compression conditions, is also inherently fixed and facility dependent. This is important because no matter how fast the compression, there is always some reaction progress during the compression, and hence, the intermediate species buildup at the end of compression is
strongly dependent on the thermodynamic path of the compression. The facility-to-facility variability of the thermodynamic path of compression, arising from the facility-to-facility variability in heat transfer characteristics and the compression trajectory is one of the major sources of facility-to-facility variability in the experimentally reported auto-ignition characteristics and severely limits the reproducibility of experimental data reported by any facility. This problem has been recognized and reported in the literature and more recently it has become a prevalent practice to supplement the auto-ignition experiment data with simulation results accounting for the facility specific thermodynamic path [20], [24], [33]–[36].

1.2 Controlled Trajectory Rapid Compression and Expansion Machine (CT-RCEM)

The controlled trajectory rapid compression and expansion machine developed at the University of Minnesota – Twin Cities addresses these limitations with the unique capability of precise control over piston trajectory and presents a new perspective for chemical kinetics and auto-ignition investigations. The desired piston motion profile is sent electronically to a high bandwidth position feedback controller which controls an electro-hydraulic actuator, driving the piston.
1.2.1 Unique Advantages of the CT-RCEM

The key to overcoming these limitations is the use of an actuator with feedback motion control. The reference piston trajectory can be fed to the controller electronically, eliminating the need for mechanical intervention for changing the operating parameters. Thus, the proposed CT-RCEM offers two major improvements over the current state-of-the-art conventional RCM:

1) With electronic piston motion control, the CT-RCEM offers ultimate flexibility of operation by eliminating the need for mechanical intervention and subsequent re-calibration. It not only allows a wider operating range with higher resolution and, but also provides exceptional repeatability of the piston trajectory and hence the gas pressure.

2) It enables a whole new paradigm of experimental investigation for chemical kinetic studies which is currently not possible using any other experimental facility. The thermodynamic path of the fuel mixture in the combustion chamber during an RCM investigation (essential pressure and temperature history) is a function of the heat transfer characteristics of the chamber assembly as well as the piston trajectory. Hence, by suitable selection of the piston trajectory, the CT-RCEM allows not only the capability to set the end of compression thermodynamic state (compressed pressure and temperature), but also the flexibility to tailor the entire thermodynamic path, during and after the compression.
1.2.2 Challenges for Design of the CT-RCEM

An electro-hydraulic actuation system has been selected for piston actuation in the CT-RCEM. High bulk modulus of hydraulic fluid ensures a high-power density, and hence, high specific power for electrohydraulic actuators. This makes electrohydraulic actuators the preferred choice for several servo applications that require precise motion control [37], [38], including piston actuation for CT-RCEM. While the use of a hydraulic actuator with feedback control of piston TDC position has been reported before, it has been limited to small stroke and compression ratios [21], [30], [39]. Moreover, CT-RCEM offers complete control of the piston trajectory and not just the piston TDC position. However, the use of an electro-hydraulic actuator for CT-RCEM involves three major challenges.

1) For large combustion force and large stroke, fluid compressibility is no longer negligible. The long and slender fluid column behind the hydraulic piston behaves as an oil spring if the combustion force is sufficiently high. Hence, the piston is excited into high frequency vibrations when the combustion occurs. These vibrations are challenging to control even with active motion control and their severity increases rapidly with increase in stroke and combustion force.

2) Piston actuation for CT-RCEM is both a high force and high-speed application with a relatively large working stroke. Hence, the actuator requires a large flow rate with low flow throttling. This imposes the requirement of a large spool size and stroke on the servo-valve which in turn tends to slow the response of the actuator. This makes the precise high speed motion control of the system extremely challenging [40]–[43].
3) The scale of the application makes the problem even harder, leading to several practical problems. For example, the requirement of large flow rates for trajectory tracking mandates the use of a servo valve with a large rated flow matching the flow demand of the actuator during the high-speed motion. However, this forces a small signal operation of the servovalve for static position regulation of the piston, say at BDC during the fueling process. While for normal operation the nonlinearities of the servovalve arising from stiction of valve spool, hysteresis, valve undercut, etc., are too small to have a noticeable impact on the system performance, for small signal operation such nonlinearities may lead to limit cycle oscillations. Similarly, maintaining accurate tracking over a long stroke presents a challenge for deploying a suitable sensor instrumentation system in terms of sensitivity, resolution and noise immunity. For example, even a 10-mV peak-peak noise on the output of the linear variable differential transformer (LVDT) used as the displacement sensor translates to roughly 0.2 mm peak-peak noise on the piston position measurement for a stroke of 200 mm, thereby placing a practical lower bound on the tracking accuracy.

1.3 Summary of Contributions

The key contributions of this work are summarized below:

1) **Modeling and design of the CT-RCEM:** A control-oriented model is developed and is subsequently used to design a novel experimental facility, i.e. the controlled trajectory rapid compression and expansion machine. The actuation system of
the CT-RCEM is capable of handling peak hydraulic flow rate of up to 1600 $l/min$ at a supply pressure of 350 $bar$. This allows the actuation system to produce any desired trajectory with peak acceleration up to 2500 $ms^{-2}$, peak velocity up to 16 $ms^{-1}$, and stroke up to 192 mm.

2) **Development of precise motion controller for CT-RCEM:** A model-based motion controller has been developed to provide precise trajectory tracking for the CT-RCEM actuation system. The control design, however, can be extended to any generic high-force and high-speed application for electrohydraulic actuators requiring precise motion control. Additionally, a nonlinear inversion-based feedforward controller has been developed for hydraulic actuators with asymmetric piston. It has been demonstrated that the current implementation of the controller can reduce the tracing error to 0.6 $mm$ for a stroke of 131 $mm$ with a peak speed of about 12 $ms^{-1}$ with the run-to-run variability in the tracking performance about 0.2 $mm$.

3) **Characterization of the CT-RCEM:** The characterization of the CT-RCEM has been conducted using non-reactive and non-reactive mixtures to demonstrate the functionality and repeatability over the operating range. For the first time, the ability to shape the thermodynamic path of compression inside the combustion chamber by suitable choice of piston trajectory has been demonstrated. Three novel investigative capabilities facilitated by the ability to control the piston trajectory have been demonstrated – investigating the effect of compression time on ignition delay, generating isobaric dwell at the end of compression using piston creep, and, quenching of the combustion chamber
gases by rapid withdrawal of the piston. Additionally, the capability to perform detailed investigation of the combustion characteristics of a single combustion cycle of an IC engine has been demonstrated by presenting a case study pertaining for the experimental investigation of an advanced control strategy, called trajectory based combustion control, for free piston engine operation.

4) **Development of computationally efficient multi-zone model for analysis of CT-RCEM data**: A computationally efficient, multi-zone thermo-kinetic model has been developed to analyze the data obtained from the CT-RCEM. It is shown that the concurrent use of the proposed model with the CT-RCEM allows, for the first time, a systematic investigation of the effect of changing piston trajectory – and consequently – the thermodynamic path of compression on the auto-ignition characteristics of fuels. The effect of changing piston trajectory on autoignition characteristics of dimethyl-ether (DME) observed in CT-RCEM experiments has been explained using the proposed model. The study clearly shows that changing the piston trajectory can significantly affect the measured ignition delay due to the resulting change in the thermodynamic path. Also, a shorter compression time for a given compression ratio does not necessarily guarantee smaller reaction progress during compression.

**1.4 Dissertation Overview**

This dissertation consists of six chapters. Chapters 2 and 3 present the design, development and control of the CT-RCEM. In Chapter 4 the characterization of the CT-
RCEM and demonstration of its unique capabilities for fundamental and applied combustion research have been presented. Chapter 5 presents the development of a multi-zone model and the use of reaction path analysis to show the effect of piston trajectory on ignition delay. Finally, Chapter 6 summarizes the dissertation and suggests the future research directions. A brief overview of each chapter is given below:

**Chapter 2:** In this chapter, first the system architecture of the CT-RCEM is presented showing the relationship between the various submodules. Next, a control-oriented dynamic model is developed for the CT-RCEM with combustion dynamics, hydraulic actuator dynamics and piston dynamics. The combustion dynamics consists of a simplified mean value HCCI combustion model converted from crank-angle to time domain, couple with a modified Woschni correlation for heat transfer, instead of detailed chemical kinetics. Then, simulation results and analysis are presented delineating the relationship between various geometrical parameters and physical quantities and hence identifying critical design tradeoffs. Based on this, the selected final design parameters have been presented.

**Chapter 3:** In this chapter, the development of the motion controller for the CT-RCEM is presented. The chapter starts with a discussion of the control philosophy for the CT-RCEM followed by the design of the repetitive controller for the dynamic model and the iterative learning control for the hardware setup. Next, a nonlinear inversion-based feedforward controller has been developed for hydraulic actuators with asymmetric piston for further improvement in tracking performance since CT-RCEM uses a hydraulic
actuator with asymmetric piston. After this, the control implementation and experimental results are presented, including initial limit cycle behavior of the system, its mitigation, and the controller performance for typical RCM and RCEM trajectories.

**Chapter 4:** In this chapter, the characterization of the CT-RCEM for reactive and non-reactive mixtures has been presented. First, a brief discussion about the importance of the thermodynamic path of the test mixture in the combustion chamber is presented along with how the ability to control the piston trajectory can be used to design special thermodynamic paths. Next the operational flexibility of the CT-RCEM is demonstrated. After this, the repeatability of the piston position and pressure data over successive repetitions is established for both non-reactive and reactive mixtures. The characterization for reactive mixtures is done for three different fuels – di-methyl ether (DME), butane and ethanol. Following this, three novel investigative capabilities enabled by shaping of the thermodynamic path have been demonstrated – ability to investigate the effect of compression time on ignition delay over a range of temperatures, ability to quench the combustion chamber contents by rapidly pulling back the piston at a desired time, and, ability to create an isobaric dwell post compression by slow creeping of the piston to offsets the wall heat loss. Finally, the utility of the CT-RCEM for in-depth analysis of the combustion characteristics for IC engine applications has been demonstrated by presenting a case study for experimental investigation of an advanced combustion control strategy for free piston engines (FPE) previously proposed in our group – trajectory based combustion control.
Chapter 5: In this chapter, the development of a computationally efficient, physics based multi-zone model of the combustion dynamics of the CT-RCEM is presented which accounts for detailed chemical kinetics, heat loss and piston crevice flows. A systematic method is presented next, which involves the concurrent use of the CT-RCEM and the model, for investigation of the relationship between the piston trajectory, the thermodynamic path of compression, and autoignition. Experimental results for the autoignition testing of DME showing the effect of piston trajectory, and hence, the thermodynamic path, have been presented and explained using a reaction path analysis. It is explained why a shorter compression time for a given compression ratio does not necessarily guarantee smaller reaction progress during compression.
CHAPTER 2  Mechanical Design

In the previous chapter some of the major challenges for the design of the actuation system of the CT-RCEM were discussed in detail. To design a system that subverts these challenges requires a systematic study of the impact of various design parameters of the system on the important physical quantities. Such a study also enables us to identify the major design tradeoffs and bottlenecks. The systematic development of the mechanical design of the CT-RCEM is based on simulation studies conducted using a physics based dynamic model which has been presented here in detail.

First, the architecture of the CT-RCEM is shown, which delineates the relationship of the various subsystems of the CT-RCEM with one another. Next, the physics based dynamic model of the CT-RCEM is developed which is subsequently used for simulation study for the design. The chapter concludes with the final mechanical design of the CT-RCEM and the simulation results pertaining to the final design.

2.1  System Architecture

The overall system architecture of the CT-RCEM is shown in Figure 2-1. The system can be divided into five sub-units – hydraulic actuator unit, combustion chamber unit, control module, fueling and exhaust gas purging system, and diagnostics system.
**Hydraulic Actuator Unit**

The hydraulic actuator unit consists of the hydraulic supply unit, hydraulic actuator a high speed servovalve and the associated accessories. The hydraulic actuator consists of a double acting piston moving inside a custom designed manifold. A high bandwidth servo valve is fitted on top of the manifold. The design of the manifold ensures minimum dead volume between the servovalve and the hydraulic piston. Ports are provided in the manifold to accommodate pressure sensors at the two ends of the piston chamber to monitor the chamber pressure. Additionally, a pressure sensor is provided at the entry of the manifold.

![System architecture of CT-RCEM showing relationship between various submodules](image)

*Figure 2-1: System architecture of CT-RCEM showing relationship between various submodules*
to monitor the supply pressure. The piston trajectory control is achieved by real time control of the servo valve. The hydraulic supply unit consists of a pump that charges two 10-gallon (~ 40 l) accumulators rated for a peak flow rate of 800 l/min each. While the pump is rated for 350 bar, lower working pressure can be achieved through a relief valve installed downstream of the pump. The two accumulators are connected in parallel to the hydraulic actuator to provide a peak flow rate of up to 1600 l/min. The hydraulic circuit has a kidney loop cooling unit connected to the hydraulic sump to dissipate the heat generated from operating the hydraulics. The unit is operated from the centralized controller in two operating modes – ON-OFF operation or set point temperature regulation. The hydraulic piston and the combustion chamber piston are attached to the two ends of a common connecting rod.

**Combustion Chamber Unit**

The combustion chamber assembly consists of a combustion cylinder and head bolted together with the combustion piston moving inside it. Depending on the requirement, a steel head or optical head can be used. The optical head allows for a side view and a front view of the inside of the combustion chamber. The piston in the combustion chamber is screwed on to the connecting rod. The assembly allows for simple replaceability of the piston to enable the use of different kinds of piston designs such as flat piston, creviced piston, bowl-shaped piston etc. as per requirement. A creviced piston design, for instance, ensures containment of the “roll-up” vortex due to piston motion during compression of air-fuel mixture. This design ensures a near quiescent core of the
mixture in the center of the combustion chamber minimizing the effect of turbulence on chemical kinetics [20], [34], [44].

Control Module

The centralized data logging and motion controller is implemented on a dSPACE DS1007 unit with a dual core 2.0 GHz processor. The nature of the application involves dealing with three different kinds of signals in terms of desired sampling frequency and hence a multi rate sampling scheme is being used for this application. The combustion chamber pressure signal can have significant high frequency content and is hence sampled at 25 kHz. The piston position signal, the hydraulic pressure signals, and the servovalve spool position feedback signal are all sampled at 5 kHz. The actuation system control loop operates at a frequency of 5 kHz. The signals that require low speed sampling include the temperature and pressure signals from the fueling and exhaust unit and are sampled at 2 Hz. A linear variable differential transformer (LVDT) position sensor which is connected to the hydraulic piston is used for piston position feedback to the controller. A Kistler pressure transducer is used to record the combustion chamber pressure. Separate PID temperature control modules are used to control the heating tapes used for maintaining the fueling system and combustion chamber at set temperature if pre-heating is required.

Fueling and Exhaust Purging System

The fueling and exhaust purging system is used for introducing fuel, extracting exhaust gases, and purging the combustion chamber. Coupling the three systems into one allows for a quick, efficient way of moving the gases simply by operating different sets of
check valve as per requirement. The fuel tank is a 10 liter custom designed vessel fitted with various ports to accommodate sensors and gas inlets. A magnetic stirrer inside the tank is used to ensure homogenous mixing of the fuel. For gaseous fuels, the fuel-mixture preparation is manometric using a Baratron pressure gauge. For liquid fuels, the fuel is metered volumetrically and introduced into the fuel tank at room temperature and then the temperature is raised to a pre-determined value to ensure the complete vaporization of the liquid fuel, the oxidizer and diluent gases are added next, manometrically, to the fueling tank. A vacuum pump is used to create negative pressure to assist moving gasses around such as, moving the exhaust out of the combustion chamber, evacuating the combustion chamber before fueling, evacuating the fuel tank, etc.

**Diagnostics System**

The diagnostic unit consists of an Agilent 7890B gas chromatography unit coupled with an Agilent 5977A Mass Spectrometry Detector. The GCMS system with a dedicated sampling system and can be used for ex-situ chemical species detection and measurement. The laser diagnostic unit consists of a planar laser induced fluorescence (PLIF) system, from TSI, with an Nd-YAG laser, with maximum pulsed output 120 mJ/pulse, coupled with a high resolution CCD camera. The PLIF system can be used with a special combustion chamber head with optical windows for in-situ species measurements.
Figure 2-2: Controlled Trajectory Rapid Compression and Expansion Machine (CT-RCEM) developed at University of Minnesota – Twin Cities

Figure 2-2 shows the actual setup of the CT-RCEM with the major sub-systems after commissioning.

2.2 Dynamic Model of the System

This section presents the dynamic model of the CT-RCEM developed to capture its essential dynamics. The aim of this model is twofold – first to understand the impact of various design parameters of the CT-RCEM on its performance, thereby tuning them to obtain a suitable mechanical design; and second to design a suitable controller that can achieve the objective of real time control of the piston trajectory for the CT-RCEM. The later part is addressed in the next chapter.
The model essentially consists of combustion dynamics, piston dynamics and the hydraulic actuator dynamics. The combustion dynamics aims at relating the pressure trace inside the combustion chamber to the piston trajectory. Piston assembly dynamics aims at relating the load trace, for a given piston trajectory, for the hydraulic actuator to the pressure trace in the combustion chamber and inertial forces of the piston assembly. Hydraulic actuator dynamics aims at relating the load trace to the pressure and flow requirements for the hydraulic fluid inside the hydraulic actuator.

2.2.1 Combustion Chamber Dynamics

As stated before, the aim of the combustion chamber dynamic modelling is to relate the pressure trace inside the combustion chamber to the piston trajectory. The fueling system and combustion chamber design ensures that the fuel-air mixture inside the combustion chamber is homogeneous before the start of the compression and the chamber wall temperature is held constant. The gas state in the combustion chamber is calculated using the first law of thermodynamics for closed system and ideal gas law. The rate of change of internal energy of the gas $\dot{U}$ is given as

$$\dot{U} = \dot{Q}_{comb} - \dot{Q}_{loss} - P_c \dot{V}_c$$

(2-1)

$$\dot{U} = mC_v \dot{T} = \frac{mRT}{\gamma - 1} = \frac{\dot{P}_c V_c + P_c \dot{V}_c}{\gamma - 1}$$

(2-2)
where, $\dot{Q}_{\text{comb}}$ is the rate of heat released during combustion and $\dot{Q}_{\text{loss}}$ is the rate of heat loss from the gas, $m$ is the mass of the fuel-air mixture, $C_v$ is isochoric specific heat capacity, $R$ is the specific gas constant, $\gamma$ is the ratio of specific heats and $P_c$ and $V_c$ are the combustion cylinder pressure and volume respectively. Term $P_c V_c$ is the rate of work done by the gas. Hence, time derivative of chamber pressure, $\dot{P}_c$, can be expressed using (2-1) and (2-2) as

$$\dot{P}_c = \frac{\gamma - 1}{V_c} (\dot{Q}_{\text{comb}} - \dot{Q}_{\text{loss}}) - \frac{\gamma P_c V_c}{V_c} \tag{2-3}$$

To estimate $\dot{Q}_{\text{loss}}$ the modified Woshini correlation for heat transfer in IC engines is used [45], which is given as

$$\dot{Q}_{\text{loss}} = h_{\text{loss}} A_S (T_c - T_w) \tag{2-4}$$

$$h_{\text{loss}} = \alpha L^{-0.2} P_c^{0.8} T_c^{-0.73} v_{ht}^{0.8} \tag{2-5}$$

$$v_{ht} = C_1 \bar{S}_p + \frac{C_2}{6} \frac{V_c}{V_0} (P_c - P_{\text{mot}}) \tag{2-6}$$

where $h_{\text{loss}}$ is the convective heat transfer coefficient, $A_S$ is the total surface area of the combustion chamber, $T_w$ is the wall temperature of the chamber, $\alpha$ is a scaling factor, $L$ is the instantaneous height of the combustion chamber, $C_1$ and $C_2$ are constants, $\bar{S}_p$ is the average piston velocity, $P_{\text{mot}}$ is the motoring pressure, and $P_0$, $T_0$ and $V_0$ are initial pressure temperature and volume respectively.

To account for $\dot{Q}_{\text{comb}}$, the progress of the combustion reaction is modeled using the mean value model for HCCI combustion proposed in [46], converted from crank-angle
domain to time domain. This model predicts the start of combustion (SOC), combustion duration, and the heat release for a given fuel, air fuel ratio and piston trajectory. This model assumes that the entire heat of combustion is released instantaneously at the end of combustion.

The effect of piston trajectory on combustion, particularly the SOC timing, can be clearly noticed from (2-3) through the rate of volume change term ($\dot{V}_c$) which is the control input. While this is a fairly simplified control-oriented combustion model that does not capture the details of combustion kinetics, it suffices to provide enough information for the design of hydraulic actuator.

### 2.2.2 Hydraulic Actuator and Piston Dynamics

As noted in [42], the valve dynamics in electro hydraulic actuators is faster than the rest of the system and hence can be neglected without significant loss of performance. Hence the dynamics of the hydraulic actuator is modelled essentially using orifice equation, fluid compressibility equation and Newton’s second law.

The rate of pressure change in the left and the right chambers of the hydraulic cylinder is given as

\[
\dot{p}_l = \beta \left( q_{\text{servo}_l} + A_l \dot{x} \right) \frac{1}{V_l} \tag{2-7}
\]

\[
\dot{p}_r = \beta \left( q_{\text{servo}_r} - A_r \dot{x} \right) \frac{1}{V_r} \tag{2-8}
\]
where $\beta$ is the bulk modulus of the fluid, $P_l$, $P_r$, $V_l$, and $V_r$ are the fluid pressures and volumes in the left and right chambers, respectively. $A_l$ and $A_r$ represent the area of hydraulic piston on left and right side respectively. $\dot{x}$ is the piston velocity which is considered negative when piston is travelling towards TDC. The flow rate through servo valve to left and right chambers is denoted by $q_{servo_l}$ and $q_{servo_r}$ respectively and is modeled using the orifice equation between the hydraulic power supply and the chamber as

$$q_{servo_l} = u_c \cdot K_m \cdot \text{sign}(P_l - P_1) \frac{\sqrt{2|P_l - P_1|}}{\rho}$$

(2-9)

$$q_{servo_r} = u_c \cdot K_m \cdot \text{sign}(P_r - P_2) \frac{\sqrt{2|P_r - P_2|}}{\rho}$$

(2-10)

$$P_1 = \begin{cases} P_{acc}, & \text{if } u_c \leq 0 \\ P_{sump}, & \text{if } u_c > 0 \end{cases} ; P_2 = \begin{cases} P_{sump}, & \text{if } u_c \leq 0 \\ P_{acc}, & \text{if } u_c > 0 \end{cases}$$

(2-11)

where, $u_c \in [-1,1]$ is the control signal to the servo valve, $K_m$ represents the maximum effective orifice area of the servo valve and $\rho$ is the fluid density. $P_{acc}$ is the hydraulic supply pressure and $P_{sump}$ is the sump pressure. The supply pressure is held constant during the operation of the CT-RCEM. The dynamics of piston assembly can now be written as

$$m_p \ddot{x} = P_l A_l - P_r A_r - P_c A_c - k_v \dot{x}$$

(2-12)

where $m_p$ is the mass of the piston assembly consisting of hydraulic piston, combustion chamber piston and the connecting rod, and $A_c$ is the combustion chamber piston area. The
term \( k_v \dot{x} \) accounts for the viscous friction in the system, where \( k_v \) is the coefficient of viscous friction. It is interesting to note that the quantities \( V_c \) and \( V_c \dot{\gamma} \) in (2-3) are directly related to system states \( x \) and \( \dot{x} \).

### 2.2.3 Mechanical Stop

Due to the compressibility of fluid, the oil column in the hydraulic chambers behaves as a stiff spring and this effect becomes significant at high combustion pressures. The piston is held in equilibrium at TDC by equal and opposite fluid force from the hydraulic chamber and gas force from the combustion chamber. The system thus essentially behaves as a spring mass system as shown in Figure 2-3 (left). However, when combustion occurs, the force in the combustion chamber rises suddenly and the piston is perturbed from its equilibrium into a high frequency vibration, called ringing. Piston ringing is highly undesirable because it disturbs the fluid dynamics and hence the chemical kinetics inside the combustion chamber. Due to inherent uncertainty of combustion, no matter how good or fast the controller is, the piston will inevitably see some non-zero net force for a short duration and this will induce piston ringing for this configuration. Since the amplitude of ringing will depend on the stiffness of the oil spring, the hydraulic actuator design must aim at maximizing the oil spring stiffness to minimize the severity of ringing. Oil spring stiffness can be written as

\[
k_{oil} = \frac{\beta A_{hyd}^2}{V_{hyd}}
\]

(2-13)
where $A_{h,yd}$ is the cross sectional area of the liquid column in the hydraulic chamber and $V_{h,yd}$ is the volume of the liquid column behind the piston [37]. Thus, to minimize the ringing amplitude we can

i. Use higher bulk modulus fluid

ii. Increase the cross-sectional area of the hydraulic chamber (increase bore)

Minimize the dead volume in the cylinder

However, there are practical limitations on increasing the fluid spring stiffness through design alone and this calls for a change in the system configuration.

A new system configuration has thus been proposed which uses a mechanical stop built into the hydraulic chamber. As can be seen from Figure 2-3 (right), the system is no longer a spring-mass system. In this configuration, a mechanical stop is placed at the TDC and the piston trajectory is designed such that the piston is seated smoothly on the stop at
the end of the stroke. Thereafter, the actuator holds the piston against mechanical stop with maximum actuation force. The system is now described by (7)

\[
F_h - F_N - F_{gas} = 0
\]  

(2-14)

where \(F_h = P_l A_l - P_r A_r\) and \(F_{gas} = P_c A_c\)

here, \(F_h\) is actuation force, \(F_{gas}\) is the force due to gases in combustion chamber, and \(F_N\) is the normal reaction applied by the stop on the piston. As \(F_{gas}\) increases with the progress of combustion, \(F_N\) reduces, while \(F_h\) stays constant. Hence, \(F_N\) acts as a reserve force. The condition for no ringing, i.e. piston always staying in contact with the stop, is that \(F_N > 0\).

It may be noted that addition of a mechanical stop does not limit the flexibility of the CT-RCEM in changing the compression ratio, or the shape of the piston trajectory, as the choice of the starting position of piston, i.e. BDC for the stroke, is still available.

### 2.2.4 Simulations Studies and Parameter Selection

As mentioned before, the dynamic model is used to identify the impact of various design parameters on system performance. The two most important operational parameters that define the usability space of the RCEM for combustion experiments are the compression ratio, and the compression time. For our design, the maximum compression ratio and minimum compression time has been chosen to be 25 and 20 ms respectively – typical of the current state-of-the-art RCM. For the CT-RCEM, the maximum compression ratio represents the compression ratio achieved when the combustion piston travels the total usable stroke of the actuator. The minimum time required to travel the full usable stroke of
the actuator represents the minimum compression time. Since the position of the TDC must be fixed to implement the mechanical stop, a lower compression ratio can be implemented by moving the BDC position closer to TDC, in other words, using only a part of the usable stroke. Similarly, a higher compression time may be obtained by lowering the speed of the actuator during the stroke. Hence, by suitable selection of the piston trajectory, the CT-RCEM can be used to investigate practically any combination of compression ratio, compression time, and shape of piston trajectory for a given compression ratio and compression time, within the operating space.

The geometric parameters of the combustion chamber that define the actuation requirement are the combustion chamber bore and the TDC clearance. To investigate the effect of bore size on combustion, (2-3) can be rewritten as

$$\dot{P}_c = \frac{\gamma - 1}{x} \left( \frac{\dot{Q}_{comb}}{A_c} - \frac{h_{loss} A_s \Delta T}{A_c} \right) - \frac{\gamma P_c x}{x} \tag{2-15}$$

where $h_{loss}$ is the convective heat loss coefficient and $\Delta T$ is the difference between the instantaneous temperatures of the gas and the chamber wall and $A_s$ is the surface area of the chamber. $\dot{Q}_{comb}$ is directly proportional to the initial mass of the charge in the combustion chamber [46], which in turn is directly proportional to $A_c$. This implies that $\dot{Q}_{comb}/A_c$ is independent of the bore size. Also, while $h_{loss}$ and $A_s/A_c$ are both functions of bore size, simulations show that the effect of change in $h_{loss}A_s/A_c$, due to change in bore size, on the gas pressure is relatively small. Accordingly, the net change in $P_c$ due to change in bore size is relatively small. Hence, the effect of combustion bore size on actuator dynamics is manifested predominantly through the area term $A_c$ in the gas force $P_c A_c$. 
The effect of TDC clearance is more subtle and is difficult to interpret directly from (2-3) or (2-15). However, simulations show that for same compression ratio and compression time, the gas pressure profile is relatively similar for different TDC clearances as well. The gas force remains relatively the same if the TDC clearance is increased, but to maintain same compression ratio and compression time, the stroke and the piston speed must be increased, leading to the higher inertial force for the piston motion. An increase in gas force or inertial force demands an increase in the actuation force. This in turn implies, from (2-7) to (2-11), a requirement of higher flow and a larger servo valve. Simulation results presented below further illustrate the above discussion. HCCI combustion has been simulated for gasoline, with air fuel ratio 36:1 at 300 K, with initial pressure 1.25 atm. The chamber wall temperature has been set to 500 K.

Figure 2-4 shows the effect of combustion bore size on the actuation force and flow rate requirement, for a constant TDC clearance of 8 mm for a relatively aggressive trajectory for the RCEM piston - stroke 192 mm, compression ratio 25, compression and expansion time 20 ms. The peak piston velocity is 15 m/s and the peak acceleration (deceleration) is 2360 m/s^2 at the start (end) of stroke. The resulting combustion chamber pressure is nearly same for all three. The bottom left plot shows the corresponding actuation force required to realize this trajectory for three different combustion chamber bore sizes – 40, 50, and 60 mm. Assuming a constant hydraulic supply pressure of 350 bar, the minimum required hydraulic actuator bore size which can just provide the maximum required actuation force would be 30.24, 37.81, and 45.36 mm respectively. The required
hydraulic flow rate for each case, respectively, has been shown in the bottom right plot.

Figure 2-5 shows the effect of TDC clearance on actuator dynamics, for a constant combustion bore size of 50 mm. Three different trajectories required to achieve a compression ratio of 25, in 20 ms compression time, have been shown for three different TDC clearances- 5mm, 8mm and 10mm. Again, the gas pressure profile is almost same for all three cases. The required peak flow rate for the actuator, assuming actuator bore size of 40 mm is shown in the bottom right plot.
The analysis presented above brings forward the main design tradeoff for the actuation system. The practical constraint for the actuation system design is the selection of a servovalve large enough to meet the peak flow demand. However, since a larger servovalve will have larger spool, and hence higher spool inertial, and, a larger spool stroke, it will tend to have a slower response. Hence, the selection of the combustion chamber bore, TDC clearance and subsequently the hydraulic actuator bore is a tradeoff between actuation force and actuator bandwidth subject to the selection of a suitable servovalve. Once the combustion chamber bore and the TDC clearance are selected, which determines the hydraulic actuator bore and the peak flow. The fastest commercially

Figure 2-5: Effect of TDC clearance on actuation dynamics. The plots show trajectory, resulting gas pressure and corresponding flowrate requirement for TDC clearance 5 mm (blue), 8 mm (red) and 10 mm (yellow)
available servovalve that can meet this flow demand is then selected to ensure fast response of the actuator.

### 2.3 Final Design

Table 2-1 summarizes the design parameters of the CT-RCEM finalized based on rigorous analysis of simulation results from the dynamic model. For the selected bore size of 40 mm the maximum actuation force will be about 44kN, and the maximum fluid flow rate required, for a peak velocity of 15 m/s will be about 1130 l/min. For more aggressive trajectories, the peak velocities can be even higher. The system has been designed to handle

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Combustion Pressure</td>
<td>250 bar</td>
</tr>
<tr>
<td>Minimum Compression Time</td>
<td>20 ms</td>
</tr>
<tr>
<td>Maximum Compression Ratio</td>
<td>25</td>
</tr>
<tr>
<td>Combustion Chamber Bore</td>
<td>50.8 mm</td>
</tr>
<tr>
<td>Maximum piston travel</td>
<td>192 mm</td>
</tr>
<tr>
<td>TDC Clearance</td>
<td>8 mm</td>
</tr>
<tr>
<td>Hydraulic Working Pressure</td>
<td>350 bar</td>
</tr>
<tr>
<td>Hydraulic Piston Bore</td>
<td>40 mm</td>
</tr>
<tr>
<td>Mass of Piston Assembly</td>
<td>1.7 kg</td>
</tr>
<tr>
<td>Rated Flow of Servovalve</td>
<td>1000 l/min</td>
</tr>
</tbody>
</table>
peak flow rate of up to 1600 l/min.

The simulation results for two representative piston trajectories for CT-RCEM operation have been shown in Figure 2-6 and Figure 2-7.

Figure 2-6 shows a sinusoidal trajectory with stroke of 152 mm and compression ratio 20. The compression and expansion times are 20 ms each. The HCCI combustion is simulated for gasoline, with air fuel ratio 20:1, preheated to 75°C, with initial pressure 1.25 atm. This is a relatively moderate trajectory and it can be seen that the peak flow rate is about 900 l/min.

Figure 2-6: Simulation results for RCEM operation. Top plots show a representative sinusoid trajectory, corresponding tracking error and gas pressure. Bottom plots show hydraulic pressure and flow rate in left (blue) and right (red) chambers of the actuator.
Figure 2-7 shows a trapezoidal trajectory with stroke 192 mm and compression ratio 25. The compression and expansion times are 20 ms each, while the piston dwell time at TDC is 50 ms. The HCCI combustion is simulated for gasoline, with air fuel ratio 36:1, preheated to 300 K, with initial pressure 1.25 atm. This is an aggressive trajectory involving full stroke operation of the actuator and in this case the flow rate is close to 1200 l/min.

More details about the dynamic model, simulation analysis and controller performance can be found in [47], [48].
2.4 Conclusion

A dynamic model has been developed for the CT-RCEM to guide the mechanical design. Simulation studies have been conducted to clearly understand the impact of various design parameters on the CT-RCEM performance and thereby guide the final mechanical design. It has been found that the main design tradeoff is between actuator force and actuator bandwidth which has been pertinently addressed in the final design. The development of a model based controller based on this dynamic model has been described in the next chapter.

Final design parameters of the CT-RCEM are summarized in Table 2-1.
CHAPTER 3  Controller Design

In chapter 1 the reason for the choice of electrohydraulic actuation system as well as the associated challenges were discussed. Essentially, while electrohydraulic actuators provide great power density, their application, in general, for precise motion control is usually limited to relatively low speed or small stroke applications. In chapter 2, it was shown through simulation studies that this limitation arises from the fact that the increase in the speed of operation leads directly to the increase in flow demand. This leads to the requirement of a larger servovalve with a bigger spool and larger spool stroke, which tends to increase the response time of the valve, making the control harder. Various control strategies have been suggested over time to achieve precise motion control for higher stroke and speed [40]–[42], and have documented the difficulty involved.

This chapter presents the details of the development and implementation of motion controller for the CT-RCEM actuation system. However, the application of the design methodology and principles presented here goes beyond the CT-RCEM and can be easily extended to a generic high-force high-speed application of electrohydraulic actuators, with a large stroke.

First, the control philosophy of the CT-RCEM is presented which illustrates the reasoning behind the choice of the controller for the CT-RCEM. Next, the design of the repetitive controller used for the dynamic model and the iterative learning controller used for the hardware is presented. A repetitive controller has been used for the dynamic model mainly because the dynamic model does not have a turnaround time between experiments,
Unlike the hardware. Next, the design of a nonlinear feedforward controller based on numerical inversion, for electrohydraulic actuators with asymmetric piston is presented. After this, the implementation of the control on the hardware and the experimental results demonstrating the tracking performance are shown.

3.1 Control Philosophy for the CT-RCEM

For the CT-RCEM operation, the maximum stroke can be up to 192 mm and the compression time can be as small as 20 ms. For a purely sinusoidal travel over the maximum stroke, the peak speed is about 15 m/s and the peak flow rate is 1140 l/min, for the designed CT-RCEM (as presented in detail in section V). Even higher speed and flow rate is expected for some compression profiles which deviate from the pure sinusoid [49].

For such a demanding application, the only way to accomplish precise motion control is ensure that system design and control design proceed in-tandem. While a suitably designed controller provides sufficient bandwidth for control action, a suitable system design ensures operation of the system in the most favorable operating region to provide enough capacity for executing the control action.

The selection of the control philosophy for CT-RCEM operation is dictated by three key facts. First, for a given experiment of the CT-RCEM, the desired trajectory is always known beforehand. Second, while the disturbance dynamics cannot be accurately predicted theoretically, it is fairly repeatable for different iterations of the same experiment. The source of this disturbance could be plant uncertainties, nonlinearities (orifice equation, gas...
force, etc.), leakages, friction etc. Third, the operation of the CT-RCEM is inherently cycle by cycle instead of continuous, with resetting initial conditions at the beginning of each cycle. The system must be pressurized and fueled before each experiment and depressurized and exhaust gas purged after each experiment. Moreover, the time duration of piston motion for each experimental cycle is extremely small (≈ 40 ms) which makes in-cycle convergence difficult, which in turn limits the tracking performance. Based on this, a run-to-run iterative learning control (ILC) is a suitable control strategy for this application since it relies on cycle to cycle feedback for improvement in control performance. Moreover, an ILC guarantees asymptotic reference tracking and disturbance rejection if the time period of the reference signal is constant, stability conditions are satisfied, and the disturbance dynamics is repeatable from cycle to cycle [50].

The plant (CT- RCEM) is first stabilized with a proportional controller. Next, a linear model based ILC is designed to ensure precise tracking performance. Figure 3-1 shows the control scheme for the CT-RCEM.

However, choice of the initial control signal for the first iteration has a significant impact on the number of iterations required for ILC convergence (i.e. no significant

\[\text{Figure 3-1: Control scheme for CT-RCEM}\]
improvement with further iterations). Hence, the initial signal for the ILC is generated through simulation, from the dynamic model of the CT-RCEM. Figure 3-2 shows the control scheme implemented on the dynamic model of the CT-RCEM to generate the initial control signal for the ILC. While the hardware has a minimum turnaround time (10-30 minutes) between two successive iterations which depends on the setup time (exhaust purging, refuelling, etc.) and the experiment being performed, the dynamic model does not have such a constraint. Hence, a repetitive controller has been used for this purpose. The converged signal from the repetitive controller is used as the initial control signal for the ILC. The ILC fine tunes this signal to compensate for the difference between the dynamic model and the actual hardware, within a few iterations.

3.2 Design of Repetitive Controller for the Dynamic Model

Repetitive controller is a type of iterative learning control which is used for tracking continuous periodic reference. The control structure used here is the robust prototype repetitive controller. It guarantees asymptotic rejection of tracking error if the time period

![Figure 3-2: Control scheme for dynamic model used for generating initial signal for ILC](image)
of reference is constant and stability conditions are satisfied; more information can be found in [51].

If the transfer function representing the nominal plant model is \( G_p(q^{-1}) = B(q^{-1})/A(q^{-1}) \), the control input \( u \) is calculated as

\[
  u(k) = C(q^{-1})[r(k) - y(k)]
\]

where \( r(k) \) is the current reference and \( y(k) \) is the current output. Additionally, controller \( C(q^{-1}) \) has the structure

\[
  C(q^{-1}) = \frac{R(q^{-1})Q(q^{-1})q^{-N}}{1 - Q(q^{-1})q^{-N}}
\]

where

\[
  R(q^{-1}) = \frac{K_r A(q^{-1})B^{-}(q)}{B^{+}(q^{-1})b}
\]

\[
  Q(q^{-1}) = \left( \frac{q + 2 + q^{-1}}{4} \right)^n
\]

\[
  b \geq \max |B^{-}(e^{-j\omega})|^2
\]

Here, \( N \) represents the period of the reference trajectory, \( K_r \in (0,2) \) is a tunable constant, \( b \) is a constant that adjusts the dc gain of the controller to unity. We factorize the numerator of the plant transfer function \( B(q^{-1}) = B^{+}(q^{-1})B^{-}(q^{-1}) \), such that \( B^{-}(q^{-1}) \) contains all the unstable zeros of the plant. \( Q(q^{-1}) \) is a low-pass filter included to ensure robust stability and \( n \) is the order of the filter.

To obtain the nominal plant, system identification of the stabilized dynamic model is conducted by swept sine method. Input to the system is the reference trajectory fed to
the stabilized plant while output was the piston trajectory. Several sinusoidal inputs of frequencies 1-200 Hz and amplitude equal to the maximum piston travel (192 mm) were used as reference trajectories and the simulated piston position for each trajectory was recorded. This constituted the set of inputs and outputs used to estimate a linear discrete time transfer function.

### 3.3 Design of Iterative Learning Controller for CT-RCEM

Like the case above, to implement a model based ILC for the actual RCEM, the nominal plant for the controller design is obtained through system identification of the stabilized RCEM, conducted by swept sine method. For any iteration $i$, the system is first brought to the operating point, i.e. desired pressure and piston initial position ($t = 0$). Next, corresponding to the desired piston trajectory, $r(t), t \in [0, T]$, the control signal calculated by the ILC, $u^{i}_{ILC}(t), t \in [0, T]$ is sent to the system and the actual piston position, $y^{i}(t), t \in [0, T]$, is recorded. The control signal for the next iteration, $u^{i+1}_{ILC}(t), t \in [0, T]$, is calculated using the control law

$$U_{\hat{I}LC}^{i+1}(j\omega) = U_{\hat{I}LC}^{i}(j\omega) + k_r G_p(j\omega)^{-1}\{\hat{R}(j\omega) - \hat{Y}^{i}(j\omega)\}$$  \hspace{1cm} (3-3)

where $U_{\hat{I}LC}^{i+1}(j\omega), U_{\hat{I}LC}^{i}(j\omega), \hat{R}(j\omega)$ and $\hat{Y}^{i}(j\omega)$ are the discrete time Fourier transforms of $u^{i+1}_{ILC}(t), u^{i}_{ILC}(t), r(t)$ and $y^{i}(t)$ respectively, $G_p(j\omega)$ is the frequency response of the CT-RCEM, and $k_r < 1$ is a constant included to ensure robustness against
uncertainty in $G_p(z^{-1})$. The cycle is repeated till desired accuracy is achieved or no significant improvement is observed with further iterations.

3.4 Design of Feedforward Controller

If the true plant model is available, an inversion based feedforward controller offers deadbeat performance. However, in presence of model uncertainties and external disturbances, a feedback controller can be used together with the feedforward controller to provide robustness. A combination of feedforward and feedback controller provides a tracking performance at least as good as provided by feedback controller alone as long as $|\Delta(j\omega)| \leq |G_0(j\omega)|$, where $\Delta$ is the additive plant uncertainty and $G_0$ is the nominal plant, as shown in [52]. Hence, the effect of a feedforward controller on the tracking accuracy has been investigated through simulation, using the dynamic model of the CT-RCEM.

It may be noted here that the implementation of a feedforward controller may not be necessary as the tracking accuracy obtained from ILC alone may be sufficient for a large set of the experiments to be conducted on the CT-RCEM. The value of the feedforward control design and evaluation lies in pushing the limit of state-of-the-art of high force and high speed electrohydraulic actuator technology for precise trajectory tracking performance.

The simplest approach to implement a feedforward control is to use a linear feedforward controller based on the inversion of the linear discrete time transfer function obtained using system identification from the dynamic model. Simulation studies show that
an improvement in performance is obtained when a linear feedforward controller is implemented together with the repetitive controller, compared to the repetitive controller alone. However, considering the significant nonlinearity introduced into the operation of electro-hydraulic actuators by the pressure-flow relationship (equations (2-9), (2-10), and (2-11), section 2.2.2) the effect of using a nonlinear plant inversion based feedforward controller on the tracking performance is worth being investigated.

In case of electro-hydraulic actuators with a symmetric hydraulic piston (i.e. same area on both sides), systematic method for design of a nonlinear inversion based feedforward controller has been reported in literature [41], [42]. The method relies on the fact that with certain approximations, the nonlinear dynamical model of an electrohydraulic actuator with a symmetrical piston can be proved to be differentially flat, and hence it is possible to obtain an algebraic relationship between the desired trajectory and its derivatives and the corresponding control signal. However, for actuators with asymmetric pistons, due to the loss of piston symmetry, this is no longer possible. From the CT-RCEM controller design perspective, this is important because the hydraulic actuator of the CT-RCEM has an asymmetric hydraulic piston as the diameters of the two rods connected to its two sides are not the same as per the design.

Therefore, a systematic approach has been developed to achieve nonlinear plant inversion for electrohydraulic actuators with asymmetric piston areas. The necessary and sufficient condition for the existence of a stable inverse of a nonlinear plant is that it must be a minimum phase system with finite relative order [53]. Since these conditions are met,
a nonlinear inversion of the system is possible. The proposed method involves two steps – first, the differential equation relating the control input and states, and their derivative to the desired trajectory and its derivatives is formulated. Next, this equation is solved numerically to obtain the desired control signal, for any desired trajectory, which can be fed through a feedforward unit to the plant. More details can be found in [54]

The pressure dynamics inside the hydraulic chamber can be expressed in terms of the desired trajectory and its derivatives alone as

\[
\dot{P}_r = \frac{\dot{P}_h + \dot{x} \beta (A_l - \gamma A_r)}{(x_0 - x + x_{dt})} \frac{A_r (1 + \gamma (x + x_{dr}))}{(x_0 + x_{dt} - x)}
\] (3-4)

Solution of this differential equation gives the required hydraulic chamber pressure profile which must be maintained to track the desired trajectory. Moreover, since the combustion chamber pressure trace is known, we know the desired actuation force \(F_h\) and its derivative \(\dot{F}_h\) from (5). This, in turn, provides us the control signal that is needed to track the desired trajectory since the control signal can be expressed as an algebraic expression in terms of the hydraulic chamber pressure from as

\[
u_c = \frac{A_r}{k_m} \left( \frac{\dot{P}_r x}{\beta} + \dot{x} \right) \sqrt{\frac{\rho}{2|P_r - P_{sump}|}}
\] (3-5)

The control signal so obtained can be fed to the actuator through a feedforward unit to achieve precise tracking. The simplest method of implementation is to solve for the control signal offline for a given trajectory and have it stored in memory for use during the experiment.
3.5 Control Implementation and Experimental Results

The implementation of the controller involves two steps- first, stabilizing the system by closing the proportional feedback loop; second, implementation of the iterative learning controller for the stabilized system. The supply pressure is set at 240 bar (3500 psi) and TDC clearance is 8.37 mm for the tests reported in this section.

3.5.1 Servovalve Sizing and Limit Cycles

On implementing a proportional controller on the piston position signal, limit cycle oscillations were observed when a constant reference signal was sent to the proportional controller - the hydraulic piston and the servovalve spool were executing low frequency, small amplitude oscillations around a constant mean position. Figure 3-3 shows this limit cycle behavior of the piston and the servovalve spool for proportional controller gain $K_p = 3$. The servovalve spool position data has been obtained from the built-in spool position sensor of the servovalve. On further testing, it was observed that the amplitude and frequency of oscillations depended on the gain of the proportional controller- increase in the proportional controller gain reduces the amplitude and increases in the frequency of the oscillations. The root cause of this instability is phase-delay in the servovalve response arising from friction characteristics of the servovalve spool.
The friction characteristics of the servovalve spool impose a small delay in the response of the servovalve which depends on the control signal received by the servovalve. This is because the driving force for the valve spool must increase beyond the spool stiction before the motion is started. However, the spool driving force depends on control signal and the relationship depends on the internal valve dynamics. Hence, for large changes in the command signal, this time delay is too small to significantly affect the system. However, for small signal operation of the servovalve, this time delay introduces close to 90° phase delay which causes the closed loop system to go unstable. A 90° phase lag between spool motion and control signal can be clearly seen in Figure 3-4 when the piston is executing limit cycle oscillations for $K_p = 3$. The required valve opening is barely 0.5%.

*Figure 3-3: Piston and servovalve behavior for proportional gain $K_p = 3$*
It is important to note that this limit cycle behavior induced by servovalve spool stiction is different from the limit cycle behavior observed due to piston stiction. Latter is a relatively common and well documented behavior which is observed in hydraulic actuators where the stick-slip motion of the piston leads to limit cycle oscillation [55]–[57]. The former, however, is a phenomenon exclusive to hydraulic actuators designed for extremely high-speed application. The servovalve is chosen for a given application based on the peak flow requirement of the actuator during operation. Hence, high speed applications must use a larger servovalve, with a higher rated flow. However, small signal operation becomes unavoidable for such systems and there is a possibility of limit cycle behavior depending on the relative sizing of the actuator and the valve.

Figure 3-4: Servovalve command signal and actual spool position during limit cycle oscillation of the piston. A $90^\circ$ phase lag between the command signal and actual signal can be observed.
3.5.2 System Stabilization

The limit cycle behavior has been mitigated by eliminating spool stiction using a dither signal. A sinusoidal signal of amplitude 300mV and frequency 500Hz is superimposed over the control signal determined by the proportional control. The dither signal maintains the servovalve spool in sustained high frequency oscillations of small amplitude while following the command signal from the proportional controller. Since the spool is constantly in motion, stiction is practically eliminated and the delay in the small-signal valve operation is eliminated. The frequency and amplitude of the dither signal has been tuned by trial and error. Figure 3-5 shows the piston behavior and the spool behavior with the use of dither.

Figure 3-5: Piston and servovalve behavior with dither superimposed on the signal from proportion controller for constant reference
It may be noted that the purpose of the inner loop control here is stabilization alone and the bandwidth of the system is enhanced by the outer loop ILC. Simulation studies have shown that the use of a higher order (and bandwidth) controller for the inner loop increases the complexity of the outer loop controller without providing significant improvement in the tracking performance. Moreover, for safety, during the system preparation for each experiment (i.e. positioning of piston at bottom dead center, exhaust gas purging, fueling, etc.), the outer loop high bandwidth control is deactivated, and the actuator is operated only through the inner loop control. The outer loop ILC is activated only when the system is completely ready for the experiment. Hence an overdamped proportional controller is a preferred choice for inner loop control.

Figure 3-6 shows the step responses of the system recorded after limit cycle behavior was mitigated, for proportional controller gains $K_p = \{1,3,5\}$. While for $K_p = 5$, the system behaves as slightly underdamped, for $K_p = 3$ the system exhibits slightly over-damped behavior. Hence the proportional controller gain is selected as $K_p = 3$. 
3.5.3 Implementation of Iterative Learning Controller

After stabilization of the system, the frequency response of the hydraulic actuator, without combustion chamber, was obtained. The input to the stabilized system was the reference position signal that consisted of sinusoids from 1-130 Hz, and amplitude of 4 mm. The output was the actual piston position. Based on this data, a linear discrete time transfer function was identified to describe the frequency response of the CT-RCEM. This transfer function, $G_p(q^{-1})$ shown below, has eleven stable poles and one stable zero.

Figure 3-6: Response of hydraulic actuator to a step command of 50 mm, for different proportional controller gains
\[ G_p(q^{-1}) = \frac{B(q^{-1})}{A(q^{-1})} \]  

(3-6)

where \( B(q^{-1}) = 10^{-7}(-1.368 q^{-1} + 3.357 q^{-2}) \)

\[ A(q^{-1}) = 1 - 8.776 q^{-1} + 36.04 q^{-2} - 91.84 q^{-3} + 162.1 q^{-4} - 208.9 q^{-5} \]
\[ + 200.9 q^{-6} - 144.2 q^{-7} + 75.51 q^{-8} - 27.38 q^{-9} \]
\[ + 6.155 q^{-10} - 0.6465 q^{-11} \]

For comparison, a frequency response of the CT-RCEM dynamic model was also obtained after removing the combustion chamber dynamics and using proportional controller with gain \( K_p = 3 \), (same as that used on the actual hardware). Figure 3-7 shows the experimentally obtained frequency response data, the frequency response of the identified transfer function, and the frequency response of the dynamic model.

Next, the iterative learning controller has been implemented, as described in section 3.3, to obtain the precise tracking performance. The implementation scheme is same as shown in Figure 3-1 before.
Figure 3-8 shows the change in system performance with subsequent iterations for a geometric compression ratio 14.15 (stroke 121 mm) and compression time 20 ms. However, since a creviced piston has been used in the combustion chamber to minimize the piston motion generated turbulence [44], the crevice volume acts as dead volume for the chamber and lowers the effective compression ratio to 11.21. The learning process is started by using the initial signal generated by the repetitive controller of the dynamic model. The combustion chamber is filled with a mixture of dry air and CO₂ for each iteration. The controller convergence is achieved in five learning iterations. Drastic reduction in the tracking error is observed with each learning iteration. The peak error for
the fifth iteration is less than 0.6 mm, about 9 ms after the start of compression. The peak piston speed is 9.5 m/s and the corresponding peak flow rate through the actuator is 700 l/min. Moreover, the tracking error was less than 0.3 mm during the final 20% of the stroke which contributes to about 90% of the pressure rise.

Next, the tracking performance for a higher stroke of 131 mm, corresponding to an effective compression ratio of 12.3, and compression time 20 is demonstrated for a compression trajectory which is different from a true sinusoidal compression. Figure 3-9 shows the comparison between the piston position reference signal and the corresponding piston velocity for the chosen trajectory and a trajectory with a sinusoidal compression
while the chosen trajectory has a higher peak piston speed, the initial acceleration and the final deceleration is lower compared to the trajectory with sinusoidal compression. The compression profile of this trajectory corresponds to $\Omega = 1.2$ as defined in [58]. It is interesting to note that even for the same compression ratio and same compression time, the effect of the two trajectories on the flow pattern of the gases inside the combustion chamber will be different due to difference in the piston speeds. This phenomenon is explained in more detail in the next chapter.

The combustion chamber is filled with similar air-CO$_2$ mixture as in the previous case. The controller convergence is achieved again in five iterations and the peak error is about 0.6 mm. The tracking performance after controller convergence is shown in Figure 3-10. The peak piston velocity is close to 12 m/s and the corresponding peak flow rate through the hydraulics is close to 900 l/min.
3.6 Combustion testing

Figure 3-11 shows the combustion data recorded for four repetitions of compression of combustible mixture of air, nitrogen and di-methyl ether (DME), for the trained trajectory shown in Figure 3-8. The composition of the mixture was DME: O$_2$: N$_2$ = 1:4:40. The initial temperature and pressure were 300 K and 15 psi (absolute) respectively. The compression pressure profile is highly repeatable, and the run to run
difference between the peak compression pressure is within 3 psi. More detailed analysis of the repeatability has been presented in chapter 3.

One of the unique advantages of CT-RCEM over conventional RCEM lies in the ability to generate comparative data as shown in Figure 3-12, representing the impact of changing the piston trajectory on the pressure trace generated inside the combustion chamber. The three trajectories shown in the figure have the same stroke but different compression times – 20 ms, 25 ms, 30 ms. The pressure data, for each trajectory, is the average of four repetitions. The difference in the observed ignition delays for different compression times is attributed to the progress of pre-ignition reactions during compression and the effect of heat loss near TDC.

Figure 3-11: Combustion pressure for DME: O₂: N₂ = 1: 4: 40, effective compression ratio 11.21, compression time 20 ms, four repetitions
As mentioned before, the ability to generate such data is extremely useful for various combustion research avenues, including but not limited to autoignition investigations, knock studies, kinetic mechanism validations and experimental investigation of the effect of piston trajectory on combustion.

### 3.7 Conclusion

A precise motion controller has been developed for the actuation system of the CT-RCEM and its performance has been demonstrated experimentally. Since the actuation requirements of the CT-RCEM are quite demanding in terms of high-force and high-speed
speed the control design must leverage the key advantages available from the system design. Since the reference trajectory for a given experiment is always known beforehand and the disturbance dynamics are highly repeatable, a frequency domain iterative learning controller has been chosen for this application. A nonlinear plant inversion based feedforward controlled has also been developed to further improve the tracking performance for extreme operating conditions involving higher flow rates at which the system nonlinearity starts to become more prominent. Additionally, the control design principles used for the development of the CT-RCEM can also be extended to a generic electrohydraulic control application involving high-force and high-speed over a large stroke.
A combustion system is essentially a high dimensional, non-linear dynamical system, and assuming spatial homogeneity for simplicity, the time evolution of the system can be represented as trajectories in state space, where the state variables are pressure and temperature (thermodynamic states), and the species concentration (chemical states) [59]–[62]. From this perspective, chemical kinetic mechanism development, improvement and validation, and reduction, essentially involves identifying the key reaction pathways, discerning the governing rate equations of the pathways, and identifying the coefficients of these governing equations, over a wide range of temperature and pressure conditions using experimental data [63], [64]. The ability to precisely control the piston motion in the combustion chamber effectively translates into the ability to prescribe the instantaneous volume profile in the combustion chamber, which in turn allows for creating special thermodynamic paths in the combustion chamber to extract chemical kinetics information which is otherwise inaccessible through conventional means.

In this chapter, three unique investigative capabilities enabled by the selecting special thermodynamic paths in the CT-RCEM have been demonstrated.

First, the ability to investigate the effect of the thermodynamic path of compression in RCM investigation on the ignition delay measurements is demonstrated. Chemical kinetics data pertaining to autoignition investigations obtained from RCM experiments, at different pressure and temperature conditions, is crucial for detailed as well as reduced kinetic mechanism development [65], [66]. However, the facility dependence of this
ignition delay data due to a fixed and facility dependent thermodynamic path for a given set of end-of-compression temperature and pressure conditions, reduces the robustness of this identification process [33], [34], [36]. Use of ignition delay data collected over similar range of conditions, but attained by several different thermodynamic paths, can effectively decouple the effect of the thermodynamic path on the chemical kinetic parameters inferred by experiments on a CT-RCEM. This is because while the thermal states (pressure and temperature) at the end of compression of compression may be (almost) same, but the different paths lead to different levels of pre-ignition reaction progress and hence different intermediate species pool, as shown in Figure 4-1.

Next, the ability to produce a thermodynamic path such that the chemical kinetics in the combustion chamber is quenched at a specified stage is demonstrated. This is accomplished by retracting the piston at an extremely high speed, such that the resulting
sudden increase of the combustion chamber volume leads to an extremely rapid drop in temperature. The quench products can be subsequently sampled for species diagnostics with gas chromatography and mass spectroscoopy (GCMS) or other techniques.

After this, the ability to experimentally compensate for the heat loss after the end of compression by creating isobaric conditions inside the combustion chamber is demonstrated. During autoignition investigations in RCM, especially when the ignition delay is large, there can be considerable heat loss from the fuel mixture while the pre-ignition reactions are in progress, which means that the thermodynamic state at the time of ignition can be considerably different from the thermodynamic state at the end of compression. The conventional practice to account for this heat loss is through simulation. In the CT-RCEM, it is possible to execute a piston trajectory where the piston, at the end of the rapid compression, starts to ‘creep’ forward at a rate which offsets the rate of heat loss, allowing isobaric dwell to be created. This ability will be particularly useful for exploring the boundary of autoignition for fuels, by avoiding thermal quenching of ignition reactions due to heat loss.

Finally, the use of the CT-RCEM for in-depth analysis of the combustion characteristics for IC engine applications is demonstrated. A desired reference trajectory corresponding to an engine can be fed to the controller and a single combustion cycle can be analyzed in detail. The unique advantage offered by the CT-RCEM for such investigations comes from the ability to precisely regulate parameters such as initial charge temperature, wall temperature, boost pressure, charge composition etc. to accuracies which
are difficult to achieve on a running engine. Moreover, a multitude of operating scenarios in terms of compression ratio, operating speed and the shape of piston trajectory can be investigated with a small turnaround time since the trajectories are changed electronically. To this effect, a case study is presented for experimental investigation, using the CT-RCEM, of an advanced combustion control strategy for free piston engines (FPE) previously proposed in our group – trajectory based combustion control [58], [67]–[69]. Extensive simulations have shown significant efficiency benefits and emissions reduction achieved using this control scheme for the FPE by implementing optimal piston trajectories.

The objective of the work presented in this chapter is twofold – first, characterizing the CT-RCEM for non-reactive and reactive testing for conventional RCM operation; and second, to demonstrate the unique capabilities of the system. More details can be found in [70].

4.1 Characterization of CT-RCEM

Characterization of any newly commissioned RCM/RCEM aims at establishing the following:

1. The facility can produce fast compression to ensure minimum heat loss and progress of reactions before end of compression.

2. The pressure and temperature history produced by the facility, inside the combustion chamber, is highly repeatable. In other words, the thermo-chemical
state at the end of compression does not change substantially from run to run for same operating parameters.

3. The facility can provide the desired functionality over the entire operating range.

The above-mentioned characteristics can be achieved only if the actuation system, fuel preparation system, and the fueling system are working as designed. Hence, the characterization experiments must consist of testing with both non-reacting and reacting mixtures. The non-reactive testing allows the characterization of the actuation parameters like minimum compression time, range of compression ratio achievable, repeatability of piston motion, etc., as well as the thermodynamic characteristics such as heat transfer characteristics and repeatability of pressure curves for various operating parameters, etc.

The reactive testing builds upon the non-reactive testing by establishing the repeatability of the pressure trace as well as the ignition delay measurements which depends, in addition to the actuation characteristics, on the fuel preparation system and the fueling and exhaust handling system.

As mentioned earlier, the ability to set and control the piston trajectory through software allows the CT-RCEM to offer extreme flexibility for achieving desired operating conditions. Figure 4-2 shows eight different piston trajectories for the compression of a non-reactive mixture (air-CO2) and the corresponding combustion chamber pressure profile. The piston trajectories represent compression events where four different geometric compression ratios – 12.2, 14.2, 15.5, and 16.7 – are achieved in two different compression times, 20 ms and 30 ms, each. The actual compression ratios were lower due
to the use of a creviced piston in the combustion chamber. This change in the compression ratios and compression times was achieved through software alone, without any mechanical or hardware intervention.

While this data is a good way to demonstrate the operational flexibility of the CT-RCEM, the key value of this data lies in being able to capture the heat transfer characteristics of the combustion chamber over a wide variety of operating conditions which is subsequently quite useful for calibrating of the heat transfer dynamics in the simulation models which are used to analyze the experimental data.

Figure 4-2: Piston trajectory and corresponding pressure profile for CR 12.4, 14.2, 15.5, and 16.7. The compression starts at t=5 ms, and ends at 25ms and 35 ms, for compression times 20 ms and 30 ms, respectively.
Figure 4-3: Repeatability of trajectory and corresponding pressure for CR 16.7 and compression time 20 ms (top), the trajectory tracking error (middle), and deviations of individual pressure trace from ensemble average (bottom) for four repetitions.

The operational flexibility, however, is of little use unless each operating condition
is highly repeatable. Figure 4-3 shows the piston trajectories and the corresponding pressure profiles for four repetitions of a test where a non-reactive mixture is compressed in 20 ms, over a compression ratio of 16.7. The tracking error is also shown in the figure which is essentially the difference in the desired piston position at a given time instant, sent to the controller, and the piston position measured from the sensor. While the peak tracking error is close to 0.6 mm, the cycle to cycle variability is within 0.2 mm. The effect of such a precise and repeatable piston motion control is immediately evident from the cycle to cycle variation in the pressure profiles which is barely distinguishable from the noise level of the pressure sensor. The flexibility in the choice of operating conditions, however, is not limited to the ability to change the compression ratios and time. It is also possible to change just the shape of the piston trajectory for the same compression ratio and compression time. Figure 4-4 shows an example of such an investigation showing the piston position and piston velocity for two different shapes of the piston trajectory, for same CR (15.5) and the compression time (25 ms). Case I represents a piston trajectory typical of a conventional RCM, involving a large acceleration, period of almost constant velocity, and a period of large deceleration. Case II represents a trajectory with a relatively higher peak velocity but more gradual acceleration and deceleration.

It can be seen in Figure 4-4 that the effect of a sharp deceleration in case I is manifested as a sharp pressure rise accompanied by pressure pulsations in the combustion chamber, despite the lower peak velocity. The probable cause of these pressure pulsations is the bulk fluid motion caused by inertia during sudden stopping with high deceleration.
While a sharp pressure rise corresponds to a smaller $t_{50}$ and $t_{50T}$, i.e. time for final 50% pressure rise and time for final 50% temperature rise, which implies less pre-ignition

![Image](image.png)

**Figure 4-4:** Effect of shape of piston trajectory on pressure trace, for same CR and compression time. Top plot shows the piston trajectories with same CR and compression time, but different shape. Middle plot compares the pressure trace for the two trajectories and bottom plot compares the pressure trace near the end of compression.
reaction progress during the compression, the accompanied fluid motion has two side-effects. First, such bulk fluid motion inside the chamber adversely affects the homogeneity of the combustion chamber core, even for a well-designed creviced piston. This would make the localized effects of temperature gradients even more pronounced and aggravate deviations from the conditions of the “adiabatic core” hypothesis. Second, the bulk fluid motion increases the overall rate of heat loss which is evident from the fact that the despite the higher peak pressure, by the time the pressure pulsations die out, the pressure for case I is lower than in case II.

This observation was found repeatable for other combinations of compression ratios and compression times as well, i.e. – a large deceleration at the end of the piston stroke leads to increased pressure pulsations inside the combustion chamber. It may be noted here that data from four different sensors – piston position sensor, combustion chamber pressure sensor, hydraulic actuator pressure sensors and accelerometer – was rigorously corroborated with each other to eliminate any the possibility of piston bounce in the cases presented above.

Another interesting observation made during this investigation was that the optimal seating velocity of the hydraulic actuator – i.e. the velocity with which the hydraulic actuator piston approaches the mechanical stop at the TDC – was found to be between 0.4 m/s to 1 m/s. Higher the seating velocity, larger the impact generated. Slower seating leads to a tailing pressure curve at the end of compression which reduces the repeatability of compression time. However, as the seating velocities are increased beyond 1 m/s, the
pressure pulsations as described above start to appear, due to sudden and high impact stopping.

Next, the reactive mixture testing was conducted to ensure the repeatability of the combustion characteristics. Three different fuels have been selected for this purpose – dimethyl ether (DME), butane and ethanol; i.e. two gaseous fuels and one liquid fuel.

Figure 4-5 demonstrates the repeatability of combustion characteristics for these three fuels, for a geometric compression ratio 15.5 (actual 12.2) and compression time 20 ms. Four repetitions are presented for each case. For this compression ratio DME does not require pre-heating to achieve autoignition. Hence, the initial temperature of the fueling system and the combustion chamber is maintained at 300K. The mixture composition is $DME: O_2: N_2 = 1:4:40$ (molar), i.e. slightly lean and with extra nitrogen. However, pre-heating of the fuel mixture is required to achieve autoignition at this compression ratio for

![Figure 4-5: Repeatability of pressure trace and ignition delay measurement. Four repetitions of autoignition testing of three different fuels for geometric compression ratio 15.5 and](image-url)
butane, and hence the fuel mixture and the setup is maintained at an elevated temperature of 350K. Stoichiometric mixture of Butane and air has been used, with no dilution. Fuel-mixture for ethanol is prepared by metered liquid ethanol by volume at room temperature into the fuel tank, followed by heating of the tank to 368K (90°C) and the fueling system and combustion chamber was maintained at this temperature. The fuel mixture for Ethanol is also stoichiometric, with no extra dilution.

The initial pressures were adjusted to achieve compressed pressure of about 25 bar for DME and ethanol and 20 bar for butane. The initial pressure and temperature can be accurately controlled to within ±10 mbar and ±1°C, respectively. The run-to-run

![Figure 4-6: Zoomed-in view of the piston position and gas pressure towards the end of compression for autoignition of DME presented in the previous figure](image)
repeatability of the compressed pressure is generally within ±0.3 bar and the temporal spread in the peak compressed pressure is generally about ± 0.2 ms. Figure 4-6 shows the piston position and the chamber pressure for the DME autoignition near TDC for the autoignition case shown in the previous figure.

4.2 Effect of Compression Time on Ignition Delay

The effect of the progress of preignition reactions during compression and the subsequent intermediate species buildup on the ignition delay measurements have been recognized and previously reported in the literature [33], [36]. The CT-RCEM provides a systematic way of investigation of such effects allowing ignition delay measurements for similar end of compression conditions achieved along different thermodynamic paths of compression.

To investigate the effect of piston trajectory on the ignition delay we investigated the autoignition of DME for six different compression ratios, each with two different compression times – 20ms and 30 ms. The mixture composition was $DME:O_2:N_2 = 1:4:40$ and the initial temperature was maintained at 300K. The initial pressure was adjusted for each CR to attain a compressed pressure of about 24.5 bar (± 0.3 bar) for the 20 ms compression. Figure 4-7 shows the combustion pressures for all six compression ratios and table T shows the summary of the results. The compressed temperatures were estimated through adiabatic core hypothesis, using non-reactive pressure traces for each test. Several repetitions were performed for each test to ensure repeatability of the results.
While counterintuitive, it can be immediately seen from the results here that a faster compression does not necessarily produce a longer ignition delay. For the CR 12.4 and 13.5, the faster compression produces a shorter ignition delay whereas for CR 14.2 and 14.7, the faster compression produces a longer ignition delay. For higher compression ratios, the difference in the ignition delays is rather small, however the trend seems to reverse again, and the faster compression has the shorter ignition delay.

Figure 4-7: Effect of compression time on the ignition delay of DME at various compression ratios. The solid blue line represents a compression time of 20 ms and the dashed red line represents the compression time of 30 ms.
A simulation analysis of this effect at higher compression ratios was conducted using a multi-zone thermo-kinetic model of the combustion chamber and it was found that higher compression ratios, a faster compression produces a thermodynamic path where the average temperature over the final couple of milliseconds, of the combustion chamber core, is higher than that in the thermodynamic path produced by a slower compression [71], [72].

The effects at lower CR, however, may be more complicated, including complex interaction effects between chemical kinetics, and fluid mechanics involving possible

*Table 4-1: Autoignition characteristics of DME for two different compression times for seven different compression ratios. For each CR, the case with lower total ignition delay is highlighted*

<table>
<thead>
<tr>
<th>CR</th>
<th>Temp (K)</th>
<th>ID1 (ms)</th>
<th>ID total (ms)</th>
<th>Temp (K)</th>
<th>ID1 (ms)</th>
<th>ID total (ms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.4</td>
<td>625.4</td>
<td>53.52</td>
<td>56.92</td>
<td>622.4</td>
<td>77.64</td>
<td>80.96</td>
</tr>
<tr>
<td>13.5</td>
<td>641.4</td>
<td>11.8</td>
<td>14.9</td>
<td>641.0</td>
<td>12.7</td>
<td>15.8</td>
</tr>
<tr>
<td>14.2</td>
<td>660.0</td>
<td>12</td>
<td>15.2</td>
<td>658.0</td>
<td>8</td>
<td>11</td>
</tr>
<tr>
<td>14.7</td>
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<td>3.88</td>
<td>7.36</td>
<td>666.7</td>
<td>3.76</td>
<td>7.16</td>
</tr>
<tr>
<td>15.5</td>
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<td>3.06</td>
<td>5.72</td>
<td>677.6</td>
<td>3.16</td>
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<td>690.2</td>
<td>0.84</td>
<td>4.58</td>
</tr>
</tbody>
</table>
localized ignition kernels [35], [73]. A detailed and systematic analysis of this effect is a work in progress.

### 4.3 Quenching chemical kinetics

Another capability enabled by piston motion control in the CT-RCEM is the capability to quench the chemical reactions in the combustion chamber by rapidly pulling back the piston from the top dead center. The resulting increase in the chamber volume leads to a sharp decrease in the combustion chamber temperature leading to the quenching of the chemical kinetics. The quench products can subsequently be sampled and analyzed using GCMS.

For quenching studies, the conventional RCM have relied on using high speed valves or burst disks [20], [22], [24], [74] connecting a quench system to the combustion chamber aimed at sampling and quenching a part of the combustion chamber gases. The quenching approach in the CT-RCEM involves quenching of the entire combustion chamber. With the actual chamber pressure and piston position measurements from the quenching experiments the chemical kinetics can be simulated to estimate the quantities of various quench products which can directly compared with the results from the GCMS.

Figure 4-8 demonstrates the piston position profile and the gas pressure for quenching chemical kinetics at various stages of combustion. The fuel mixture is DME with composition same as before. The initial temperature was 300K and initial pressure was 1.03 bar. A flat piston was used instead of a creviced piston to avoid back flow of
gases during expansion. While for the test results shown above, the piston was retracted back by 8 mm in 2 ms from the start of quenching, quenching up to twice as fast can be achieved if required.

### 4.4 Isobaric dwell for compensating heat loss at TDC

During autoignition investigation of fuels at conditions where the ignition delay is large, effect of heat loss can be significant leading to a large drop in the combustion chamber temperature and pressure from the end of compression to the eventual ignition. Moreover, since the heat transfer characteristics of RCMs vary from facility to facility, the temperature and pressure drop profile after the end of compression, even for same compressed state can vary significantly. This in turn leads to large variability in the reported ignition delays measured on RCMs especially when the ignition delays are large.
This problem is well documented in the literature and the common practice is to account for this heat loss using chemical kinetic simulations with heat loss.

The CT-RCEM provides an experimental way to account for the effect of heat loss. The piston trajectory can be designed such that at the end of the rapid compression, the piston is still slightly far from the top dead center and creeps forward during the rest of the stroke at a rate which offsets the heat loss, allowing an isobaric dwell to be maintained inside the combustion chamber till the autoignition of the fuel. Figure 4-9 demonstrates use of such a creeping trajectory for autoignition of a stoichiometric mixture of butane and

![Piston trajectory and Combustion pressure graphs]

*Figure 4-9: Achieving isobaric dwell using a creeping piston trajectory in CT-RCEM to compensate for the heat-loss. The dotted lines (purple and yellow) represent two repetitions of the conventional RCM trajectory while the solid lines (blue and red) represent two repetitions of the creep trajectory.*
compares it to a base case of conventional RCM trajectory for compression ratio 12.4. For the creeping trajectory case, the piston creeps forward the final 1mm of the stroke to achieve isobaric dwell.

The initial temperature and pressure were adjusted for the creep trajectory to attain the same compressed state as the base case. For the base, it can be seen that the pressure drop due to heat loss is more than 5 bar. Using a creep trajectory, on the other hand allows an almost isobaric dwell where the pressure drop is less than 1 bar. From the ideal gas law, it follows that a similar reduction is expected in the temperature drop as well.

4.5 Investigation of IC engine trajectories

With the ability to track any desired reference trajectory in the combustion chamber, the CT-RCEM provides the ability for an in-depth analysis of a single combustion cycle of an IC engine. The unique advantage of using the CT-RCEM for such an analysis comes from the fact that with only a single cycle being investigated, it is possible to precisely regulate the initial and boundary conditions, such as the initial wall temperature, initial charge temperature, the boost pressure, charge composition, etc. with accuracies which are difficult to achieve on a running engine. Moreover, several operating conditions in terms of compression ratio, operating speed and even shapes of piston trajectories can be investigated with a small turnaround time since any changes to the piston trajectory are made electronically. Additionally, the in-situ and ex-situ capabilities for chemical species diagnostics coupled with the quenching capability provide a unique
opportunity for a deeper investigation of the chemical kinetics and especially the emissions formations such as soot, NOx, etc.

The current fueling system of the CT-RCEM is tailored to provide the capabilities closer to those of a conventional RCM for autoignition investigation of pre-mixed fuel mixtures, and hence does not have an intake and exhaust manifold, a fuel injector or a spark plug. Hence the investigations are currently limited to autoignition of premixed charge over the compression and expansion stroke. However, it may be noted that the simulation studies have shown that the actuation system is perfectly capable of producing a full four stroke cycle with intake and exhaust stoke as well and hence, if required, with requisite modifications in the fueling system or the cylinder head the CT-RCEM can also be used for conventional SI and CI modes of engine operation as well.

In this section, it is demonstrated that the CT-RCEM can be used for advanced IC engine investigation by providing a case study involving experimental validation of a combustion control strategy for HCCI combustion in free piston engines – trajectory based combustion control.

Free piston engine is an alternative architecture of IC engines which does not have a mechanical crankshaft and the combustion energy is either directly converted into compressed fluid or electricity [75]–[78]. By eliminating the constraint imposed on the piston motion by the mechanical crankshaft and connecting rod setup, the free piston engine provides several advantages over the conventional IC engines such as variable
compression ratio, reduced friction losses, modularity, etc. and hence shows a promising potential for efficiency improvement and emissions reduction.

The key challenge for the FPE operation lies in the control of the piston motion in the absence of a mechanical crankshaft. Several control strategies have been used in past to achieve sustained operation of the FPE, however, many of these strategies rely on calibration to be effective [76], [77], [79], [80]. The inherent complexity of the combustion and the gas exchange processes in the engine together with the dynamic coupling between the gas dynamics and the piston trajectory makes such calibration a tedious task.

An active motion controller has been previously developed in our group for the robust operation of the FPE [43], [81]. By precisely tracking any desired piston trajectory and rejecting external disturbances, the motion controller, called the virtual crankshaft mechanism, has been shown to provide reliable starting and stable operation of the FPE as well as the ability to recover from any misfires or variability in combustion.

Hence, the FPE when operated using a virtual crankshaft mechanism allows the piston trajectory to be used as an extra control means to control the combustion process inside the combustion chamber. The piston motion is used to modulate the pressure and temperature history of the air-fuel mixture inside the combustion chamber and thereby modulate the chemical kinetics. This is the core idea of trajectory based combustion control for the FPE [49], [58], [67], [68]. Extensive simulations have shown the efficiency benefits and emissions reduction achieved using this control scheme for the FPE by implementing optimal piston trajectories.
The CT-RCEM offers a natural means for an in-depth experimental investigation of the concept of trajectory based combustion control.

Figure 4-10 shows the combustion pressures and average temperatures corresponding to three different piston trajectories tested on the CT-RCEM with the same compression ratio and operating speed. The equivalent crank angle scale corresponding to time scale during the cycle has also been plotted. The compression ratio is 12.1 corresponding to a stroke of 131 mm and operating speed is 1500 rpm corresponding to compression and expansion time 20 ms each. The shape of the piston trajectories has been characterized using parameter $\Omega$, introduced previously. For $\Omega = 1$, the trajectory represents a pure sinusoidal motion between the TDC and BDC. As the $\Omega$ decreases, the piston spends lesser time near TDC and vice versa. More details about the geometrical properties of $\Omega$ can be found in [67].

The fuel mixture is DME-air with fuel-air equivalence ratio $\phi = 0.6$. The mixture and the chamber walls are preheated to $343K$ ($70°C$) and the initial pressure in the combustion chamber at the start of compression stroke is $1.034 \text{ bar (15 psi)}$.

The mass of air fuel mixture inside the combustion chamber at the start of compression stroke is $311.8 \text{ mg}$, estimated using ideal gas law.

The mass of DME is $19.6 \text{ mg}$ based on the equivalence ratio and the corresponding amount of chemical energy per cycle is $561 J$, assuming a lower heating value of $28.8 MJ/kg$ for DME.
A special bowl shape piston has been used to ensure that the fluid dynamics inside the combustion chamber is closer to that expected in a real engine [82]. The combustion
pressure measurements have been obtained at a sampling frequency of 25 kHz. The average temperature in the combustion chamber has been estimated using ideal gas law. The results of the further analysis of the pressure data are summarized in the Table 4-2.

The start of combustion is defined as the time when the rate of heat release becomes positive and the end of combustion is defined as the time when the rate of heat release becomes zero. This definition of combustion duration has been used since the duration of combustion is about 0.5 ms, for all three trajectories, with the low and high temperature

| Table 4-2: Combustion characteristics for different piston trajectories for combustion of DME air mixture for CR: 12.1, φ: 0.6 and 1500 rpm |
|---------------------------------|-----------------|-----------------|-----------------|
|                                | Ω = 0.8         | Ω = 1.0         | Ω = 1.2         |
| SOC time                       | 18.92 ms -9.72° | 18.60 ms -12.60° | 18.28 ms -15.48° |
| Temperature at SOC             | 647 K           | 630 K           | 627 K           |
| Peak pressure                  | 74 bar          | 76 bar          | 78 bar          |
| Peak temperature               | 1990 K          | 2097 K          | 2186 K          |
| Combustion duration            | 0.56 ms         | 0.52 ms         | 0.52 ms         |
| Combustion heat release        | 430 J           | 470 J           | 515 J           |
| Combustion efficiency          | 77 %            | 84 %            | 92 %            |
| Net work                       | 113 J           | 101 J           | 106 J           |
| Work as % of comb heat         | 26 %            | 22 %            | 21 %            |
| Indicated thermal efficiency   | 20 %            | 18 %            | 19 %            |
heat releases being quite close. The time difference between the peak of the low temperature heat release rate and the peak of the high temperature heat release rate is about 0.2 ms. The combustion heat release $Q_{comb}$ has been calculated by integrating the apparent heat release $dQ_r$ between the start and end of combustion given as

$$dQ_r = \frac{\gamma}{\gamma - 1} P dV + \frac{1}{\gamma - 1} V dP$$  \hspace{1cm} (4-1)$$

$$Q_{comb} = \int_{t_{soc}}^{t_{eoc}} dQ_r$$ \hspace{1cm} (4-2)

The net work output during the cycle is given as $\int PdV$ over the compression and the expansion stroke. The pumping losses have been neglected in the calculations here.

Combustion efficiency is defined as the ratio of the amount of heat released during combustion ($Q_{comb}$) and the amount of chemical energy introduced into the chamber with the fuel. The quantity, work as a percentage of heat release, indicates how much of the combustion heat is converted into work. The indicated thermal efficiency is the ratio of the work obtained to the chemical energy introduced into the chamber.

From these results, two trends regarding the effect of the piston trajectory on combustion characteristics are immediately obvious; first, the combustion efficiency increases with the omega, and second, the efficiency of conversion of combustion heat to work decreases with $\Omega$. Also, for the chosen combination of the initial temperature and the compression ratio the major heat release occurs during the compression stroke, i.e. is significantly advanced.
Figure 4-11 shows the piston velocity profile in the combustion chamber for the three piston trajectories investigated here. For the trajectory with $\Omega = 0.8$ the velocity of approach to the TDC and the velocity of receding from the TDC is the relatively the highest and hence the mixture spends the least amount of time near the TDC, i.e. at high temperature and pressure conditions. Intuitively, on one hand it means that the less time available for the mixture in this case for the progress of the pre-ignition reactions during the compression stroke leads to a relatively delayed ignition. On the other hand, a relatively faster expansion prevents the completion of the combustion reactions leading to a lower combustion efficiency. However, due to the less time spent at the high temperature and pressure conditions, the heat loss is also lower leading to relatively the highest conversion of combustion heat to work.

*Figure 4-11: Piston velocity profile corresponding to the piston trajectories*
Similar explanation can be extended to explain why the trajectory with $\Omega = 1.2$ which has the slowest approach and recede velocities for the TDC and spends the largest time at the high temperature and pressure conditions has the fastest ignition, highest combustion efficiency and lowest conversion efficiency of combustion heat to work.

It may be noted that the intuitive explanation offered above must be substantiated with simulation studies using a dynamical model which includes the interaction effects of piston trajectory, heat transfer and chemical kinetics. Such an analysis is in the scope of future work. It may also be noted that the given the low indicated thermal efficiencies, more operating points must be investigated, potentially with relatively delayed ignition to lower the heat loss during the cycle to benchmark the highest achievable indicated thermal efficiencies and to delineate the individual effects of the parameters, i.e., compression ratio, initial temperature, equivalence ratio, and shape of the trajectory. While the framework for the optimization of the piston trajectory for each operating point has been previously developed [83], the experimental validation of the framework also remains a key avenue for future work.

The case study presented in this section demonstrates the capability of the CT-RCEM for conducting performance analysis of IC engine trajectories, in general. It also demonstrates the unique capability to offer experimental validation and in-depth investigation of advanced combustion mode and combustion control techniques such as trajectory based combustion control.
4.6 Conclusion

The novel capabilities of the CT-RCEM have been demonstrated and it has been shown that the ability of achieve precise piston motion control allows the CT-RCEM to offer extreme flexibility of operation and a high repeatability and throughput time since the changes in the operating conditions can be achieved by electronically changing the piston trajectory sent to the controller. However, the uniqueness of the CT-RCEM lies in the capability of tailoring the thermodynamic path, essentially the pressure and temperature history, inside the combustion chamber which in turn allows for a host of new investigative capabilities which cannot be offered by conventional combustion research apparatus. Three different capabilities have been demonstrated – the capability to investigate the effect of compression trajectory on autoignition characteristics, ability to quench the chemical kinetics in the combustion chamber, and the ability to create an isobaric dwell inside the combustion chamber. Additionally, the capability to perform detailed investigation of the combustion characteristics of a single combustion cycle of an IC engine has also been demonstrated.
CHAPTER 5  Multizone Model of CT-RCEM Combustion Chamber and its Application

Since the temperature measurement in an RCM is not straightforward, the temperature history is generally estimated from the pressure data, using a numerical model. While the computational fluid dynamics (CFD) based models are relatively the most accurate, the computational cost can be prohibitive even for relatively simple fuels. This has led to the widespread use of multi-zone models that are computationally tractable but can still provide reasonable accuracy. However, for CT-RCEM, the requirement of computational efficiency is even more pronounced. For an effective use of CT-RCEM, a numerical model is required to quickly predict, with reasonable accuracy, the evolution of the thermo-kinetic states in the combustion chamber for different piston trajectories. Analyzing the combustion characteristics for different trajectories through simulation allows the user to not only interpret the experimental results, but also to select the best suited trajectory, corresponding to a desired thermodynamic path, for a given experiment. High computational complexity of the model would make the analysis time prohibitive and reduce the overall turnaround time of the CT-RCEM. A physics based multi-zone model has been developed to meet the aforementioned requirements for the CT-RCEM.

In this chapter, we present, a systematic framework for the investigation of the effect of changing the piston trajectory – and hence, the thermodynamic path – on the combustion characteristics of fuels. This framework involves a concomitant use of the CT-
RCEM and the proposed multizone model to leverage this extra degree of freedom. This allows us to obtain further insight into the chemical kinetics of combustion, especially the low temperature chemistry and auto-ignition dynamics. From application perspective, such insight is critical for enabling advanced combustion modes, such as HCCI, RCCI, etc. especially for renewable fuels [84], [85]. Additionally, this capability makes the CT-RCEM naturally suitable for investigation pertaining to trajectory based combustion control [49], [58], [67], [86]

In the following sections, first the multi-zone model which has been developed for the CT-RCEM is presented. Next, the simulation results from the model are benchmarked with non-reactive and reactive mixture tests to verify its fidelity. After this, an investigation of the effect of piston trajectory on auto-ignition characteristics of dimethyl ether (DME), observed experimentally on the CT-RCEM, is presented. The change in the shape of piston trajectory has been realized, for this work, by changing the compression time for a constant CR. A reaction path analysis based on the simulation results from the model is presented next to interpret the experimental results. The study clearly shows a smaller compression time does not necessarily provide a smaller intermediate species buildup at the end of compression. Finally, the importance of systematic evaluation of the thermodynamic path of compression corresponding to the piston trajectory is highlighted, followed by the conclusion.
5.1 Modelling Approach

Irrespective of the level of detail and complexity, all dynamic models for RCM simulations include three key elements—compression trajectory, heat transfer, and reaction mechanism. While the reaction mechanism is the property of the fuel, the compression trajectory and heat loss are the characteristics of the RCM. The compression trajectory completely defines the path taken by the piston from start to end of compression and hence the compression parameters such as compression ratio, total compression time, 50% pressure rise time, etc. for a given RCM. It can be implemented in the model either as the trajectory to be provided by the actuation system as per the design [44], [87], [88], as the measured piston position data [39], [89], or as an empirical correlation in terms of RCM operating parameters obtained during its characterization [90], [91]. Modeling the heat loss, however, is a more involved task due to its complex dependence on the RCM geometry, fuel mixture properties, piston trajectory and level of turbulence inside the chamber.

The simplest, and most popular model, for RCM simulations is the adiabatic core hypothesis model, which relies on the assumption that with a carefully designed creviced piston, a relatively quiescent core is obtained inside the combustion chamber that undergoes almost adiabatic compression with minimal piston motion generated bulk fluid motion or turbulence [20], [44], [92]. The chemical kinetics is simulated assuming the core to be a homogeneous reactor with adiabatically changing volume [24], [33], [88], [93], [94]. The deviation from the adiabatic condition, due to heat loss, is accounted for by a
volume correction term determined from non-reactive experiments. While this model has proven fairly reliable it has three fundamental limitations. First, every reactive mixture test must be supplemented with a non-reactive mixture test, which is a time and resource intensive process. Second, the accuracy of the post compression temperature history predicted by the model for reactive mixtures tests is limited, especially for fuels with multi-stage ignition. Third, due to the lack of an explicit trajectory and heat loss sub-model, the volume of this adiabatic core does not have a well-defined physical relationship with the combustion chamber volume and hence the model cannot predict the pressure and temperature profile for a given piston trajectory. This severely limits the utility of this model for CT-RCEM which needs a reliable prediction of the thermodynamic path corresponding to the piston trajectory.

The physics based model proposed by Goldsborough et al. [90] builds upon the adiabatic core hypothesis based model and eliminates the need for a non-reactive experiment for every new test point. The volume correction term is obtained by a separate multizone model that simulates a non-reactive mixture compression, instead of actual experiment. By exchange of state information between the two sub-models periodically during the simulation, higher accuracy can be achieved compared to the original adiabatic core model by accounting for the heat release from chemical reactions, especially for fuels with multi-stage ignition. However, the volume of the assumed adiabatic core is still not representative of the entire combustion chamber. The multi-zone model proposed by Wilson et al. [95] builds upon the non-reactive sub-model of Goldsborough’s model to
include chemical kinetics such that the evolution of the thermal and chemical states can be simulated together, in the entire combustion chamber, instead of simulating the core region separately.

However, for both the physics-based models mentioned above, detailed modeling of the fluid flow dynamics between the main chamber and piston crevice, and the fluid flow inside the piston crevice leads to high computational complexity for efficient use with the CT-RCEM. The proposed model simplifies the modeling of the fluid flow processes to reduce computational complexity by using approximations and empirical correlations. The dissipative energy loss due to wall friction for fluid flow from combustion chamber to the crevice as well as inside the crevice is lumped together with the heat loss. This allows us to model the system dynamics without explicitly using the momentum equation for the flow from chamber to crevice and for the flow inside the crevice. Moreover, the zoning scheme used here enables us to avoid re-gridding of the chamber zones after every time step, as required in [95]. This provides a considerable boost in computational efficiency, especially when using reaction mechanisms with a large number of species and elementary reactions.
5.2 Dynamic Model

The overall schematic of the model is shown in Figure 5-1. The dynamic model is divided into two parts - combustion chamber volume and the crevice volume. The combustion chamber is sub-divided into annular zones of which shrink along the direction of piston motion during compression. Mass exchange between the zones ensures pressure uniformity in the combustion chamber. The detailed description of the dynamics is given in the following sections. The main assumptions in modeling the dynamics of the combustion chamber are listed below:

1. The combustion chamber is free of bulk fluid motion and turbulence generated due to piston motion during and after compression. Roll up vortex is completely captured by the piston crevice and the residual vorticity at the end of compression is negligible [20], [44], [90], [95]–[97].
2. Pressure equilibrium is maintained inside the combustion chamber by mass transfer between the zones.

3. Mass transfer between the zones is accompanied by exchange of corresponding enthalpy.

4. Conductive heat transfer occurs across the zone boundaries between adjacent zones.

5. Heat loss from the outermost combustion chamber zone to the chamber walls is conductive alone.

6. Heat loss from inside the piston crevice is convective alone.

7. The mass transfer from the combustion chamber to the piston crevice comes equally from all zones [90], [95].

8. Mass transfer among the combustion chamber zones and from chamber zones to the piston crevice is driven by pressure differential alone. The effect of concentration gradient is negligible [20], [44], [90], [95].

9. Dissipative loss of energy from the fluid flow due to wall shear friction (during flow to the crevice and inside the crevice) is lumped together with the heat loss from the crevice.

10. Chemical reactions progress inside the piston crevice is insignificant [20], [90], [95].
**Combustion Chamber Volume**

To model the thermal and compositional non-homogeneity inside the combustion chamber, it is divided into $N_z$ zones shaped as concentric annular cylinders, as shown in figure 6. While the temperature and composition vary from zone to zone, each zone is assumed to be homogeneous and described by a single set of thermo-chemical states. Each zone $i$ has two boundaries, inner and outer boundary; except the innermost zone ($i = N_z$) which has only an outer boundary. The outermost zone ($i = 1$) shares its outer boundary with the chamber walls, head and the piston top. For each zone, while the zone thickness is different along the height ($b_i$) and along the diameter ($a_i$), the thickness ratio ($\lambda = a_i/b_i$) is a constant. The zone thickness $a_i$ and $b_i$ grow in a geometric progression with the same growth rate $r$ from the chamber walls towards the core to account for the sharper thermal gradient near the walls, as suggested in [95], [98], [99]. The innermost zone represents the core region of the chamber, which attains the highest temperature, and is free of the boundary layer effects. The outer zones $i = \{1, \ldots, N_z - 1\}$ completely contain the boundary layer.

**Gridding Combustion Chamber into Zones**

Gridding of the combustion chamber into zones involves selection of four parameters - thickness of the outermost zone along chamber height ($b_1$), the zone thickness ratio ($\lambda = a_1/b_1$), number of zones ($N_z$), and the volume of the innermost zone as a fraction of chamber volume at TDC ($\eta$). This gridding of the zones completely defines the zone geometry and its relationship to the piston trajectory. The zone thickness and the
zone boundary diameters remain constant after gridding. The piston motion is accounted for by axial compression of the zones along the height.

The thickness ratio accounts for the higher heat transfer to the chamber walls near the side of the chamber compared to the center due to higher surface area, especially if the aspect ratio (ratio of diameter to height of chamber) at TDC is large. The effect of thickness ratio on the geometry of zones for CT-RCEM is shown in Figure 5-2. Thickness ratio of unity corresponds to the case of uniform thickness. The volume fraction $\eta$, is typically set to a fraction of the total chamber volume which maintains a relatively homogeneous

\[ \eta = \frac{\text{innermost zone volume}}{\text{total chamber volume}} \]

Figure 5-2: Zone shapes for various thickness ratios, at TDC, for six zones with innermost zone occupying 20% of the total chamber volume

The thickness ratio accounts for the higher heat transfer to the chamber walls near the side of the chamber compared to the center due to higher surface area, especially if the aspect ratio (ratio of diameter to height of chamber) at TDC is large. The effect of thickness ratio on the geometry of zones for CT-RCEM is shown in Figure 5-2. Thickness ratio of unity corresponds to the case of uniform thickness. The volume fraction $\eta$, is typically set to a fraction of the total chamber volume which maintains a relatively homogeneous
temperature distribution unaffected by the post compression thermal boundary layer growth. The thickness of the outermost zone $b_1$ determines the distribution of the boundary layer among the outer zones since the growth rate $r$ of the zone thickness is determined from $b_1$, $\eta$ and $N_z$. The number of zones $N_z$ determines the spatial resolution of the thermal gradient between the core and the chamber walls. Since the computational time increases roughly as $O(N_z^3)$ with the number of zones for most chemical kinetics solvers, selecting the number of zones is a trade-off between computational time and accuracy. For this work, $b_1, \lambda,$ and $\eta$ were chosen to be 0.25 mm, 2, and 0.75 respectively based on a CFD study conducted during the design of the creviced piston [97]. The number of zones was limited to $N_z = 3$ to keep the model computationally tractable while using a detailed reaction mechanism.

Once $b_1$, $\lambda$, $N_z$ and $\eta$ have been chosen, the growth rate of zone thickness $r$ can be calculated from equations (5-1)-(5-3).

$$V_{N_{tdc}} = \eta V_{chamb_{tdc}} \quad \text{(5-1)}$$

$$\frac{p_i}{4} (d_{chamb} - 2\sum_{i=1}^{N_z} a_1 r^{i-1})^2 (h_{tdc} - 2\sum_{i=1}^{N_z} b_1 r^{i-1}) = \eta V_{chamb_{tdc}} \quad \text{(5-2)}$$

$$a_i = \lambda b_i \quad \text{(5-3)}$$

The zone thicknesses $a_i = a_1 r^{i-1}$ and $b_i = b_1 r^{i-1}$ can now be calculated for $i = \{1, \ldots, N_z - 1\}$. Hence, the zone boundary diameters $(d_i)$ can be calculated as
\[ d_i = \begin{cases} \frac{d_{chamb}}{d_{chamb} - 2\Sigma_{j=1}^{i-1}a_j}; i = 1 \\ d_{chamb} - 2\Sigma_{j=1}^{i-1}a_j; i = \{2, 3, \ldots, N_z\} \end{cases} \]  \tag{5-4}

and the instantaneous height \( h_i(t) \) of a zone boundary is defined by the instantaneous piston position \( x(t) \),

\[ h_i(t) = \begin{cases} x(t); i = 1 \\ x(t) - 2\Sigma_{j=1}^{i-1}b_j; i = \{2, 3, \ldots, N_z\} \end{cases} \]  \tag{5-5}

**Dynamics of Combustion Chamber Zones**

The dynamics of the combustion chamber zones is described mainly by four governing equations – the ideal gas law, and, mass, energy and species conservation. The ideal gas law for each zone can be written as:

\[ P_i V_i = \sum_k \left( \frac{m_{ki}}{M_k} \right) R T_i \]  \tag{5-6}

Where \( P_i, V_i, \) and \( T_i \) are the pressure volume and temperature of the zone \( i \), \( R \) is the universal gas constant. \( m_{ki} \) is the mass of species \( k \) in zone \( i \), and \( M_k \) is the molar mass of species \( k \).

The mass conservation for each zone can be written as:

\[ \dot{m}_i = \dot{m}_{i-1,i} + \dot{m}_{i+1,i} - \dot{m}_{i,cr} \]  \tag{5-7}

where \( \dot{m}_i \) is the rate of change of mass of zone \( i \). The terms on the right-hand side represents the mass flow rate from zone \( i - 1 \) to \( i \), zone \( i + 1 \) to \( i \), and zone \( i \) to the piston crevice respectively. Depending on the individual pressures of zones at any particular solver step, the mass flow rates may be positive or negative. The mass flow rate between
adjacent zones in the combustion chamber is assumed to be directly proportional to the pressure difference between the zones with a large constant of proportionality. The calculation of mass flow rate from each zone to the crevice is described in the crevice volume dynamics.

The energy conservation equation for the combustion chamber zones can be written as:

\[
\dot{U}_i = \frac{d}{dt} \left( m_i \sum_k X_{ki} u_{ki}(T_i) \right) = -P_i \dot{V}_i - \dot{Q}_{cond} + \sum_{l=1}^{n_{in}} \dot{m}_l h_l + \sum_{p=1}^{n_{out}} \dot{m}_p
\]  (5-8)

where \( U_i \) is the total internal energy of zone \( i \), \( X_{ki} \) is the species concentration (mass fraction) of species \( k \) in zone \( i \) and \( u_{ki} \) is its specific internal energy which is a function of the zone temperature. The terms on the right in equation (5-8) represent the piston work, conductive heat loss, enthalpy inflow and enthalpy outflow respectively for each zone. The term \( n_{in} \) represent the total number of enthalpy inflow sources into zone \( i \), and \( \dot{m}_l, h_l \) represent the mass flow rate and specific enthalpy from source \( l \) to zone \( i \). The term \( n_{out} \) represents the total number of enthalpy outflows from zone \( i \) and \( \dot{m}_p \), represents the mass flow rate and specific enthalpy from zone \( i \) to outflow \( p \). (Note that \( \dot{m}_p \) is a negative quantity since it represents an outflow of mass). From equations (5-4) and (5-5), the rate of change of volume for the zone \( i \) is given as:

\[
\dot{V}_i = \frac{\pi}{4} \left( d_{i-1}^2 - d_i^2 \right) \dot{x}
\]  (5-9)
where \( \dot{x} \) is the piston velocity, which is a negative quantity when piston is moving forward from BDC to TDC. The conductive heat loss term (\( Q_{\text{cond}_i} \)) for each zone is modelled according to Fourier’s law, as

\[
\dot{Q}_{\text{cond}_i} = k_i A_{i,i-1} \frac{(T_i - T_{i-1})}{a_i + a_{i-1}} + k_i A_{i,i+1} \frac{(T_{i+1} - T_i)}{a_{i+1} + a_i} \tag{5-10}
\]

where \( k_i \) is the thermal conductivity of the gas, \( A_{i,i-1} \) and \( A_{i,i+1} \) are the surface area of the and \( a_i \) is the zone thickness for zone \( i \).

The species conservation equation for each zone is written as:

\[
\frac{d}{dt} (m_i X_{k_i}) = \sum_{l=1}^{n_{in}} \dot{m}_l X_{k_i} + X_i \sum_{p=1}^{n_{out}} \dot{m}_p + \dot{m}_{k_i,\text{gen}} \tag{5-11}
\]

where the first two terms on the right represent the species flux in and out of the zone. (Again, note that \( \dot{m}_p \) is a negative quantity). The third term (\( \dot{m}_{k_i,\text{gen}} \)) represents the species generation given as:

\[
\dot{m}_{k_i,\text{gen}} = V_i \Lambda_{k_i} M_k \tag{5-12}
\]

\[
\Lambda_k = \sum_{j=1}^{N_r} v_{k,j} R_j \tag{5-13}
\]

where \( \Lambda_{k_i} \) is the net molar production rate per unit volume of the species \( k \) in zone \( i \); \( v_{k,j} \) is the stoichiometric coefficient of species \( k \) in \( j^{th} \) chemical reaction; \( R_j \) is the reaction rate per unit volume for \( j^{th} \) chemical reaction; and \( N_r \) is the total number of chemical reactions.
**Piston Crevice Volume**

The governing dynamics for the piston crevice volume involves the ideal gas law, equation of mass flow from combustion chamber to the crevice and the energy conservation equation as chemical reaction progress is considered negligible inside the piston crevice.

The ideal gas law is written as

\[ P_{cr}V_{cr} = \sum_k \left( \frac{m_{kcr}}{M_k} \right) RT_{cr} \]  

(5-14)

The total mass flow rate from the combustion chamber to the crevice is calculated using compressible orifice equation and divided equally among the combustion chamber zones.

\[ \dot{m}_{net} = C_d A_{crev} \left[ \frac{2}{gRT_{ch}} \right]^{\frac{1}{2}} P_{ch} \left( \frac{P_{cr}}{P_{ch}} \right)^{\frac{1}{2}} T_{ch} \left[ 1 - \left( \frac{P_{cr}}{P_{ch}} \right)^g \right]^{\frac{1}{2}} \]  

(5-15)

\[ g = \frac{\gamma_{ch} - 1}{\gamma_{ch}} \]

\[ \dot{m}_{i,cr} = \dot{m}_{net}/N_z \]

where \( \dot{m}_{net} \) is the total mass flow rate from the combustion chamber to the piston crevice, \( C_d \) is the orifice constant, \( A_{crev} \) is the total area available for fluid flow into the crevice, \( P_{ch}, P_{cr} \) are the average pressure of the combustion chamber and the pressure in the piston crevice, respectively, \( T_{ch} \) is the mass averaged temperature and \( \gamma_{ch} \) is the ratio of averaged specific heats of the combustion chamber zones. As mentioned in assumption (7) before, the mass flow from chamber to the crevice is equally divided among all zones.
The energy conservation equation for the piston crevice is simpler due to the absence of piston work and chemical reaction progress and is given as

\[
\dot{U}_{cr} = -h_{cr}A_{scr} (T_{cr} - T_{wall}) + \frac{\dot{m}_{net}}{N} \sum_{i=1}^{N} h_i
\]  

(5-16)

where \( h_{cr} \) is the convective heat transfer coefficient for the piston crevice, \( A_{scr} \) is the total surface area available for heat transfer including the crevice wall and the chamber wall area enclosing the crevice gas. \( T_{cr} \) is the crevice gas temperature and \( T_{wall} \) is the wall temperature of the piston crevice and chamber wall. The heat transfer coefficient is evaluated using Nusselt number correlation, suggested in [90], [95], [100], as

\[
Nu_{cr} = \frac{h_{cr} l_{cr}}{k_{cr}} = \frac{c_1 Pr_{cr}^{c_2}}{1 + \frac{c_3 \Theta}{c_4 \Theta^{-3}}}
\]  

(5-17)

\[
\Theta = \frac{\zeta_{cr} Ra_{cr} Pr_{cr}}{l_{cr}}
\]

where \( \zeta_{cr} \) is the surface area to volume ratio of the crevice and \( l_{cr} \) is the length of the crevice, \( Nu_{cr}, Ra_{cr}, Pr_{cr} \) are the Nusselt, Reynolds and Prandtl numbers respectively; the constants \( c_1, c_2, c_3 \) and \( c_4 \) are constants calibrated experimentally using non-reactive compression data for several compression ratios and compression times.

The model has been implemented in MATLAB and CANTERA has been used for solving chemical kinetics. On a desktop with Intel i7 5960k Haswell processor, with clock speed 3.0 GHz, and 32 GB RAM, the model, with combustion chamber divided into three zones, runs non-reactive simulations in under a minute, while the reactive simulation using detailed chemical mechanism Aramco 2.0 (493 species) takes about 4.8 hours.
5.3 Experimental Results and Model Validation

The experimental validation of the model was done using both non-reactive and reactive mixtures. Figure 5-3 shows the comparison of the model prediction with the experimentally obtained pressure profile for the compression of air-CO2 mixture for geometric compression ratios 14.2, 15.5 and 16.7, for compression time 20 ms and 30 ms. It may be noted that due to the presence of piston crevice the actual compression ratio is lower than the geometric compression ratio – 8.9, 9.6 and 10.4, respectively. An excellent agreement can be seen between the experimental pressure data and the pressure predicted.
by the model.

Figure 5-4 shows the corresponding zone temperatures for geometric (actual) compression ratio 16.7 (10.4) and the peak temperature predicted by the adiabatic core hypothesis model. This establishes that the model can accurately predict the thermodynamic states for a given trajectory.

Figure 5-4: Zone temperatures (top) for geometric compression ratio 16.7 and compression time 20 ms - z1, z2 and z3 represent the outermost, middle and core zone of the combustion chamber respectively. Bottom plot shows comparison of core temperature predicted by the proposed multizone model and the simple adiabatic core hypothesis based model
Figure 5-5 shows the experimentally obtained combustion pressure and the corresponding piston trajectory for reactive mixtures testing for geometric compression ratios 16.7, and compression time 20 ms and 30 ms. The fuel mixture was prepared by manometric mixing of dimethyl-ether, dry air and nitrogen to obtain molar composition **DME: O₂: N₂ = 1:4:40**. It is evident that the measured first stage ignition delay is shorter for 20 ms compression compared to 30 ms compression. Several repetitions (6-9) of the experiments have been conducted to ensure that the observed difference in the ignition delay is both repeatable and statistically significant. The variability in the ignition delay measurements was less than 0.3 ms. The initial pressure and temperature for both cases were set at 1.034 bar (15 psi) and 300 K respectively. The uncertainty in the initial

![Combustion pressure and piston trajectory](image)

*Figure 5-5: Experimentally obtained pressure trace and piston trajectory for compression of DME mix (DME:O₂:N₂ = 1:4:40) for compression times 20 and 30 ms and CR 16.7*
temperature and pressure is $\pm 1^\circ C$ and $\pm 3\, \text{mbar}$ respectively. Same batch of fuel has been used for the two cases for each test condition to minimize the effect of variability in the fuel composition. The measured compressed pressure was almost same, i.e. 23.2 bar, for both 20 ms and 30 ms case while the compressed temperature was estimated using the proposed model as 692.8 K and 691.3K. The uncertainty of the dynamic gas pressure measurement is $\pm 0.1\, \text{bar}$. The corresponding uncertainty in the estimated peak temperature is $\pm 5K$. For this work, the end of compression (EOC) is defined as the time instant at which a pressure maximum is attained inside the chamber, i.e. $\frac{dp}{dt} = 0$ which is a customary practice for conventional RCM data. Henceforth, the data pertaining to reactive mixtures (both experimental and simulation) has been presented with EOC as $t = 0$.

Moreover, to further validate the observed trend, further testing was conducted by varying two conditions – 1) slightly reduced compression ratio (to reduce the peak compressed temperature); and 2) increased the dilution of the fuel mixture with extra nitrogen (to make the ignition delay more observable).
Figure 5-6: Experimentally obtained pressure trace and piston trajectory for compression of DME mix (DME:O2:N2 = 1:4:40) for compression times 20 and 30 ms and CR 15.5

Figure 5-6 shows the data obtained for compression ratio 15.5, and compression times 20 & 30 ms. The initial temperature and pressure were 300K and 0.99 bar (14.4 psi) and mixture composition was DME:O2:N2 = 1:4:40. The compressed pressure was almost the same, i.e. 21.3, bar for both 20 ms and 30 ms case and the compressed temperature was estimated to be 682.6K and 681.1K for 20 ms and 30 ms compression respectively. Reduced compression ratio results in a reduced compressed temperature, however, the 20ms compression still leads to a shorter ignition delay compared to 30 ms.

Figure 5-7 shows the combustion pressure profile obtained for compression ratio 16.7 and compression times 20 ms and 30 ms, for mixture composition DME:O2:N2 =
The initial temperature and pressure were 300K and 1.034 bar (15 psi). It can be seen that due to increased dilution the ignition delay times have increased, however, 20 ms compression still produces a shorter ignition delay than 30 ms compression. Figure 5-8 shows the comparison of model predictions and experimental results for the first reactive mixture, i.e. **DME:O\textsubscript{2}:N\textsubscript{2} = 1:4:50**. Aramco 2.0 detailed mechanism was used for this simulation. It can be seen that the model over predicts the first stage ignition delay and the peak combustion pressure. However, the agreement between the change in the ignition delay with the change in compression time from 20 ms to 30 ms is remarkably accurate. While the experimentally recorded difference in the first stage and total ignition delay is 0.5 ms and 0.8 ms respectively, the model predicts a difference of 0.7 ms and 0.9 ms respectively.

**Figure 5-7**: Experimentally obtained pressure trace compression of DME mix with increased dilution by nitrogen (DME:O\textsubscript{2}:N\textsubscript{2} = 1:4:50) for compression times 20 and 30 ms for CR 16.7

**1:4:50**. The initial temperature and pressure were 300K and 1.034 bar (15 psi). It can be seen that due to increased dilution the ignition delay times have increased, however, 20 ms compression still produces a shorter ignition delay than 30 ms compression.
In the following sections we show, using reaction path analysis performed using species concentration data obtained from simulations that a faster compression in an RCM experiment does not necessarily mean a smaller intermediate species buildup at the end of compression. This, however, further emphasizes the key advantage of CT-RCEM over conventional RCM. Since the ignition delay measurements on an RCM are heavily path dependent, the capability to produce different thermodynamic paths to achieve the desired set of pressure and temperature conditions is vital for chemical kinetic investigations of auto-ignition which is the uniqueness of the CT-RCEM.

![Experiment v/s Simulation](image)

*Figure 5-8: Model prediction vs experimental data for compression ratio 16.7 and compression times 20 ms & 30 ms*
5.4 Reaction Path Analysis

As mentioned before, a reaction path analysis has been performed to investigate the reason for shorter ignition delay with 20 ms compression compared to 30 ms compression.

Figure 5-9 shows the comparison of the pressure and temperature profiles for the two cases as predicted by the model. The end of compression in both cases is considered $t = 0$. A zoomed-in plot of the temperature and displacement profile of these two cases near the end of compression are shown in Figure 5-10. Seven time-instants have been selected for investigating the reaction pathways, as indicated by numbers 1 to 7 on the displacement and temperature plots shown in Figure 5-10. The first three of the selected time-instants, i.e. 1, 2, and 3 are during the compression process – i.e. 6ms, 4ms and 2ms.

*Figure 5-9: Comparison of pressure and core temperature for 20 ms and 30 ms compression predicted by the dynamic model*
before the end of compression, respectively. The time-instant 4 is at the end of compression (i.e. t=0 ms). The remaining three time-instants, i.e. 5, 6, and 7, are during the post compression period –i.e. 1ms, 2ms and 3ms after the end of compression, respectively. The specific reaction paths and the corresponding chemical kinetics analysis for each of the selected time-instants is presented below. The reaction rates in the path diagrams presented in this section are scaled with respect to the most prominent reaction at the particular time-

*Figure 5-10:* Zoomed-in figure of displacement and core temperature for 20 ms and 30 ms compression predicted by the dynamic model
instant. The reaction rate threshold for the diagrams is set at $10^{-5}$ times the diagram scale, i.e. any reaction with a rate that is more than five orders of magnitude slower than the most prominent reaction at a given time-instant is considered insignificant and not shown on the path diagram. The net rate of a reaction represents the difference of the forward and reverse reaction rates, and hence, a negative net rate indicates that the net reaction is progressing in the reverse direction. The reverse rate is not indicated when it is slower by more than five orders of magnitude relative to the forward rate.

**Time-instant 1 (6 ms before end of compression):**

At this time-instant, the temperature of the combustion chamber core for the 30ms compression case is higher than the 20ms compression case – 551K and 521K respectively. This is because, the piston is closer to the TDC and as a result, the combustion chamber volume is smaller in 30ms compression case at this time-instant. As a result, the reaction rates for the 30ms case, in general, are higher than the 20ms case, which is evident from the reaction path diagrams for the two cases, shown in Figure 5-11. The most prominent reaction for both the cases is the conversion of CH$_3$OCH$_3$ (the DME molecule) to CH$_3$OCH$_2$. However, the rate of this reaction is more than an order of magnitude higher in 30 ms case compared to the 20 ms case. It is also obvious that more intermediate reactions have been triggered by this time in the 30ms case, particularly, the pyrolysis of CH$_3$OCH$_2$O$_2$ to CH$_2$O and CH$_3$OCH$_2$O$_2$H. However, since the temperatures are still relatively low in both cases, the absolute reaction rates are very small, which is indicated by the scale number ($1 \times 10^{-10}$), for both the cases.
By this time - instant 2 (4 ms before end of compression): the combustion chamber volume is almost the same for the 20 ms and the 30 ms cases. The corresponding combustion chamber core temperatures are also almost the same – 607.5K and 607.3K respectively. As can be seen from Figure 5-12, again the involved reaction pathways are identical in both cases.

Figure 5-11: Reaction path diagram for 20 ms and 30 ms compression, 6ms before the end of compression

Time-instant 2 (4 ms before end of compression):

By this time-instant, the combustion chamber volume is almost the same for the 20 ms and the 30 ms cases. The corresponding combustion chamber core temperatures are also almost the same – 607.5K and 607.3K respectively. As can be seen from Figure 5-12, again the involved reaction pathways are identical in both cases.
Figure 5-12: Reaction path diagram for 30ms compression, 4 ms before the end of compression
The most prominent reaction for both the cases is the conversion of CH$_3$OCH$_2$O$_2$ to CH$_2$OCH$_2$O$_2$H. Moreover, the reaction rates are also similar, as is evident from the two diagrams scales $7.8 \times 10^{-9}$ for 20ms case and $7.6 \times 10^{-9}$ for 30ms. The most significant difference between the two reaction path diagrams, however, comes from the following reaction:

$$CH_3OCH_2 + O_2 \rightleftharpoons CH_3OCH_2O_2$$

The conversion of CH$_3$OCH$_2$ to CH$_3$OCH$_2$O$_2$, shown in the above reaction is reversible with very similar reaction rates for the forward and the reverse reaction. As a result, the reaction is very sensitive to both –temperature and the species concentration. In the 20ms case, the reaction goes mainly in forward direction, which leads to the accumulation of OH radical. To the contrary, in the 30ms case the reaction goes mainly in reverse direction, causing a relatively slower accumulation of OH radical.

**Time instant 3 (2 ms before end of compression):**

After time-instant 2, the core temperature in 20 ms case remains a bit higher compared to 30 ms case. At time-instant 3, the core temperatures are 672.1 K and 657.8 K for the 20 ms and 30 ms case, respectively. The higher core temperature in 20 ms case is caused by higher pressure rise rate, as well as lower heat loss, due to faster compression.

<table>
<thead>
<tr>
<th></th>
<th>CH3OCH2O2</th>
<th>HO2</th>
<th>O2</th>
<th>OH</th>
</tr>
</thead>
<tbody>
<tr>
<td>20 ms</td>
<td>3%</td>
<td>3%</td>
<td>88%</td>
<td>6%</td>
</tr>
<tr>
<td>30 ms</td>
<td>1%</td>
<td>2%</td>
<td>95%</td>
<td>2%</td>
</tr>
</tbody>
</table>
The main reactions are still identical and the general reaction rate is still slightly higher, with scales $6.0 \times 10^{-6}$ and $1.3 \times 10^{-6}$ for 20 ms and 30 ms case, respectively (Figure 5-13). The most prominent reaction is still the conversion of CH$_3$OCH$_2$O$_2$ to CH$_2$OCH$_2$O$_2$H, for both the cases. However, the most significant difference between the two cases lies in the pathways for H abstraction for conversion of CH$_3$OCH$_3$ to CH$_3$OCH$_2$.

Table 5-1 summarizes the contribution of four different pathways for H abstraction for the 20 ms and the 30 ms case. Reaction pathway involving O$_2$ is relatively the slowest.
while the pathway involving OH is relatively the fastest since O2 and OH are the most stable and unstable species, respectively, among all the four species listed in Table 5-1. Hence, it is reasonable to conclude that the H abstraction is progressing at a relatively faster rate in 20ms case compared to the 30ms case, which facilitates a faster and larger accumulation of intermediate species in 20ms case.

**Time instant 4 (end of compression):**

At this time-instant, i.e. at the end of compression, the core temperature for both the cases is almost the same again, i.e. 692.8K and 691.3K for 20 ms and 30ms, respectively. The corresponding combustion chamber volumes are almost the same as well. From the reaction path diagram shown in Figure 5-14, three things are obvious. First, the reaction rates for 20ms case (scale: $1.8 \times 10^{-3}$) are already about an order of magnitude larger compared to 30ms case (scale: $2.1 \times 10^{-4}$). Second, some reactions are considerably more prominent in the 20ms case. The reactions pertain to the pyrolysis of larger reaction intermediates to relatively smaller molecules and radicals and are listed below:

\[
OCH_2OCHO \rightleftharpoons HOCH_2OCO
\]

\[
HOCH_2OCO \rightleftharpoons HOCH_2O + CO
\]

\[
HOCH_2OCO \rightleftharpoons CH_2OH + CO_2
\]

\[
CH_3OCH_2O_2H \rightleftharpoons CH_3OCH_2O + OH
\]

The net result of this pyrolysis is to speed up the subsequent reactions involving the smaller intermediate species which are critical for initiating the chain reactions for ignition.

Third, the contributions of the various reaction pathways for H abstraction are different.
Table 5-2 summarizes the relative contribution of the four different reaction pathways for H abstraction for 20 ms and 30 ms case at this time-instant. It can be seen that H abstraction through the path involving O$_2$ is relatively far lower for 20 ms case compared to 30 ms case. Hence, Table 5-2 precisely explains why the H abstraction is proceeding at relatively faster rate for 20 ms case, as indicated by the net reaction rate for
Time instant 5: (1 ms after the end of compression)

At this time-instant, the temperature for both cases have dropped a bit, due to heat loss, to 691.0 K and 689.0 K for 20 ms and 30 ms case, respectively. The probable cause of a slightly higher temperature for 20ms case is that the chemical reactions by this point have started to turn exothermic due to large intermediate species buildup.

From the reaction path diagram shown in Figure 5-15, besides a higher reaction rate and more contributions of faster reaction pathways for H abstraction, there are two additional reactions that have started adding to the intermediate species pool for 20ms case:

\[
HOCH_2O \rightleftharpoons HOCHO + H
\]

\[
CH_3OCH_2O_2H \rightleftharpoons CH_3OCH_2O + OH
\]

The effect of faster buildup of intermediate species culminates into a large enough pool to eventually start the ignition earlier for the 20 ms case.
Time instant 6: (2 ms after the end of compression)

At this time-instant, the first heat release has already been triggered in the 20ms case, where the temperature rises to 812.4 K. However, the 30ms case is still undergoing the accumulation of the intermediates for ignition, and the temperature is only 688.7 K.

(a) 20 ms compression

(b) 30 ms compression

Figure 5-15: Reaction path diagrams, 1ms after the end of compression
From the reaction path diagram in Figure 5-16, we see that the species CH$_3$OCH$_2$O, which is being produced in the 20ms case via the pyrolysis of CH$_3$OCH$_2$O$_2$H, becomes the parent molecule for a lot of smaller molecules, as CH$_3$O, CH$_3$OCHO, CH$_2$O, and radicals such as HO$_2$ and H.

**Figure 5-16: Reaction path diagrams, 2ms after the end of compression**
The chain reactions which cause the first heat release have already started in the 20ms case. Further effect is cumulative and the chain reactions continue until the pool of intermediate species responsible for the first stage heat release have been exhausted. However, in 30ms case, the pyrolysis of CH₃OCH₂O₂H to produce CH₃OCH₂O hasn’t started yet, indicating that more time is needed for accumulation of intermediates, leading to delayed first stage heat release for 30 ms case.

**Time instant 7: (3 ms after the end of compression)**

At this time-instant, while the induction reactions for second stage ignition are well underway for the 20 ms case, the first stage ignition has just been completed in the 30 ms case. The temperature is higher for the 20 ms case compared to 30 ms – 889.1 K and 874.3K, respectively – due to the exothermic nature of the reactions. Moreover, the reaction rates for 20 ms case are, again, an order of magnitude higher than 30 ms case, indicated by the scale values — $8.4 \times 10^3$ and $5.2 \times 10^2$ respectively (Figure 5-17). The higher reaction rate in 20ms certainly will trigger the second ignition sooner compared to the other one.

To summarize the reaction path analysis, we see that even though the 30ms case has relatively higher temperature and less combustion chamber volume at the beginning, i.e. before time-instant 1, the relative impact of this on the chemical kinetics is small since the absolute temperature is low in both the two cases.

However, chemical kinetics is more significantly affected by the thermal state near the end of compression when the absolute temperature is higher, as can be seen from the
reaction path analysis from time-instant 2 onwards. While the total time of the stroke is lower for 20 ms compression, because of the specific trajectory of this case, a consistently higher temperature is attained in the final 2 ms of the compression process. This leads to a relatively higher degree of reaction progress in the 20 ms case compared to 30 ms case, resulting in a higher accumulation of reaction intermediates consisting of both, relatively larger molecules as well as highly reactive radicals. This leads to a shorter induction time.

Figure 5-17: Reaction path diagrams, 3ms after the end of compression
to accumulate enough intermediate species to trigger the chain reactions of the ignition process leading to a shorter ignition delay measurement in the 20ms case.

This analysis clearly highlights the importance of the thermodynamic path of compression for autoignition investigation studies on rapid compression machines. It also demonstrates the unique advantage provided by the ability to tailor the thermodynamic path of compression in the CT-RCEM. Systematic investigation of auto-ignition along different thermodynamic paths on the same experimental apparatus, can provide valuable information for developing, improving, and validating chemical kinetics mechanism.

Validation of this analysis at other operating points and the further investigation of the effect of the thermodynamic path on the ignition characteristics, especially variation in influence of the low temperature chemistry, over a wide range of compressed pressure and temperatures (as shown in section 4.2, figure 4-7) is an ongoing work and is in the scope of future work. Moreover, for the proposed framework, while the multi-zone model offers computational efficiency, for a more detailed study, the analysis could be further improved using a CFD model with chemical kinetics which captures the dynamics more accurately. Efforts to develop a CFD model are also ongoing and the detailed analysis is a work in progress [101].

5.5 Conclusion

A multi-zone thermo-kinetic model for combustion chamber dynamics of a controlled trajectory rapid compression and expansion machine (CT-RCEM) has been
developed. While the ability to precisely control the piston trajectory in the CT-RCEM allows for tailoring the thermodynamic path of compression, a multi-zone model is required for both — selecting a suitable piston trajectory to achieve a desired thermodynamic path as well as to investigate the effect of thermodynamic path on the auto-ignition characteristics. After, experimental validation for compression of non-reactive and reactive mixtures over a range of operating conditions, the model is used to explain the experimentally observed effect of changing compression time on the ignition delay for dimethyl ether.

The reaction path analysis at various time-instants, during and after the compression, clearly reveals that a faster compression does not necessarily ensure a smaller intermediate species buildup at the end of compression. It also demonstrates how the CT-RCEM can be used for a systematic investigation of auto-ignition along different thermodynamic paths but similar end of compression conditions which can provide critical information for developing, improving, and validating chemical kinetics mechanism.
CHAPTER 6  Conclusions and Future Works

6.1  Conclusions

This dissertation presents the modelling, design, control and characterization of a novel, controlled trajectory rapid compression and expansion machine (CT-RCEM) with the unique capability of precise motion control of the piston. While in a conventional RCM/RCEM, changing the operating parameters such as compression ratio and compression time requires mechanical alteration of the hardware, the same can be achieved in the CT-RCEM merely by changing the reference trajectory fed electronically to the controller. More importantly, the CT-RCEM offers a new paradigm of investigative capabilities by providing, for the first time, the ability to directly tailor the thermodynamic path of the test mixture inside the combustion chamber by appropriate selection of the piston trajectory.

A control oriented dynamic model of the CT-RCEM has been developed. Simulation studies and analysis is used to understand the relationship between the various physical quantities and the geometrical parameters, and, to identify the major design tradeoffs. The dynamic model and the simulation studies are used to guide the mechanical design, design of the subsystems and the development of the model based controller used for precise tracking performance. The actuation system of the CT-RCEM has been designed for a peak flow rate of 1600 l/min at a working pressure of 350 bar which
makes the CT-RCEM capable of tracking any trajectory with peak speed up to $16 \text{ ms}^{-1}$ and peak acceleration up to $2500 \text{ ms}^{-2}$ over a maximum stroke of 192 mm.

A precise motion controller has been developed to provide high accuracy tracking of the reference profile by the piston in the CT-RCEM. While a repetitive controller is developed for the dynamic model an iterative learning control is developed for the hardware. This is because while the hardware has some turnaround time between successive runs, the dynamic model has no such constraint. A nonlinear inversion based feedforward controller has also been developed for hydraulic actuators with asymmetric which is the case with CT-RCEM actuator. The control scheme has been shown to provide excellent tracking performance reducing tracking error to about 600 microns for CT-RCEM operation for piston trajectory with stroke of 131 mm and compression time of 20 ms and peak speed of about $12 \text{ ms}^{-1}$.

The CT-RCEM has been characterized using both non-reactive and non-reactive mixtures establishing the functionality and repeatability of the system. The ability to tailor the thermodynamic path of test mixture inside the combustion chamber by suitable selection of the piston trajectory has been demonstrated. Three novel investigative capabilities enabled by the CT-RCEM have been demonstrated – investigating the effect of compression time on ignition delay, generating isobaric dwell at the end of compression using piston creep, and, quenching of the combustion chamber gases by rapid withdrawal of the piston. It has been shown using autoignition data for dimethyl ether (DME) that there exists a strong coupling between the thermodynamic path of compression and the ignition
delay, leading to an important insight – while the species pool resulting from reaction progress during the compression process cannot be eliminated, it is possible to account for this species pool and potentially reduce the uncertainty of further analysis by using several different compression paths on the CT-RCEM. In addition to this, the utility of the CT-RCEM for IC engine investigations has also been demonstrated by presenting a case study pertaining to the experimental investigation of an advanced control strategy called trajectory based combustion control for the operation of the free piston engine.

A multi-zone thermo-kinetic model for combustion chamber dynamics of a controlled trajectory rapid compression and expansion machine (CT-RCEM) has been developed. While the ability to precisely control the piston trajectory in the CT-RCEM allows for tailoring the thermodynamic path of compression, a multi-zone model is required for both — selecting a suitable piston trajectory to achieve a desired thermodynamic path as well as to investigate the effect of thermodynamic path on the auto-ignition characteristics. After, experimental validation for compression of non-reactive and reactive mixtures over a range of operating conditions, the model is used to explain the experimentally observed effect of changing compression time on the ignition delay for dimethyl ether. The reaction path analysis at various time-instants, during and after the compression, clearly reveals that a faster compression does not necessarily ensure a smaller intermediate species buildup at the end of compression. It also demonstrates how the CT-RCEM can be used for a systematic investigation of auto-ignition along different
thermodynamic paths but similar end of compression conditions which can provide critical information for developing, improving, and validating chemical kinetics mechanism.

6.2 Future works:

In the future, CT-RCEM would be used to further investigate the dynamic relationship between the thermodynamic path inside the combustion chamber and the autoignition. New thermodynamic paths will be designed to further enhance the investigative capabilities of the CT-RCEM aimed at facilitating better development improvement and validation of chemical kinetic models.

6.2.1 Investigation of low temperature chemistry for fuels

While the shock tubes are the main source of chemical kinetics data at high temperatures, the chemical kinetic models of low temperature chemistry (LTC) heavily rely on the data from RCM experiments given the operating range of typical RCM. However, as discussed in previous chapters, the experimental data obtained from conventional RCM is that it is highly facility dependent and a large facility-to-facility variability has been reported in the chemical kinetic data obtained from RCMs, leading to large uncertainty in the subsequently developed LTC kinetic models.

The CT-RCEM will be used in future studies to mitigate this uncertainty for LTC models. Besides the highly repeatable operation for a given test condition, the CT-RCEM will be used to obtain data pertaining to similar end of compression temperature and
pressure conditions but achieved with different thermodynamic paths. This will help to better account for the effect of piston trajectory and heat transfer on the autoignition during LTC model validation and improvement.

Additionally, by using special thermodynamic paths created by using a combination of rapid compression, piston dwell, creep and rapid expansion, it may be possible to improve the quality of direct measurement of key intermediate species which are otherwise difficult to detect. This will be a major aspect of the future investigations.

6.2.2 Investigation of trajectory based combustion control

The ability of the CT-RCEM to conduct performance analysis for a single cycle of an internal combustion engine has been demonstrated previously. This ability has been used for a case study to demonstrate that the CT-RCEM is capable of experimental investigation of the concept of trajectory based combustion control, previously proposed in our group [49], [58].

With the flexibility of piston motion due to the absence of a mechanical crankshaft based mechanism, the FPE offers great flexibility in terms of compression ratio as well as the shape of the piston motion profile. For trajectory based combustion control, the controllable piston trajectory in the FPE is used as a control means such that the instantaneous volume profile of the combustion chamber is used to shape the pressure and temperature history and thereby regulate the autoignition for each combustion cycle.
Extensive simulation work has been performed previously which shows the ability of trajectory based combustion control, enabled by FPE, to reduce engine-out emissions and increase engine thermal efficiency [49], [58]. The CT-RCEM offers the unique opportunity to experimentally validate the relative gain in efficiency and reduction in emissions offered by trajectory based combustion control. With the ability to precisely control the initial and boundary conditions, the experimental data obtained from the CT-RCEM for different piston trajectories would be invaluable for benchmarking study.
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