CFD ANALYSIS OF NOVEL VARIABLE COMPRESSION RATIO
ROTARY ENGINE

by

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Abstract

In compression ignition engines, the soot-NOx paradox is an extremely challenging unresolved issue. Homogeneous Charge Compression Ignition (HCCI) is one of the most promising solutions that combine the benefits of both Spark ignition and Compression ignition combustion modes. Fuel-lean premixed combustion helps to reduce or eliminate the formation of NOx and soot. HCCI engines have a high heat release rate at high load that results in knock. A unique variable compression ratio rotary engine based on the HCCI combustion mode (patented by Customachinery Inc) is under development at Queen’s University. The present study includes a computational fluid dynamics analysis of the air induction and compression, fuel injection, fuel and air mixing, and ignition process using Ansys Fluent. A unique dynamic mesh was adopted that allowed for the modeling of a fixed stator and rotating lobed rotor, as well as novel gates that extend and retract. A default Fluent fuel spray model was used and the optimum fuel injector location and orientation were determined. Two different combustion models (single-step and detailed chemistry) were investigated, and it was found that the results have significant differences. The detailed chemistry predicted a two-stage ignition process typical for heptane fuel that a single-step model cannot predict. The effect of other parameters such as compression ratio, fuel load, and fuel injection time on the ignition and combustion process were also studied.
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List of Abbreviations

IC = Internal combustion
ms = milliseconds
NTC = Negative Temperature coefficient
TDC = Top Dead Center
BDC = Bottom Dead Center
CI = Compression Ignition
HCCI = Homogenous Charge Compression Ignition
EGR = Exhaust Gas Recirculation
LTC = Low Temperature Combustion
DPM = Discrete Phase Model
SOI = Start of Injection
Chapter 1

Introduction

The invention of the internal combustion (IC) engine has had an intense impact on human life. The internal combustion engine is a small lightweight source of power. Internal combustion engines are used in many applications ranging from small model airplanes to big trucks and power generation stations. The most widely used application for IC engines is transportation. The basic principle of the IC engine remains the same, it converts the chemical energy contained in the fuel into mechanical work. The energy is released by combustion that also creates emissions via the exhaust gases. The efficiency by which the chemical energy is converted into mechanical energy is very important and governs the fuel economy of the vehicle.

1.1 Fuel Economy and Emission Standards

In simple words, fuel economy is defined as the power produced per unit mass of fuel consumed. It is one of the important factors that needs to be improved because fuel consumption plays a significant role in air pollution and consumption of the available fuel resources. Fuel energy is required to propel the vehicle and overcome vehicle drag and rolling resistance. There are many factors that affect fuel economy, such as, the aerodynamic design of the automobile, engine design, type of engine, usage pattern of vehicle etc.

The internal combustion engine produces exhaust, which contributes to air pollution due to presence of nitrogen oxides (NOx), soot, hydrocarbons, carbon monoxides, etc. Every country has emission standards, which regulates the permissible air pollutants released by the engine into the atmosphere. These standards are designed to preserve the air quality in the environment and to protect human health.

“According to the IEA, Canada’s CO2 emissions from fuel combustion in 2010 accounted for
approximately 1.8% of global emissions. Global emissions of CO2 from fuel combustion have increased by 44% between 1990 and 2010. Over the same period, Canadian CO2 emissions from fuel combustion have increased by less than 24%. Canada’s share of total global emissions, like that of other developed countries, will continue to decline in the face of rapid emissions growth from developing countries, particularly China and India. By 2005, China had overtaken the U.S. as the world’s largest overall greenhouse gas emitter, and in 2010 accounted for 24% of total global CO2 emissions from fuel combustion as shown in Figure 1.1.” [1]

Figure 1.1 Distribution of world carbon dioxide emission [1]

1.2 Basics of Internal Combustion Engines

Internal combustion engines produce mechanical power from chemical energy of the fuel. Energy is released from the burning of fuel in the presence of oxygen. Fuel-air mixture before combustion and burned products after combustion are the working fluids. There are different classifications of internal combustion engines, the most common being the spark ignition and compression ignition engines have
wide application in automotive and power generation due to their simplicity, higher power output and easily accessible fuel. Spark ignition engines are generally called gasoline (or petrol) engines and compression ignition engines are often referred to as diesel engines. The internal combustion engine can be classified by:

1. Fuel: gasoline, diesel, natural gas, liquid petroleum gas (LPG), dual-fuel, hydrogen
2. Working cycle: Four-stroke and two-stroke
3. Method of ignition: Spark ignition and compression ignition
4. Basic engine design: Reciprocating or rotary
5. Method of cooling: Air cooled, water cooled, uncooled

All of the above classifications are important but because this thesis approaches the engine design and emissions characteristics of internal combustion engines from a fundamental point of view, the method of ignition and engine design was selected as the key classifying feature. The remainder of this chapter will review the basic concepts of reciprocating engines.

### 1.3 Four Stroke Reciprocating Diesel Engine (Conventional Diesel Engine)

Reciprocating IC engines are the most widely used automotive engines. Power is transmitted through a connecting rod to the drive shaft by using the back-and-forth movement of the piston. Four stroke reciprocating diesel engines use compression for ignition of the fuel. Figure 1.2 shows the four strokes of the conventional diesel engines. Each thermodynamic cycle, that includes one power stroke, requires two complete revolutions of the crankshaft.
The following is a description of the processes that occur in each of the four strokes for a diesel engine; refer to the schematics in Figure 1.2:

**Intake stroke** - When piston starts moving from top dead center (TDC) to bottom dead center (BDC), the intake valve opens and air is drawn into the cylinder. Valve timings can be varied to increase or decrease the mass of air inducted.

**Compression stroke** - At the end of the intake stroke the intake valve closes and the piston starts moving from BDC to TDC. The air in the cylinder is compressed and the pressure and temperature increases. When the piston approaches TDC diesel is injected in the form of spray directly into the compressed air. The diesel fuel is ignited upon injection and the combustion process begins due to the high temperature of the air.

**Power stroke (or expansion stroke)** - The piston starts moving from TDC to BDC by the high pressure produced by the release of heat from the combustion of the fuel. This in turn forces the crank to rotate via the connecting rod. About five times as much work is done on the piston during the power
stroke compared to the work done by the piston during the compression stroke. As the piston reaches BDC, the exhaust valve opens to initiate the exhaust process and cylinder pressure starts to drop.

**Exhaust stroke** - This is the last stroke where all the burned gases are swept out by the piston when it moves from BDC to TDC. As the piston approaches TDC, the inlet valve opens and just after TDC the exhaust valve closes and the cycle starts again.

The four strokes described above can be modelled as an Air-standard Diesel thermodynamic cycle. The system is taken to be the air contained inside of the cylinder contained by a fixed single ended cylinder and a frictionless piston. Figure 1.3 shows the four thermodynamic processes involved in Diesel cycle on a PV and TS diagram.

**Figure 1.3 PV and TS Diagram of four stroke diesel engine**

**Process 1-2** Isentropic compression: In this process, the piston moves from BDC to TDC. Air is compressed isentropically inside the cylinder during which time work is done on the system. During this process entropy remains constant.
Process 2-3 Constant pressure heat addition: heat is added at constant pressure from an external heat source whereby work is done by the system on the piston. $Q_{in} = mC_p(T_3 - T_2)$

Process 3-4 Isentropic expansion: Pressure of air decreases in this process and work is done by the system.

Process 4-1 Constant volume heat rejection: This constant volume heat rejection process is used to complete the cycle

The compression ratio is defined as the ration of swept volume to the clearance volume ($V_1/V_2$), is an important parameter that governs the cycle efficiency and in an actual engine controls the start of ignition.

CFD analyses can be used to demonstrate the effects of various engine parameters on engine performance. Umakant and Vivek [3] worked on the combustion analysis of direct injection diesel engine using ANSYS Fluent. The fuel spray was modeled in using a spray breakup model, wall spray interaction model and turbulence model as well. The diesel combustion was modelled using the species model with a single reaction model. Rate of pressure rise and heat release rate were calculated. The CFD results showed good agreement with experimental results, as shown in Figure 1.4.

![Figure 1.4 Rate of pressure rise versus crank angle [3]](image-url)
Brijesh and coworkers [4] performed a parametric study on the combustion and emission characteristics of CI engine. They showed that at lower compression ratios, production of NO decreases drastically while specific fuel consumption increases and soot emissions increases. Change in spray cone angle was shown to have no effect on emissions. Increased injection pressure, and hence small injection duration, proved to increase both NO and soot. Figure 1.5 shows the Nox and soot formation and specific fuel consumption for varying compression ratios.

![Figure 1.5 (a) Emissions and (b) ISFC comparison for different compression ratio](image)

1.4 Homogenous Charge Compression Ignition (HCCI)

HCCI engines have a similar configuration as conventional diesel engines but they work by a different combustion mode. Figure 1.6 shows the difference in fuel air mixing and combustion in Gasoline, Diesel and HCCI engines. In a gasoline spark ignition engine, the fuel is sprayed and mixed with the air in the intake system (commonly referred to as port injection). As a result, combustion occurs in a fuel-air premixed state with flame propagation from the spark plug. In conventional diesel engines, fuel is injected directly into the cylinder. In comparison to spark ignition engine, the fuel is not uniformly mixed into the air. The liquid fuel evaporates first around the periphery of the spray where it premixes with the air. Diesel combustion includes rich premixed combustion (near the injection point) that is responsible for producing soot; and diffusion flame combustion where combustion occurs at stoichiometric conditions producing very high temperature which creates NOx in to the exhaust gases [5].
NOx and Soot are the most harmful pollutants in the engine exhaust, which needs to be reduced for cleaner combustion and exhaust. Diesel engine emissions are difficult to control because measures taken to reduce soot, such higher combustion temperature, increases the amount of NOx, or vice versa.

![Figure 1.6 Air-fuel distribution in Gasoline, Diesel and HCCI engines [5]](image)

HCCI combines characteristics of conventional gasoline engine (premixed combustion) and diesel engines (compression ignition). Fuel is homogenously mixed throughout the volume. This can be achieved by different ways, such as using port injection to form a premixed fuel air mixture, or early fuel injection during compression. HCCI engines can work with variety of fuel, which has significant effect on both design and control strategy for the engine [6]. The system features lower-temperature lean premixed-combustion compared to ordinary gasoline engines, resulting in nearly no NOx emissions. There is no soot formation because there are no fuel rich areas in the cylinder.

HCCI offers the highest potential heat efficiency among internal-combustion engine systems, leading to projections of major cuts in CO2 emissions [6]. Majid and Reza [7] did a parametric study for the reduction of emissions and improvement in the efficiency of HCCI combustion. A few important
parameters like injection timing, equivalence ratio, injection rate profile and exhaust gas recirculation (EGR) were investigated. From the studies conducted, they concluded that emissions increased with increase in equivalence ratio, and early injection helps to lower the NOx emissions. They also showed that the injection rate shape can change the start of combustion. Due to reducing temperature and amount of oxygen in cylinder, EGR rate is very useful to decrease NOx emissions.

Magnus and coworkers [8] demonstrated the multi-fuel capability of a HCCI engine with variable compression ratio. The study was performed with a single-cylinder reciprocating engine with a modified cylinder head. Variable compression ratio was used to get auto-ignition at TDC without preheating of inlet air. Specifically, the compression ratios for each fuel were: 11:1 for n heptane, 21.5:1 for iso-octane and 22.5:1 for gasoline.

Current HCCI technology allows clean efficient stable combustion at low and middle load conditions. Hyvonen et al. [9] characterized the operating range, in terms of load and engine speed, of a four stroke multi-cylinder engine with variable compression ratio capabilities and preheating of the inlet air. They showed that to increase the combustion efficiency at intermediate and high speeds, or at intermediate loads, lower compression ratios are used; whereas, at low loads, maximum compression ratio and high initial temperature of air is used to increase the combustion efficiency.

At high load conditions the high heat release rate produces “knock,” which is associated with an undesirable rate of pressure rise that can damages the engine. Current HCCI research is focused on extending the operating range using novel approaches, including charge stratification and exhaust gas recirculation (EGR)-diluted low temperature combustion (LTC). Karthikeya [10] et al. experimentally studied the effect of different parameters like swirl ratio, EGR, equivalence ratio, piston design and engine speed to control the peak pressure of an HCCI engine. The results show that the use of higher EGR concentration, lower engine speeds, reduced equivalence ratios and increased swirl ratios result in a reduction of the peak cylinder pressure.
Conventional SI combustion is dependent on flame propagation, whereas diesel combustion is highly dependent on fuel-air mixing. HCCI combustion is mainly governed by chemical kinetics, with little influence from the flow conditions. HCCI combustion is driven by the temperature, in-cylinder pressure and chemical composition of the charge [11] [12] Because of this, CFD gives nearly realistic results when detailed chemical kinetics is used to model combustion. [6]

The following points summarize the advantages and limitations of HCCI engines over conventional gasoline and diesel engines.

1.4.1 Advantages of HCCI engines

1. HCCI engines are low temperature combustion engines due to its fuel lean combustion. It works on diesel like high compression ratios which helps to achieve around 30% higher efficiency as compared to gasoline engines.

2. The use of fuel-lean homogenous mixture gives low combustion temperature compared to typical SI engines that operate at stoichiometric conditions. As a result, NOx levels are almost negligible. There is no incomplete combustion, typical of fuel-rich combustion, which produces soot particles. So HCCI engines are basically high efficiency, low emission internal combustion engines.

3. HCCI engines can be operated with gasoline, diesel and most of the alternative fuels due to the advantages [6].

4. Since there is no throttle HCCI engines don’t have any pumping loses which improves efficiency in comparison with SI engines.

1.4.2 Limitations of HCCI engines

1. Due to constant volume combustion HCCI engines have very high pressure rise rates (associated with high heat release rates) at high loads where the mixture approaches stoichiometric conditions
that increases the knock tendency which is not good for an engine. High rate of pressure rise causes the engine to wear and decreases engine life.

2. Ignition control is the main problem with HCCI engines. Ignition is very sensitive to intake air temperature which may be different in each cylinder. EGR and variable compression ratio are the two main techniques to control the start of combustion [6].

3. Cold start is sometimes difficult for HCCI engine because it operates under fuel-lean conditions.

4. HCCI engine works on lean fuel mixtures and low combustion temperature, which leads to incomplete oxidation. So, pre-catalyst emissions like carbon monoxide and hydrocarbons are higher than the typical diesel engines.

1.5 Rotary Engines

Rotary engines have a long history dating back to 1588, when Italian inventor Agostino Ramelli invented a rotary piston type water pump. In 1759, James Watt invented the first steam powered rotary engine. In 1954, in cooperation with German auto company NSU, Dr. Felix Wankel created a rotary internal combustion engine. [13]. The Cosmo Sport, which Mazda released in May 1967, was the first dual-rotor rotary engine car. Mazda began using rotary engines in its sedans and coupes in 1968, and the vehicles hit the U.S. market in 1971. In addition to Mazda, a number of other companies licensed the Wankel engine during the 1960s and 1970s, including Daimler-Benz, Alfa Romeo, Rolls Royce, Porsche, General Motors, Suzuki and Toyota. Rotary engine research slowed down for a few decades because of the low efficiency of the engines, although Mazda continued to develop the rotary engines for automobiles until tightening of the emission standards stopped their production. The rotary engine studied in this thesis does not use the same technology as the Wankel engine (other than it is a rotary engine and uses very similar sealing techniques), and therefore only broad aspects of the Wankel engine will be reviewed. One of the main advantages of the rotary engines is it possesses higher power to weight ratio compared to reciprocating engines. Rotary engines are comparatively quieter than the reciprocating
engines because they use ports for gas intake and exhaust valves and their associated drivetrain. Rotary engines use a balanced mechanical design that produces less vibration compared to reciprocating engines; which includes a reciprocating piston that produces inertial forces at TDC and BDC where acceleration is maximum. Thermal efficiency of the Wankel engine is lower because it operates as a spark ignition engine and thus the compression ratio is lower than that of a diesel reciprocating piston engine.

There are several CFD research papers in the literature on the rotary IC engine that are pertinent to the rotary engine studied here. For example, Asela [13] performed a CFD analysis of a direct injection spark ignition rotary engine. The basic concept of the Wankel engine was investigated computationally to study the optimization of fuel injectors and spark locations resulting in optimum power output. The turbulence models, injection modeling and discretization techniques used are relevant to this study and will be discussed in detail in the Chapter 2. Also of use is the pre- and post-processing for the CFD results.

Michael [14] performed a computational investigation of a HCCI rotary engine. A CFD analysis of a 3D rotary engine was performed to study the feasibility of HCCI combustion in such an engine. A parametric study was performed to observe the effect of pressure, equivalence ratio, engine speed, temperature on the HCCI combustion. The study showed that the amount of premixed fuel within the chamber significantly affects the pressure and temperature rise within the chamber. Variations of the test parameters resulted in auto-ignition of n-heptane fuel, governed by the fuel-air reaction kinetics, resulted in a consistent ignition time over the engine speed range. Michael [14] also showed that the HCCI rotary engine is more fuel efficient and produces less emissions than a spark ignition rotary engine.

The rotary engine studied does not use the same technology as the Wankel engine and therefore its operating principles will not be reviewed.
1.6 Fanara Rotary Engine

The patented design of a rotary engine that approaches the Homogeneous Charge Compression Ignition (HCCI) combustion mode is an initiative by the Canada based start-up company Customachinery Inc. The research and development activities conducted have resulted in two provisional patent applications (April and August 2014), then combined in a Patent Cooperation Treaty (PCT) application the following year (March 2015). Mr. Fanara actively sought academic partnerships to further development of the patent pending proprietary technology. This thesis is based on the project initiated between Customachinery and Queen’s University to perform a CFD study of the operation of the engine. Figure 1.7 shows the 3D printed model of a Fanara rotary engine.

![3D printed Fanara rotary engine model](image)

**Figure 1.7 3D printed Fanara rotary engine model [15]**

A schematic showing the basic engine concept is shown in Figure 1.8. The engine consists of a stator that remains fixed and a rotor with a lobe that rotates and is connected to the output shaft. There are two gates at the top of the engine (intake gate to the left and the exhaust gate to the right) that are opened and closed during different phases of the cycle. One of the novelties of the engine is the ability to vary the compression ratio in real time by varying the height of the combustion gate (located between the intake
and exhaust gates). A cycle consists of four processes similar to a four-stroke engine. Air is inducted into the left side of the combustion chamber through an intake port and fuel is injected via an injector (see Figure 1.8 #1 and #2). The fuel-air mixture is compressed as the volume between the rotor lobe and the intake gate decreases (see Figure 1.8 #3). Combustion starts once the autoignition temperature is reached and combustion occurs at roughly constant volume (see Figure 1.8 #4). The high pressure and temperature combustion products expands pushing on the rotor lobe (see Figure 1.8 #5). Once the rotor lobe passes the exhaust port, the high-pressure combustion products blowdown to a final pressure of 1 atmosphere. Not shown in the schematic is that at some point during the expansion processes the exhaust gate opens and the intake gate closes trapping exhaust gas (commonly referred to as residual gas) enclosed between the three gates. The cycle is completed with one full rotation of the rotor, similar to a two-stroke engine, resulting in more power compared to a four-stroke engine.

The Fanara rotary engine is a low emission engine as it employs the fuel-lean mode of combustion. However, unlike the HCCI engine the Fanara rotary engine has good ignition control due to its ability to vary the compression ratio in real time using the combustion gate position. Variable compression ratio allows the engine to operate with varying load applications. Due to the high compression ratio, thermal efficiency is predicted to be similar to that of a conventional diesel engine. Gate timing is an important feature of the Fanara rotary engine, e.g., the amount of residual gas can be varied by changing the gate timing on the fly. The suggested strategy is particularly useful when transitioning from low to higher load regimes. At high load conditions, lower compression ratios and higher residual values are necessary to minimize the risk of knock.
Figure 1.8 Engine Concept of Fanara Rotary Engine [15]
Chapter 2

Methodology

In this study a concept design of a rotary type compression ignition engine was investigated with the objective to establish the optimum fuel injector location and orientation based on the analysis of the fuel and air mixing and combustion processes. Experimentally, it is very expensive and time consuming to test different designs. The most practical and economical approach is to model the engine, including fuel injection, using CFD. In the present study AutoCAD was used for the 2D modeling of the flow volume, Ansys Gambit was used to generate a computational mesh and Ansys Fluent 17.0 was used for carrying out the flow simulation. CFD techniques are very useful when it comes to design optimization. CFD is a tool that is used for efficiently predicting what happens under a given set of circumstances, i.e., it can quickly answer many ‘what if’ questions. It can predict how a design will perform, and allow testing of many variations, eventually arriving at an optimal design.

CFD is beneficial because it can simulate real engine operating conditions in a shorter time than experiments. Ansys 17.0 workbench has a built-in code Fluent, that has many functions to solve different fluid mechanics problems. Fluent has different fluid functions to model turbulence, heat transfer, combustion, fuel injection, etc. The turbulence, combustion and injection models were used for modeling the fuel and air mixing, compression and combustion within chamber.

2.1 Turbulence Modeling

In 1937, Taylor and von Karman proposed the following definition of turbulence:

"Turbulence is an irregular motion which in general makes its appearance in fluids, gaseous or liquid, when they flow past solid surfaces or even when neighboring streams of the same fluid flow past or over one another" [16].

Most flows occurring in nature and in engineering applications are turbulent. In general, turbulence is a continuum phenomenon which is governed by the equations of fluid mechanics. Turbulence modeling
is the construction and utilization of a model to consider the effects of turbulence. A turbulent fluid flow has features on many different length scales, which all interact with each other. A typical approach is to average the governing equations, to address the large-scales and non-fluctuating features of the flow. However, the effects of the small-scales and fluctuating components must be modeled. Turbulence models are categorized as zero-equation model, one-equation model, two-equation model and second-order closure models. Two-equation models are most widely used for solving engineering and analysis research problems. These models provide self-governing transport equations for both the turbulence length scale and the turbulent kinetic energy (k). With the specification of these two variables, two-equation models work without the requirement of additional information on the turbulence for a given flow scenario. The k-ω and k-ε are two-equation turbulence models which are widely used to solve industrial fluid dynamic problems.

2.1.1 k-ε Turbulence Model

The k-ε turbulence model utilized in the present study is the most widely utilized CFD model to simulate mean flow characteristics for turbulent flow conditions. The novelty of the k-ε model was to amend the mixing-length model and to find a substitute to algebraically model the turbulent length scales in moderate to high turbulent flows. Unlike earlier turbulence models, k-ε model addresses the mechanisms that affect the turbulent kinetic energy, i.e., the mixing length model lacks this kind of generality. The underlying assumption of this model is that the turbulent viscosity is isotropic, in other words, the ratio between Reynolds stress and mean rate of deformations is the same in all directions.

The exact k-ε equations contain many unknown and unquantifiable terms. Being more practical to the problem, the standard k-ε turbulence model is utilized which is predicated based on the understanding of the pertinent processes, thus reducing unknowns and presenting a set of equations which can be applied to an extremely large number of turbulent applications. [17]
For turbulent kinetic energy $k$,

$$
\frac{d}{dt}(\rho k) + \frac{d}{dx_i}(\rho ku_i) = \frac{\partial}{\partial x_j}\left[\mu_t \frac{\partial k}{\partial x_j}\right] + 2\mu_t E_{ij}E_{ij} - \rho \varepsilon \quad (1)
$$

For dissipation $\varepsilon$,

$$
\frac{d}{dt}(\rho \varepsilon) + \frac{d}{dx_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j}\left[\mu_t \frac{\partial \varepsilon}{\partial x_j}\right] + C_1\varepsilon E_{ij}E_{ij} - C_2\rho \frac{\varepsilon^2}{k} \quad (2)
$$

These equations can be interpreted as:

Rate of change of $k$ or $\varepsilon$ + Transport of $k$ or $\varepsilon$ by convection

= Transport of $k$ or $\varepsilon$ by diffusion + Rate of production of $k$ or $\varepsilon$

- Rate of destruction of $k$ or $\varepsilon$.

where,

$u_i$ represents velocity component in corresponding direction

$E_{ij}$ represents component of rate of deformation

$\mu_t$ represents eddy viscosity

and the Fluent default values for the constants are:

$C_\mu = 0.09, \sigma_k = 1.00, \sigma_\varepsilon = 1.30, C_{1\varepsilon} = 1.44, \text{ and } C_{2\varepsilon} = 1.92.$

2.1.2 Realizable $k$-$\varepsilon$ model

The Realizable $k$-$\varepsilon$ model represents an improvement over the standard $k$-$\varepsilon$ turbulence model. It is a relatively modern development and differs from the standard $k$-$\varepsilon$ model in two approaches. The realizable $k$-$\varepsilon$ model contains a formulation for the turbulent viscosity and a transport equation for the dissipation rate, $\varepsilon$, which is derived from an exact equation for the transport of the mean-square vorticity fluctuation. The benefit of the realizable $k$-$\varepsilon$ model is that it provides more accurate predictions of the spreading rate of both planar and round jets. Additionally, it exhibits noteworthy
performance for flows involving rotation, boundary layers under strong adverse pressure gradients, disunion, and recirculation. Realizable k-ԑ demonstrates the ability to capture the mean flow around intricate structures. The realizable k-ԑ model includes a few extra terms like the generation of turbulence kinetic energy due to the mean velocity gradients, the generation of turbulence kinetic energy due to buoyancy and the contribution of the fluctuating dilatation which are not considered in standard k-ԑ model. [17]

2.2 Injection Modeling

Ansys Fluent has built-in models to simulate fuel injectors and spray patterns. In the present study the Discrete Phase Model (DPM) was used to model the spray in the form of droplets, with the appropriate breakup models for the formed droplets. A Lagrangian-Eulerian multi-phase formulation was utilized to simulate the interaction of the discrete and continuous phases. The Navier-Stokes equations are solved for the continuous gas phase using a turbulence model. At each time step, the Eulerian approach defines the flow parameters such as velocity components, pressure, density and temperature as a function of position (x,y) for the entire two dimensional flow domain. In a Lagrangian description, the droplets are assumed as single mass particles, the velocity of which is decelerated by aerodynamic interaction of the gas and droplet, the mass of which is decreased by evaporation, etc. The two phases continuously exchange momentum, energy and mass. These exchanges are accounted for by applying source terms in the conservation equations of the gas phase in each grid cell. On the other hand, the gas phase affects the dispersed liquid by employing the local values of temperature, gas velocity, etc., in the grid cell through which the droplet is passing at each time step as a boundary condition. In Eulerian-Lagrangian method it is assumed that the volume fraction of the discrete phase is small compared to the continuous phase.

The Fluent default standard wall function is used to treat the turbulence effects at the wall.

2.2.1 Type of Injection
While using the DPM model, there is no need to physically model a fuel injector for the injection of diesel spray. There are different types of injection available in the Fluent injection model. They are mainly surface injection, group injection, cone injection, pressure orifice atomizer, single injection, flat fan atomizer, and air blast atomizer. A few of them are only available while simulating for 3D problem. For the present study, Group injection is used, where fuel is injected from a point called fuel injector as shown in Figure 2.1.

![Figure 2.1 Types of injection](image-url)
The injection of fuel is in the form of droplets, which will interact with the continuous phase air and some of them will evaporate and will be converted into gas phase. In the injection panel, the properties of the injection are filled in to create a custom injection.

2.2.2 Injection Properties

After deciding on the injection type, injection properties are defined. In the present study group injection with 10 number of streams is used. For group injections, the initial positions of the particles are the location of the data points. Total Flow Rate of all particles released from the stream is defined.

For distribution of droplet diameters, there are again two available options in FLUENT. The options are uniform distribution and non-uniform distribution of the particle diameters. Generally, for a real flow study, we select the non-uniform distribution of the droplet diameters. If we have the experimental data for the range of the droplet diameter, we can easily give the minimum and the maximum diameter for the droplets and the range of droplets diameters. The main parameter is droplet diameter that has to be chosen very carefully for the proper mixing and combustion of fuel. A non uniform size distribution can be used for variable droplet diameter range.

2.2.3 Rosin-Rammler Diameter Distribution Model

The Rosin-Rammler size distribution is available for group injections. While using one of the Rosin- Rammler distributions, we designate a few more parameters under Point Properties, like minimum, maximum and mean diameter of droplets and Spread parameter. Injection is in the form of streams of particles, with diameters selected by the Rosin-Rammler distribution function. The total number of injection streams tracked is equal to the number of diameters in each distribution multiplied by the number of mesh faces on the injection surface.

2.2.4 Spray Sub Models

Spray sub-models have been implemented to account for the effects of coalescence, evaporation and droplet break-up in the fuel spray simulation. These sub models help to generate the realistic effect of fuel
spray. In the present simulation, Tylor Analogy Breakup (TAB) breakup model is used for consideration of the droplet breakup. Droplet evaporation is also considered which is been solved by defining the evaporation fuel species within injection properties. In addition, pressure and temperature dependent boiling option is enabled to account for the effects of pressure and temperature on the vaporized fuel when it reaches to boiling point.

The present study uses unsteady particle tracking with spray sub models as pressure and temperature dependent boiling and TAB droplet breakup model. The droplet distribution is Rosin Rammler distribution method with the minimum droplet diameter as 0.1 μm, maximum diameter 5 μm and mean diameter 2.68 μm. Group injection with the 10 number of streams is used which means that 10 different diameters of fuel droplet to be injected at a same time. [18]

2.3 Combustion Modeling – Species Model

Fluent 17.0 has five different models to simulate the combustion for different situations. These models are the species model, the non-premixed combustion model, the premixed combustion model, the partially premixed combustion model and the composition PDF transport model. The species model is a generalized model which has ability to model many different situations, whereas other models are case specific. For example, the non-premixed model is used when fuel and oxidizer are initially not premixed, whereas premixed and partially premixed models are used when fuel and oxidizer are premixed or partially mixed when they enter the combustion chamber. In this study, the species model was used, it can model premixed and non-premixed conditions. The Fanara rotary engine is an HCCI-like engine which can be operated with premixed air and fuel, as well as air intake with direct fuel injection. Direct fuel injection was considered in this study. Although a few case studies were performed with premixed air and fuel under adiabatic constant volume and variable volume conditions.

2.3.1 Single Reaction Model
Fluent 17.0 contains a few default reaction mechanisms for modeling combustion. One of them is a single reaction mechanism. The Fluent database has predefined single-step (or a global reaction) reaction mechanisms for a few hydrocarbons. The single-step reaction mechanism calculates the final products complete combustion products. For example, when a hydrocarbon reacts with air, it produces carbon dioxide and water as a final product. If we consider a real scenario, these final products are generated after many intermediate reactions, involving intermediate species, before the final products are produced. For large hydrocarbons, such as n-heptane, thousands of intermediate reactions and species are involved in the production of CO₂ and H₂O. The single-reaction model does not account for any intermediate species.

For the reaction of n-Heptane and air, the single-step reaction mechanism involves the following reaction equation:

\[ C_7H_{16} + 11(O_2 + 3.76N_2) = 7CO_2 + 8H_2O + 41.35N_2 \]  \hspace{1cm} (3)

Where the reaction rate is defined as:

\[ d[C_7H_{16}]/dt = kT^n[C7H16]^a[O2]^b \]  \hspace{1cm} (4)

\[ k = Ae^{(-Ea/RT)} \]  \hspace{1cm} (5)

Where,

\[ A = \text{Pre-exponential factor} \]

\[ E_a = \text{Activation energy} \]

\[ R = \text{Universal gas constant} \]

\[ T = \text{Temperature} \]

\[ n = \text{Temperature exponent} \]

The single-reaction model is not accurate as it does not account for intermediate reactions and intermediate species. Although it is useful for approximate predictions, as part of a parametric study,
because it requires less computational power. It is possible to change the reaction parameters (like pre-exponential factor, temperature exponent, stoichiometric exponents within this model) based on experimental results. The single-reaction model was used as part of a parametric study.

2.3.2 Turbulence Chemistry Interaction Model

The species transport equation has a source term which models the turbulence chemistry interaction. It predicts the change in reaction rate due to turbulence in the flow. There are a few built-in models for calculating the turbulence chemistry interaction. The models include:

1. Laminar finite rate model: This model calculates the chemical source term using Arrhenius expression, which ignores the effects of turbulent fluctuations. This model is mostly suitable for laminar flows, or flows with very low turbulence.

2. Eddy dissipation model: In this model, the chemical reaction rate is governed by large eddy mixing time-scale and combustion proceeds in the presence of turbulence. This model is computationally cheaper.

3. Eddy dissipation concept (EDC) model: This is an extension of the eddy dissipation model, and incorporates the detailed chemical mechanism in turbulence flows. It assumes that the reaction happens at fine-scales. This model uses the added source term to accurately predict the reaction rates considering effect of the turbulence. The mechanism is very stiff and computationally time consuming to integrate in a numerical simulation.

The EDC model (the most accurate model) was used to model the turbulence chemistry interaction. The model was used because high turbulence, generated by the fuel injection, exists in the combustion cavity.

2.3.3 Detailed Chemistry Model

In reality, the reaction proceeds through elementary reactions in a chain process known as chain reactions. The Species Model allows simulating the detailed chemistry that takes place during
combustion. It requires a reaction chemistry file in CHEMKIN format. CHEMKIN is a file format which contains chemical kinetics and thermodynamic data file for the chemical reaction. A thermodynamic data file, that contains thermodynamic data for each species, is also required. The chemical kinetics mechanism consists of a set of elementary reactions, and species that are produced during the elementary reactions. It reaction proceeds with chain initiation, chain propagation, chain branching and chain termination. An example of the reaction mechanism is provided below.

\[
\begin{align*}
H_2 + M &\rightarrow H + H + M \quad \text{Chain Initiation} \\
H + O_2 + M &\rightarrow HO_2 + M \\
HO_2 + H_2 &\rightarrow H_2O + OH \quad \text{Chain Propagation} \\
OH + H_2 &\rightarrow H_2O + H \\
H + O_2 &\rightarrow H_2O + H \quad \text{Chain Branching} \\
H_2 + O &\rightarrow OH + H \\
H + OH + M &\rightarrow H_2O + M \\
H + H + M &\rightarrow H_2 + M \quad \text{Chain Termination} \\
O + O + M &\rightarrow O_2 + M
\end{align*}
\]

where \( M \) is any species present that acts a collision partner.

A detailed chemistry model considers all (or a reduced number of) elementary reactions and predicts more accurate results. However, this method is very time consuming as compared to single-reaction model.

**2.4 Case Studies: Detailed Chemistry Model**

As described in the previous Section, two chemistry models (single-step and detailed chemistry) are available in Fluent. Both models were used in the study. For the detailed chemistry model the reduced University of Wisconsin n-Heptane mechanism (containing 29 species and 52 reactions) was used. There are many such mechanisms available, but as the number of species and number of reactions increases, simulation time goes up. Since the engine geometry and the use of the dynamic mesh requires large
computation power, the detailed chemistry model was used sparingly in this study. The following two case studies were carried out to see how the two models performed.

Case study I: Adiabatic Constant Volume

The main purpose of this case study was to see if the detailed chemistry model works correctly. The constant volume temperature time-history predicted by Fluent was compared to that from the combustion-specific commercial code Cosilab. The simulation involved an adiabatic box (5mm x 10 mm) initially containing a quiescent stoichiometric mixture of n-heptane and air at an elevated initial temperature. The simulation was carried out for three different initial temperatures, i.e., 1000 K, 900 K and 800 K. The Wisconsin reduced n-Heptane kinetics mechanism contained 29 species and 52 reactions. For all three cases the temperature-time history was obtained and compared with the predictions from Cosilab. The results are shown in Figure 2.2

![Figure 2.2 Time versus temperature for initial temperature (a) 1000 K (b) 900 K and (c) 800 K](image-url)
The Fluent results are little offset in time relative to the results obtained from Cosilab. The Fluent predicted temperature-history looks the same as predicted by Cosilab, specifically there is an induction period where recombination reactions taking place that result in energy release. The main energy release that results in a large increase in temperature is preceded by a small temperature rise associated with “cool flame” phenomenon typical of large hydrocarbon chemistry. For all three initial temperatures simulated, Fluent predicts a shorter ignition time (time to the start of the large temperature rise) than Cosilab, the reason for this is not clear. For 1000 K and 900 K initial temperatures, ignition time difference between Fluent and Cosilab is 0.05 ms, whereas for 800 K the ignition time difference is 0.1 ms.

2.4.1 Case Study II: Adiabatic Compression

The second case study was an adiabatic box (5mm x 10mm) with the left wall moving to the right, starting at 0 ms and stopping at 5 ms. This is a piston cylinder type of arrangement with compression of the gas mixture without any leakage. The simulation was initialized with stoichiometric n-Heptane-air mixture at an initial temperature of 633 K. The mixture gets compressed and eventually ignites. The detailed chemistry and single reaction model results were compared. The temperature contour shown in Figure 2.3 demonstrates how the temperature rises uniformly (a very narrow temperature range is shown in the contour colour legend) throughout the volume as the left wall moves.

![Figure 2.3 Temperature rise (K) with compression](image)

Ignition occurs at 2.7 ms uniformly throughout the volume. The rise in temperature is plotted in Figure 2.4 for the detailed-chemistry and the single-reaction model. As observed in the constant volume
combustion simulation, the detailed-chemistry model predicts a two-step ignition process, whereas the single reaction model is not able to reproduce the small initial temperature rise event. In addition, the ignition time predicted using the detailed chemistry model is about 1.3 ms shorter than that with the much simpler single-step model.

![Figure 2.4 Temperature versus time for (a) detailed chemistry (b) single reaction model](image)

2.5 Solver Setting

The unsteady pressure based SIMPLE solver was used for the flow simulation. Preliminary simulations were carried out with a time-step size of $1 \times 10^{-5}$ s, however, it was determined that the chemical reaction was not properly captured. After few simulations with varying time-step size, $5 \times 10^{-6}$ s was found to be the best time-step size for the simulations. The particle tracking time-step for fuel droplets was kept the same as flow time-step. The Green-Gauss cell based option was selected for the gradient. Standard wall function is used to treat the turbulence effects at the wall. Pressure was solved by the standard and PRESTO scheme, whereas all other equations like conservation of density, momentum, species, turbulent kinetic energy and energy were solved by first order upwind discretization scheme. The species transport equation and discrete phase model were solved simultaneously, which makes the simulation unstable at times. Correctly chosen under relaxation factors helped to converge and stabilize the solution. At the start of the simulation, under relaxation factors were fixed to the default value of 0.9 and then they were varied whenever the solution became unstable.
Chapter 3

Modelling and Meshing

The general procedure for the analysis is to create a solid model from which a mesh with finite number of elements is imported into the Fluent solver. A 3D model of the rotary engine was provided by the sponsor, see Figure 3.1

3.1 Modeling

Computationally complex three-dimensional engine models need to be simplified in a way that can be used in a flow analysis. The rotary engine under investigation lends itself nicely to a two-dimensional analysis. The two-dimensional flow domain replicates the engine flow paths on an XY plane. Dimensions for the flow domain were obtained from an AutoCAD drawing, shown in Figure 3.1, of the rotary engine provided by the sponsor.

Figure 3.1 3D AutoCAD model of the rotary engine

The rotary engine geometry is very complex and the combustion process requires a very short time-step. As a result, based on the computational power available a three-dimensional model was not possible.
Instead a two-dimensional flow model that includes the stationary stator, rotating lobed rotor, and sliding compression gate was created, see Figure 3.2. The main assumptions, implicit with the two-dimensional model, is that it neglects the side-wall friction effects and three-dimensional flow-field produced by the fuel injection. The size of the combustion chamber, defined by the square cavity at the top. All the simulations start when the rotor lobe position is at the bottom position.

![Figure 3.2 Two-dimensional simplified Fanara rotary engine](image)

The dimensions of the different parts of the engine are shown in Figure 3.3. The size of the combustion chamber is 8 mm x 3.74 mm. Size of the engine was based on a prototype manufactured by Customachinery. As a part of the parametric study, the compression ratio of the engine was changed by varying the height of the combustion chamber. The stator diameter was 60 mm and the rotor diameter was 40 mm. In an actual engine, seals would be located at the tip of the rotor lobe and between the bottom of the compression gate and a rotor. In the Fluent mode no seal exists, there is a small gap in between compression gate and a rotor as well as rotor and a stator producing a single zone for the entire engine. The gap is required to model the rotation of the rotor and movement of the gate. The gap dimension is
0.25 mm between the rotor lobe and the stator and as well as between the gate and the stator (minimum gap dimension). This gap size is substantially larger than the prototype gap dimension of 5 micrometer. The 0.25 mm was chosen to allow at least two elements in the gap at the start of the computation, diminishing the gap size would require a substantial increase in the number of computational elements.

**Figure 3.3 Model Dimensions**

### 3.2 Meshing

Meshing is the most important step in any flow analysis, as the results are dependent on the mesh quality. Ansys Gambit is used to generate the mesh from the AutoCAD drawing. The flow volume was divided into a finite number of computation volumes where tri- and quad-elements can be used for 2D meshing. Tri-elements are easy to fit into complex geometries, whereas quad-elements are good for simple geometries. Meshing of the engine was done using tri-elements with a “pave scheme” that is available in Gambit. A total number of 298,000 elements were used to create a fine mesh, and 178,000 elements were used in a coarse mesh. The small gap in between the rotor and stator and the rotor and...
bottom of a compression gate were meshed with a minimum of three mesh elements. Figure 3.4 shows the meshing of the two gaps.

![2D Mesh for Fanara rotary engine](image)

**Figure 3.4 2D Mesh for Fanara rotary engine**

### 3.2.1 Mesh Motion

The rotary motion of the rotor was modeled using a “moving mesh”. The concept of a moving mesh can be accomplished by the dynamic mesh option in Ansys Fluent. First the equation of a rotor rotation and the user defined function is generated to import into Fluent which can model the rotation of a rotor. Fluent provides several options for dynamic mesh like smoothing, remeshing and layering. Smoothing and remeshing were used for rotary engine meshing. The rotor and bottom gate are considered as rigid body whereas the side gate is considered as a deforming body. Lifting of the compression gate is modeled by a user-defined function that makes the bottom of the gate that follows the surface of the rotor and lobe. The mesh nodes are fixed to the stator surface and the rotor surface. When the mesh moves along with the rotor, the mesh elements get stretched, so remeshing is enabled which allows the mesh to regenerate under a set of constraints. The constraints under which the mesh gets regenerated are maximum length
scale, minimum length scale and maximum allowable skewness. Maximum allowable skewness is kept 0.7 for a mesh generated. Figure 3.5 shows the dynamic meshing that takes place between the rotor and the stator as the rotor moves and the stator remains fixed.

Figure 3.5 Moving mesh

3.3 Effect of Mesh Density

For any simulation, it is necessary to check if the results are independent of the number of mesh elements in the computational domain. If the number of mesh points are less than the required, the
resulting accuracy gets compromised. However, if the mesh is too fine more time is required for the simulation to be completed making it more computationally expensive. Grid Independence is tested with a few simulations with different number of mesh elements, aspects of the results are compared with each other and the optimum number of mesh elements are found resulting in maximum accuracy with an acceptable amount of computational time.

In this simulation, there are three important phenomena that must be considered. Firstly, the compression phase that raises the pressure and temperature in the combustion cavity that has a large effect on the ignition time, secondly, the flow-field at the time of fuel injection that governs fuel and air mixing, lastly, the combustion progress following ignition. On this last point, if it is premixed constant volume combustion the flow field including level of turbulence is not important; however, if it is turbulent flame propagation then reproducing the turbulent flow-field would be important.

In this section, the effect of mesh density on the compression process will be considered. The most important effect is the gas leakage rate through the gap between the stator and the rotor, and the rotor and the bottom of the compression gate. The leakage will be characterized by the deviation of the average volume temperature versus time before fuel injection takes place (20 ms in later simulations). Three different mesh densities were investigated, i.e., simulations were carried out with 298K, 178K and 107K elements under adiabatic wall conditions, same turbulence model, and the same rotor velocity. The meshing of the gap between the compression gate and the rotor for the 178K and 298K simulations is shown in Figure 3.6. As can be seen there are extra elements across the gap for the 298K simulation.

![Figure 3.6 Mesh elements across the gap between rotor and gate for (a) 178K elements (b) 298K elements](image-url)
The gas volume was calculated for the rotor position at each time step. The constant mass (no leakage) theoretical temperature rise was calculated assuming isentropic compression starting at an initial temperature of 350K using the following equation

\[ T(t) = T_0 \left( \frac{V_0}{V(t)} \right)^{\gamma - 1} \]

Where,

\[ T(t) \] = Temperature at any time \( t \)

\[ T_0 \] = Temperature at time zero

\[ V_0 \] = Volume at time zero

\[ V(t) \] = Volume at any time \( t \)

The theoretical results, along with the simulation results for the three mesh densities, are plotted in Figure 1.5. The temperature rise for all three mesh densities is different from the theoretical curve. Since all three simulations are adiabatic (and largely reversible), the only factor affecting the temperature rise is the leakage rate in the simulations. The results in Figure 3.7 indicate that the temperature rise for the coarser meshes (103K and 178K) are identical and more closely follow the theoretical temperature rise. This is expected as the finer mesh simulation has more mesh elements in the gap and thus results in a more parabolic velocity profile that translates into a higher mass volumetric flow rate.
Figure 3.7 Temperature rise versus time for different mesh densities
Chapter 4

Results and Analysis

In order to achieve HCCI mode combustion the fuel and air should be perfectly mixed. To this end, it was believed that placing the injector on the left stator wall and injecting early during the compression process would be ideal. Calculations were carried out with the model described section 1.6 with a rotor speed of 573 revolutions per minute. The results were not favorable as most of the fuel ended up coating the stator wall or the rotor wall depending on the fuel injection angle. As can be seen the fuel spray bends towards the stator wall by as a result of the flow generated by the rotor rotation flow. For a shallower spray angle orientation (tilted towards horizontal), the liquid spray ended up coating the rotor wall. In addition, because fuel injection occurs early during compression the air temperature is low and thus most of the fuel that impacts the wall is in liquid form. It is well known that liquid fuel wall coating results in large unburned hydrocarbon emissions and poor fuel economy, so an alternate injector position was sought. The most important contributor to the problem is the small gap between the stator and rotor wall, i.e., 10 mm. For a larger more prototypic engine this fuel injector location may be acceptable.

To overcome this wall wetting problem, the location of the fuel injector was changed to the bottom of the combustion gate, i.e., top wall of the combustion cavity. The first simulations were carried out with a vertically downward spray orientation. The liquid fuel and vapour contours as a function of time for this position are provided in Figure 4.1 and Figure 4.2, respectively. Figure 4.1 shows that, after a short time from the start of injection the fuel spray is observed to bend towards the compression gate as a result of the flow field in the combustion cavity generated before the spray starts (the flow-field will be discussed later in this chapter). The results indicate that a significant portion of the fuel vapour makes its way to the gap between the bottom of the compression gate and the rotor surface, eventually leaking out of the
combustion cavity. However, the simulation demonstrates that all the fuel evaporates before contacting any combustion cavity surface because of the higher air temperature that exists at the start of injection.

**Figure 4.1** Vertically downward liquid fuel spray (298K elements)

**Figure 4.2** Mass concentration of fuel (Vapour) for vertically downward spray (298K elements)
In order to compensate for the flow field spray bending effect, the angle of injection was changed towards the expansion gate at 30 degrees from vertical. This was found to be the most suitable position for minimum fuel leakage out of the combustion cavity and fuel-air mixing. This fuel injector location was used in all the following simulations.

4.1 Baseline Simulation

A baseline simulation was performed with 178,000 mesh elements with an initial rotor lobe position of 180 degrees (bottom position) and quiescent air between the stator and rotor at an initial pressure and temperature of 100 kPa and 350K. The simulation ends when the rotor lobe reaches the top position bounding the bottom of the combustion cavity. The compression ratio is 19. The rotor speed was 573 revolution per minute and the total simulation time was 52 milliseconds. The liquid fuel used is n-Heptane, start of injection (SOI) was at 20 ms and end of injection was at 30 ms (spray duration of 10ms). The mass of fuel injected resulted in a global stoichiometric fuel-air mixture (air to fuel mass ratio of 15.16, or fuel mass fraction of 0.062), based on the mass of air present at the start of the simulation. The heptane mass flow rate was 5.52 g/s.

Figure 4.3 shows the liquid fuel spray concentration contours during the injection process. The off-vertical liquid fuel spray can clearly be observed in Figure 4.3. The length of the liquid spray remains roughly constant, as the fuel evaporates at the tip of the spray jet due to the higher air temperature in the combustion cavity. All the fuel evaporates by 31 ms and mixing continues until the start of combustion.
As the rotor rotates it drags along with it air (no slip condition) and the lobe pushes the air in the annulus between the stator and rotor like a piston. The 573 rpm rotor rotation corresponds to a rotor surface velocity of 2 m/s. Figure 4.4 shows the velocity vectors at times when fuel is injected into the cavity. Before fuel injection starts there is no discernable vortex in the combustion cavity and the peak velocity in the computation domain is 2.05 m/s, and less than 1 m/s in the combustion cavity. Fuel injection starts at 20 ms, inducing a large counter-clockwise rotating vortex in the cavity with a circulation velocity of up to 40 m/s. After 2 ms from the start of fuel injection, a secondary clockwise rotating vortex starts to form which is clearly visible in Figure 4.4. This secondary vortex remains intact up to 42 ms and then merges with the primary vortex, as seen in Figure 4.5. This causes the shifting of the primary vortex away from the compression gate. The flow features discussed above are highlighted in the two schematics shown in Figure 4.6.
Figure 4.4 Velocity vectors showing generation of secondary vortex during fuel injection for high CR and 178K mesh.
Figure 4.5 Velocity vectors showing shifting of big vortex for high CR and 178K mesh

Figure 4.6 Schematics showing flow field at two different times
As the rotor rotates, the volume occupied by the air decreases and as a result both the temperature and pressure increases due to compression. Before the fuel is injected the temperature remains uniform throughout the volume between the rotor lobe and the compression gate, see the temperature contours at 21 ms in Figure 4.7. Note, the high temperature zones below the rotor lobe are not physical; they are a manifestation of the very high viscosity set in this region to reduce leakage past the rotor/stator gap. Once the cold fuel is injected into the combustion cavity heat is transferred from the compressed air to the liquid fuel spray. This results in a reduction of the local air temperature, as seen in the recirculation zone at 30 ms in Figure 4.7. This heat transfer into the fuel results in evaporation of the liquid droplets. As can be seen in Figure 4.8, the fuel vapour that is produced closely follows the air flow-field that is characterized by the large recirculation zone as shown schematically in Figure 4.6. There is evidence of fuel vapour convection towards the bottom of the compression gate (see contour plot at 30 ms) due to the presence of the smaller recirculation zone, as depicted in Figure 4.6. This results in leakage past the gap between the compression gate and the rotor surface, clearly seen in the fuel vapour density contours at 40 and 45 ms in Figure 4.8. The temperature contour plot at 45 ms in Figure 4.7 shows a colder region in the recirculation zone, with significantly higher temperature along the surface of the rotor where the fuel does not penetrate. The maximum temperature at this time is 890K, which is just below the ignition temperature.
Figure 4.7 Contours of temperature between the fuel SOI and ignition for high CR and 178K mesh

Figure 4.8 Contours of fuel mass fraction between the fuel SOI and ignition for high CR and 178K mesh
To better visualize the fuel vapour concentration and temperature uniformity in the combustion cavity before ignition, the distribution of these two quantities at three heights are shown in Figure 4.9. Line 1h is at the top, line 2h is in the middle and line 3h is at the bottom of the combustion cavity. The line 2h is roughly at the level of the center of the recirculation zone.

Figure 4.9 Lines at different heights in combustion cavity

Figure 4.10b shows the temperature and fuel distribution along these three lines at a time of 46 ms, just before the time when the fuel auto-ignites. Note, the combustion cavity extends from -4 mm to 4 mm. As reference, the stoichiometric combustion heptane mass fraction is 0.0621. The center of the recirculation zone is roughly at the middle of the cavity, corresponding to the peak fuel mass fraction in Figure 4.10a. The highest fuel concentration being at the middle height, where the center of the recirculation zone is located. The heptane mass fraction is fairly uniform inside the recirculation zone, with a sharp drop off at about +1 mm, at the middle and bottom heights. There actually is some fuel on the right side of the combustion cavity, outside the recirculation zone, especially at the top right-hand corner. The temperature distributions along the same three lines indicate that wherever there is fuel present the temperature is lower, the highest being on the right-hand side of the combustion cavity. The highest temperatures are at the bottom right of the cavity just above the rotor, below the line 3h.
Contour plots for temperature, fuel vapour concentration and reaction rate are provided in Figure 4.11, starting at a time of 46 ms. At this time, there is evidence of very slow chemical reacts in the area to the right of the recirculation zone, where the highest temperatures are present as well as some fuel. Note, the reaction rate is defined by the depletion rate of the heptane (and therefore is a negative quantity) and is proportional to the fuel concentration and the exponential of the temperature. As a result, although the fuel concentration is highest in the recirculation zone, the temperature is lower and thus there is no chemical reaction. There is no noticeable temperature rise associated with this slow initial reaction.

At 47 ms ignition occurs at a point just above the rotor surface (the reaction rate is four orders of magnitude times higher than the maximum at 46 ms) and the local temperature in the ignition zone reaches a maximum of 1780K. At the same time, there is a secondary ignition site at the compression gate left corner. Between 47.5 and 49.0 ms a flame front is observed to propagate across the combustion cavity from right to left at an average velocity of about 400 cm/s. Low level combustion continues on the right side of the combustion cavity past 49 ms, where very little fuel is located. Some fuel remains in the vortex following the passage of the flame due to the initial fuel rich condition. This fuel would continue to be consumed as it mixes with the high temperature air remaining in the combustion cavity. After the flame
propagates across the combustion cavity the volume continues to decrease resulting in an increase in temperature of the combustion products above 3000K.
Figure 4.11 Contours of (a) temperature, (b) fuel vapour concentration and (c) reaction rate just before and after ignition for high CR and 178K mesh

The velocity vectors for three simulation times during which combustion occurs (47-49 ms) are shown in Figure 4.12. All three images show that the strong recirculation zone persists, even while the flame propagates across the cavity. The first image at 47 ms represents the flow-field that exists at the time of ignition, and is characterized by a recirculation velocity of roughly 3 m/s. At 49 ms the flame is propagating across the cavity and the expansion of the combustion products increases the velocity on the top part of the cavity to about 5 m/s. After the flame has swept across the cavity the velocity drops back to around 3 m/s. The general shape of the recirculation zone changes slightly over this time as more of the rotor lobe enters the combustion cavity.
4.2 Effect of Mesh Density on Combustion

In this section, the effect of mesh density on the combustion process is investigated. The reaction rate contours covering the combustion times is provided in Figure 4.13 for three mesh densities, the 178K mesh being the baseline case just discussed. For the higher resolution 298K elements only a single ignition site forms, initially at roughly the same location as in the baseline case. The second ignition at the compression gate forms later at 48 ms and is less consequential. The flame propagation is qualitatively the same for the higher and baseline mesh density. The lower mesh density of 103K elements produces very similar results, with combustion from the secondary ignition playing more of a role especially at early times. Based on these results one can conclude that simulations at 178K should be accurate enough, especially since the higher resolution mesh produces more leakage as shown in section 3.3.
Figure 4.13 Reaction rate for high CR with (a) 103K elements (b) 178K elements (c) 298K elements
4.3 Variable Compression Ratio

The main purpose of the Fanara rotary engine is to get the HCCI like combustion with control of ignition timing via the variable compression ratio; this is one of the benefits of this engine compared to reciprocating engines. The compression ratio is varied by changing the height of the combustion gate, effectively changing the combustion cavity volume. The baseline case compression ratio is 19, in this section results for a compression ratio of 18.3 are reported for comparison. The temperature contours obtained for the two compression ratios at 46 ms (just before ignition) are provided in Figure 4.14. The general shape of the contours is the same for the two and temperature near the rotor, where ignition occurs, for the compression ratio of 19 and 18.3 are 900K and 850K, respectively, The reaction rate contour plots are very similar for the two compression ratios, so they will not be presented. Figure 4.15 shows the average temperature and pressure rise for the two compression ratios. The plots show that the temperature and pressure rise for the higher compression ratio is slightly higher than that obtained for the lower compression ratio. This comparison is not straightforward because gas leakage and liquid fuel injection influences the pressure and temperature rise observed during compression before ignition. There is a small difference in the ignition time of the fuel as observed by the time at which point the temperature increases rapidly at about 47 ms. The fuel ignites at 47 ms for the low compression ratio case, whereas for the high compression ratio, it ignites at around 46 ms, which is consistent with the higher temperatures observed for the larger compression ratio.

![Figure 4.14 Temperature contour at 46 ms for (a) high compression ratio (b) low compression ratio (178 K mesh)](image)

Figure 4.14 Temperature contour at 46 ms for (a) high compression ratio (b) low compression ratio (178 K mesh)

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Figure 4.15 (a) Temperature v/s time (b) Pressure v/s time for high CR and low CR with 178K mesh

4.4 Effect of detailed chemistry model

The two case studies discussed in section 2.4 showed that there are significant differences between the energy release predicted using the detailed chemistry and the single-step reaction model. The most significant is that the single-step model does not predict the first stage of ignition that includes a small temperature rise. This section provides the results obtained using the detailed chemistry model. A simulation was carried out with low compression ratio with 178K mesh elements.

Figure 4.16 shows reaction rate contours obtained during the combustion process. Starting at 46 ms a slow reaction occurs over a large section of the combustion cavity (larger than that observed using the single-step reaction model). This reaction starts outside the recirculation zone vortex where the fuel concentration is lower and the temperature is higher, working its way inward towards the centre of the vortex. The temperature distribution at the start of this slow reaction (46 ms) and just before the primary ignition (47.5 ms) are shown in Figure 4.17. One can see that the slow reaction results in a temperature increase of about 200K on the right side of the cavity, but only about 50K at the centre of the vortex. The primary ignition occurs between 47.5 and 47.75 ms at a point near the rotor surface, similar to that obtained in single step simulations. A flame propagates outwards and then stretched by the flow-field, initially around the vortex and then towards the centre. Combustion is complete by 49 ms.
Figure 4.16 Reaction rates at different times for detailed chemistry model for low CR and 178K mesh
Figure 4.17 Temperature contours for a simulation with detailed chemistry, low CR and with 178K mesh

Figure 4.18a shows the pressure rise and rate of pressure rise for single step reaction model and detailed chemistry model. The pressure rise predicted by the single step reaction model is higher than the detailed chemistry model. The main factor affecting engine longevity is the rate of pressure rise which is associated with knock. Looking at the Figure 4.18b, it is clear that the rate of pressure rise for detailed chemistry is lower than the single step reaction model. The acceptable rate of pressure rise for avoiding knock is generally taken to be around 80 bar/ms [19]. Also a qualitative comparison of the reaction rate contour plots indicates that the detailed chemistry results show a slower flame propagation which produces a more gradual increase in pressure.

Figure 4.18 (a) Pressure rise (b) Rate of pressure rise for single step and detailed chemistry mode
4.5 Effect of Injection Timing

In this section, the effect of fuel injection time on the fuel mixing and combustion is investigated. For HCCI early fuel injection is better so that there is more time to mix with air and make a homogenous fuel air mixture. Simulations were carried out with three different start of injection times, e.g., 10ms, 20ms (baseline case) and 30ms. For all three simulations, a stoichiometric amount of fuel was injected, such that the duration of fuel injection was kept constant at 10ms. Figure 4.19 shows the contours of temperature, reaction rate and fuel mass fraction at the time of ignition.

![Figure 4.19 Contours of fuel mass fraction, reaction rate and temperature for injection time at (a) 10 ms (b) 20 ms and (c) 30 ms (high CR and 298K mesh)](image)

It will be seen that ignition time is not that affected by the injection timing. In all three cases, ignition occurs just off the rotor surface but the point of ignition shifts towards the compression gate with earlier fuel injection. This is because of a shift in the center of the recirculation zone, that has the highest
concentration of fuel, to the right side of the cavity, see Figure 4.20. This results in a shift of the reduced temperature zone in the combustion cavity, as will be seen from the result given in Figure 4.21. This shift in the recirculation zone also shifts the high temperature zone on the rotor surface (that governs where ignition occurs) towards the compression gate, see Figure 4.20.

Figure 4.20 Fuel distribution within combustion chamber 298K mesh, high CR
Although the ignition time stays the same for different fuel injection times the fuel and temperature distribution change significantly, which affects the combustion process. In order to understand why the distribution changes the velocity vector contours are provided for the 10 ms and 30 ms injection cases in Figure 4.22 and Figure 4.23. The flow-field for the 10 ms fuel injection develops similar to that at 20 ms discussed in Section 4.1. i.e., a primary counterclockwise-rotating vortex forms with the start of fuel injection, followed by the formation of a secondary vortex. As the rotor lobe approaches the secondary vortex merges with the primary lobe and vortex formed shifts away from the compression gate.

For fuel injection at 30 ms the flow-field develops differently, specifically no secondary vortex forms and as a result the primary vortex does not shift away from the compression gate as the rotor lobe approaches. A possible explanation for the absence of the secondary vortex is that the velocity in the
combustion cavity up the compression gate face is significant, i.e., 1 m/s, at the time of start of fuel injection.
Figure 4.22 Velocity vectors (m/s) for fuel injection at 10 ms (298K mesh high CR)

Figure 4.23 Velocity vectors (m/s) for fuel injection at 30 ms (298K mesh high CR)
The effect of the fuel and temperature distribution on the combustion process can be assessed based on the cavity pressure development over time, see Figure 4.24a and b. The highest peak pressure is produced for the 30 ms fuel injection case and the lowest peak pressure is produced for the 10 ms injection, which indicates that fuel distribution effects combustion efficiency.

![Graph showing static pressure vs. time and rate of pressure rise vs. time for different injection times](image)

**Figure 4.24 (a) Static pressure v/s time and (b) Rate of pressure rise v/s time for different injection times**

Figure 4.24b shows that the rate of pressure-rise for fuel injection at 10 ms is lowest and that the rate is highest for the 30 ms. This can be explained by the reaction rate contours provided in Figure 4.25 and Figure 4.26. For the 10 ms, see Figure 4.25, the flame propagates around the vortex in a similar manner to that observed for the 20 ms injection baseline case (see Figure 4.11). Figure 4.26 shows the reaction rate contours for a fuel injection time of 30 ms. The flame is observed to propagate very fast across the cavity (in about 1.5 ms) which corresponds to the faster rate of pressure rise observed in Figure 4.24b. This observation is also compatible with the fact that the mixture is more uniform across the cavity, as seen in Figure 4.20c.
Figure 4.25 Reaction rate contours for 10ms fuel injection for 298K mesh high CR
4.6 Effect of Load

The load is defined by the amount of fuel that is consumed. Since the amount of air inducted into the engine is constant, a change in the amount of fuel added changes the global equivalence ratio (ER). Three different equivalence ratios were studied, all other parameters being kept the same for the comparison purposes. Simulations were performed for ER of values 1, 0.5 and 0.25 (the latter two being fuel lean conditions). The equivalence ratios are changed by changing the mass flow rate of fuel that is sprayed into the combustion cavity. For the stoichiometric mixture, the mass flow rate of fuel is kept 0.0052 kg/s. The other two cases were obtained by cutting down the mass flow rate of fuel by 50% and 75%, i.e., fuel injection duration was kept constant at 10 ms.
The reaction rate contours for the three simulations are shown in Figure 4.27. The first column of contours is the baseline case corresponding to ER=1 that shows flame propagation across the combustion cavity. The ignition time for all three cases is 47 ms, and the ignition point on the rotor surface moves slightly away from the compression gate as the equivalence ratio is lowered. At 48 ms a flame is perfectly formed for the baseline case, whereas for the other two cases a diffuse reacting region forms from which a flame initially forms in the case of ER =0.5; but eventually at 49 ms the flame thickens to the point where it can no longer be considered a flame. For the ER=0.25 a flame never forms, instead a zone of reacting gas forms that spreads out. This type of combustion is closer to a well stirred reactor where the characteristic turbulent mixing time is shorter than the characteristic chemical reaction time.
Figure 4.27 Contours of reaction rate for different equivalent ratios (a) 1 (b) 0.5 and (c) 0.25 for 298K mesh high CR

Figure 4.28a shows the pressure rise for ER values equal to 1, 0.5 and 0.25. The pressure rises slowly during the compression process and then increases more rapidly following ignition. The pressure rise
before ignition is of course the same for all three cases, which indicates that the change in specific heat ratio with the different fuel concentration is not significant. Since the compression ratio is the same for all three cases, the peak pressure following combustion increases with the amount of fuel added. Since the volume decreases over the combustion phase, and there is no heat loss, the pressure drop observed following the peak can be attributed to gas leakage associated with the very high pressures generated. The rate of pressure-rise before ignition, shown in Figure 4.28b, is the same for all three cases. The peak rate of pressure rise is largest for the ER=0.5 case, see Figure 4.28b. The peak rate of pressure rise is governed primarily by the average reaction rate over the combustion cavity volume. Figure 4.29 shows the average reaction rate for the three prescribed equivalence ratios. This plot shows that the reaction rate for the ER=1.0 is slight higher (more negative) than the ER=0.5 case, which means that perhaps the leakage rate is higher for the ER=1.0 case, since the peak rate of pressure rise observed is higher for the ER=0.5 case, see Figure 4.28b.

![Graphs showing static pressure vs time and rate of pressure rise vs time for different equivalence ratios](image)

Figure 4.28 (a) Static pressure v/s time (b) Rate of pressure rise v/s time

Figure 4.29 also shows that the combustion is very fast for all of the cases. In all three cases reaction occurs over about 2-3 ms, which corresponds to approximately 10 degrees of crank angle. The reason for such a small reaction time is the small size of combustion chamber and the strong recirculation zone.
Figure 4.29 Average reaction rate for Equivalence ratio 1, 0.5 and 0.25
Chapter 5

Conclusion

The objective of this work was to model the compression process in the Fanara rotary engine and check the combustion characteristics with varying parametric conditions. The computational modelling was done with Ansys Fluent 17.0. A dynamic mesh was adopted to model the rotor and compression gate motion. In order to model the rotor motion a small gap between the stator and the rotor lobe surface was required that resulted in gas leakage that was unavoidable. The leakage was reduced artificially by increasing the viscosity in the gap as well as on the expansion side of the rotor. Ignition was successfully achieved using both single-step and detailed combustion chemistry models. Mesh independence was checked using three different mesh densities.

From the parametric study, the following conclusions can be drawn:

1. Fuel injection directly into the combustion cavity at an angle away from the compression gate is found to be the best injector position for generating recirculation zones for good fuel-air mixing.

2. Ignition time for higher compression ratio is 1ms faster than with a lower compression ratio. The temperature and pressure rise is also proportional to the compression ratio.

3. The detailed chemistry model is able to catch the low temperature ignition which can be observed from the low temperature flame propagation before real ignition starts, whereas single step reaction model is not able to predict the same. Although the single step reaction model is not accurate, it is computationally cheap and most effective way to observe the parametric studies.

4. Varying the fuel injection time gives a small difference in the ignition time but has a big impact on the flow field and fuel distribution at the time ignition.

5. Changing the global mixture composition changes the ignition location and the ensuing combustion process. For an equivalence ratio of one flame propagation is obtained through most of the combustion cavity. For an equivalence ratio of one-quarter the fuel loading flame
propagation was not achieved, instead slow reaction rate chemistry took place. The rate of pressure rise is low for an equivalence ratio 1 and high for an equivalence ratio of 0.5.
Chapter 6 References


Appendix A

Fuel Lean Early Injection Simulation

The simulations presented in Section 4.6 showed that reducing the fuel injected at 20 ms by one half resulted in the propagation of a failing (thickening) flame, see Fig 4.27b. This could be attributed to a leaner mixture produced in the cavity. Since simulations with early injection (10 ms) resulted in the fuel settling in the vortex ring occupying a smaller volume on the left side of the cavity, it is possible that the mass fraction can be increased and thus result in normal flame propagation throughout the combustion cavity. Therefore, a simulation with ER=0.5 and 10 ms was carried out with a 178K mesh and high CR and detailed chemistry, see Fig. A1. The heptane mass fraction is evenly distributed in the vortex with a composition near stoichiometric. The maximum temperature in the cavity reaches around 700K at 43 ms, at which time low rate reaction starts on the right-hand side of the cavity. Once the temperature reaches 1000K at 44.5 ms a flame is ignited on the side of the compression gate, where lean fuel conditions exist. This is much earlier and at a different location than observed in all other simulations. Once reaction starts it depletes the fuel very quickly from the outside inwards to the center of the vortex, like that observed with the simulation carried out with 20 ms injection ER=1 and low CR, see Figure 4.16. Unfortunately, because of the multiple parameters varied for this simulation (mesh density, CR and chemistry model) it is difficult to isolate the cause of the temperature reaching 700K earlier at 43 ms.
Figure A.1 Contours of (a) Fuel mass fraction (b) Temperature and (c) Reaction rate 10 ms injection high CR and 178K elements
Appendix B
User Defined Functions

User defined function for the rotation of Rotor.

#include "udf.h"
#include "math.h"
#include "dynamics_tools.h"

DEFINE_CG_MOTION(rotor, dt, vel, omega, time, dtime)
{
    /* reset velocities */
    NV_S (vel, =, 0.0);
    NV_S (omega, =, 0.0);
    /* compute velocity formula */
    omega[2]=60;
}
User defined function for the gate movement

```c
#include "udf.h"
#include "math.h"
#include "dynamics_tools.h"

// for the left August 26 for circle stator
DEFINE_CG_MOTION(gate, dt, vel, omega, time, dtime)
{
/* reset velocities */
NV_S (vel, =, 0.0);
NV_S (omega, =, 0.0);

// -60 is omega
// for rotation -100, -1.74533 is radian for -40 is -0.698132
// for rotation -180, -3.141594 is radian
/* compute velocity formula */
if (time>.031 && time<.04)
{
    vel[1]= -0.038*( .0348*pow(-3.141594 -60*time,5) + .5505*pow(-3.141594 -60*time,4) + 4.0364*pow(-3.141594 - 60*time,3) + 15.9189*pow(-3.141594 - 60*time,2) + 31.258*(-3.141594 - 60*time) + 23.319);
}
else if (time>=.040 && time<.046)
{
    vel[1]= -0.043*( .0348*pow(-3.141594 -60*time,5) + .5505*pow(-3.141594 -60*time,4) + 4.0364*pow(-3.141594 - 60*time,3) + 15.9189*pow(-3.141594 - 60*time,2) + 31.258*(-3.141594 - 60*time) + 23.319);
}
else if (time>=.046 )
{
    vel[1]= -0.037*( .0348*pow(-3.141594 -60*time,5) + .5505*pow(-3.141594 -60*time,4) + 4.0364*pow(-3.141594 - 60*time,3) + 15.9189*pow(-3.141594 - 60*time,2) + 31.258*(-3.141594 - 60*time) + 23.319);
}
}
```
User defined function for high viscosity on the expansion side

#include "udf.h"
// rotor -180 , 16 August 2016
// viscosity every where

#define vis_HIGH 30
#define vis_MED 30
#define vis_right 30
#define vis_LOW 1.7894e-05
#define pi 3.1415926535897932
#define rotor_dia 0.0296
#define stator_dia 0.03
#define theta_a -1.26625
#define theta_b -1.804955
#define theta_c -1.575602
#define omega -60

DEFINE_PROPERTY(my_viscosity, c, t)
{
    real vis;
    real cr[ND_ND];
    real flow_time;
    real xa;
    real xb;
    real xc;
    real ya;
    real yb;
    real yc;

    flow_time = CURRENT_TIME;
    // flow_time = 0;
C_CENTROID(cr,c,t);

xa = stator_dia*cos(theta_a + omega*flow_time);
ya = stator_dia*sin(theta_a + omega*flow_time);
xb = stator_dia*cos(theta_b + omega*flow_time);
yb = stator_dia*sin(theta_b + omega*flow_time);
xc = stator_dia*cos(theta_c + omega*flow_time);
yc = stator_dia*sin(theta_c + omega*flow_time);

//if (cr[0] >= -.0025 && cr[0] <= .0005 && cr[1] >= 0) //make the gate thicker
//if (cr[0] >= -.0035 && cr[0] <= .00025 && cr[1] >= 0) //make the gate thicker
if (cr[0] >= .004 && cr[0] <= 0 && cr[1] >= 0)
{
   vis = vis_HIGH;
}
{
   vis = vis_MED;
}
{
   vis = vis_MED;
}
{
   vis = vis_MED;
}
{
   vis = vis_MED;
}
{
   vis = vis_MED;
}
{
    vis = vis_MID;
}
{
    vis = vis_MID;
}
{
    vis = vis_MID;
}
{
    vis = vis_MID;
}
{
    vis = vis_MID;
}
{
    vis = vis_MID;
}
else if (cr[0]<-.002)  //for left side of the engine
{
    vis = vis_LOW;
}
else if (cr[1]<yb)  //for bottom side of the engine (below rotor)
{
    vis = vis_LOW;
}
else
{
    vis = vis_LOW;
}

// Viscosity top right
if (cr[0]>=0.004 && cr[1]>0)
{
    vis = vis_right;
}
if (cr[0]>=0 && cr[1]<0)
{
    vis = vis_right;
}

// Viscosity left
if (cr[0]<0 && cr[1]<yb && flow_time<=.029)
{
    vis = vis_right;
}
if (cr[0]<0 && cr[1]<ya && flow_time>.029)
{
    vis = vis_right;
}

return vis;