JIMMA INSTITUTE OF TECHNOLOGY

FACULTY OF MECHANICAL ENGINEERING

THERMAL SYSTEMS ENGINEERING CHAIR

MSc. Research Thesis on: -

CFD modeling of Fast Turbulent mixing process of Ethanol in Homogeneous Charge Compression Ignition Engine with the application of Exhaust Gas Recirculation

For the partial fulfilment of MSc. Degree in Thermal Systems Engineering

BY

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November 2017

Jimma, Ethiopia

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Declaration

This MSc. research thesis is my original work and has not been presented for degree in any other university.

Name	Signature	Date

This MSc. research thesis has been submitted for an examination with my approval as University Supervisor.

Advisor	Signature	Date
Co-advisor	Signature	Date
Internal examiner	Signature	Date
External examiner	Signature	Date

January 2017

List of Abbreviations

AFR..Air fuel ratio

BDC..Bottom Dead Centre

BMEP...Break Mean Effective Pressure

CA...Crank Angle

CFD..Computational Fluid Dynamics

CI..Compression Ignition

CO..Carbon Monoxide

CR..Compression Ratio

DNS..Direct Numerical Simulation

EGRD...Exhaust Gas Recirculation Device

EVO..Exhaust Valve Open

HC..Hydro Carbon

HCCI...Homogeneous Charge Compression Ignition

IVC..Inlet Valve Closed

LES..Large Eddy Simulation

NOx...Nitrogen Oxide Molecules

PM...Particulate Matter

RANS..Reynolds Average Navier-Stoke

Re.. Reynolds Number

SI...Spark Ignition

SOFI..Start Of Injection

TKE...Turbulent Kinetic Energy

TDC...Top Dead Centre

List of Symbols

α.. Crank radius

B... Cylinder bore

l.. Connecting rod length

L... Stroke

V_l... Minimum lift

ω... .... Engine speed

K.. ....Kelvin

%.. ....Percentage

x...Combustion prefix

S_y...Stress

G_b..Buoyancy constant

S_k...Sources

Y_M..Compressibility effects

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Abstract

The importance of design the type of internal combustion engines such as Homogenous Charge Compression Ignition (HCCI) which increase efficiency while decreasing harmful emissions with low fuel consumption is steadily increasing. HCCI is a combustion concept, which is a hybrid between Otto engine and Diesel engine, which is thermodynamically favorable, leading to the benefit of high thermal efficiency.

The geometry setup for HCCI engine is drawn and mesh size is fixed for appropriate simulation setting using ANSYS 17.2 software for analyses. In this investigation, port fuel injection method is used for the homogeneous mixture preparation and injection for HCCI mode.

The research is aimed to develop the CFD modelling of fast turbulent mixing processes of ethanol in HCCI engine conditions through air-fuel mixture preparation with application of exhaust gas recirculation under various engine factors. The HCCI combustion is successfully achieved. Combustion simulations are performed by ANSYS 17.2 software for combustion and emission behavior of ethanol HCCI engine. It is found that combustion starts at intake charge temperature of 720K.

Combustion behavior investigation is carried out on addition of 0% to 30% EGR to show the alternative use of ethanol instead of conventional fuels. It is found that The Turbulent kinetic energy is increased by addition of EGR which will facilitate rapid combustion in the combustion chamber to increase engine's efficiency and fast mixing of ethanol and air for homogeneous mixture is obtained which, in turn leads the engine to 40% minimized pollution, 20% decreased fuel consumption rate and 15% increased the engine efficiency. The result obtained has been validated with experimental and theoretical research work.

Keywords: *Homogeneous Charge Compression Ignition, HCCI, Auto-ignition, Premixed Charge Compression Ignition, Combustion, Internal Combustion Engines.*

Acknowledgements

I have benefited from the kindness, experience, and technical expertise of numerous people during the writing of this thesis. I would like to begin by thanking my wonderfully supportive and encouraging thesis advisors, Asst. Prof. **Balewgize Amare Zeru** and Mr. **Dasta Goitom** (MSc). Balewgize, I always appreciated and benefited from the enthusiasm that you bring to my research. Dasta, I very grateful for the guidance and timely advice you have always given me. I feel blessed to have had two advisors that I am happy to know as both colleagues, friends and teachers.

Chapter One

Introduction

1.1 Background

One way to further improve upon IC engines is to implement a combustion cycle known as Homogeneous Charge Compression Ignition (HCCI) which has the potential to reduce fuel consumption while simultaneously drastically reducing emission of nitric oxides (NOx) and particulate matter (PM), two products of combustion known to be harmful to human health and the environment.

HCCI engine is premixed, like spark ignition (SI) engines, and compression ignited, like a Diesel engine. The premixed fuel and air mixtures are unusually lean (stoichiometric ratios around 0.3) which results in low peak temperatures thus limiting the production of NOx. Since the fuel and air in the HCCI engine are premixed, there is no diffusion flame burning (as in a diesel engine) so particulate matter (PM) emissions are also quite low. The lean nature of the combustion process also leads to a decrease in PM since excess hydrocarbons (HC) are not present. This allows for high compression ratios and therefore higher engine efficiencies.

Combining the premixed charge from the SI engine with compression ignition, the homogenous charged compression ignition (HCCI) is the result. By fully premixing fuel and air and then compressing the charge until ignition occurs, simultaneous combustion throughout all parts of the combustion chamber is ideally achieved. This auto-ignition phenomenon has been applied in IC engines as an alternative to SI and CI engines, and is generally referred to as HCCI combustion. Since under HCCI combustion the fuel/air mixture does not rely on the use of a spark plug or direct injection near Top Dead Centre (TDC) to be ignited, overall lean mixtures can be used resulting to high fuel economy. Thus, the combustion temperature remains low and therefore NOx emissions decrease significantly [20], [21] compared to SI and CI operation.

In ethanol fueled HCCI engines, a uniform charge of ethanol and air enters the combustion chamber and the compression stroke gives sufficient energy input to the mixture, so that the temperature reaches at an auto-ignition condition where then the charge (of homogeneous mixture) auto-ignited near TDC in the combustion process without any external source of ignition. The mixture is homogeneous which minimizes emission of NOx and PM, it is compression ignited using high compression ratios, has no throttling losses, also has shorter combustion duration which leads to high thermal efficiency.

In order to prevent excessive knocking during HCCI combustion, it must take place in a dilute environment, resulting from either operating fuel lean or providing high levels of either internal or external exhaust gas recirculation (EGR). Operating the engine in a dilute environment can substantially reduce the pumping losses, thus providing the main efficiency advantage compared to spark-ignition (SI) engines.

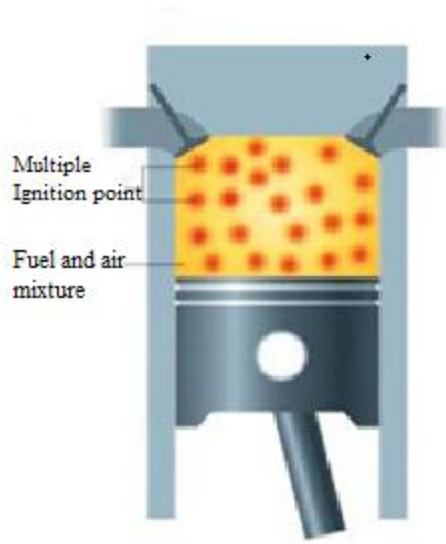


Figure 1.1 HCCI engine [2]

Implementation of HCCI means uniform distribution of fuel in cylinder volume and creation of a homogeneous air-fuel mixture with the absence of the locally rich zones (zones with low values of an air-fuel equivalence ratio). As a result of formation of nitrogen oxides, particle matters and unburnt combustibles considerably decreases. Besides due to the mixture leaning, recirculation and cooling of EGR, the level of temperatures in combustion zone remains rather low. It also promotes minimization of pollutant emissions. [17]

The ability of turbulent flows to effectively mix entrained ethanol to air is a vital part of the dynamics of such flows, with wide-ranging consequences in HCCI engine modelling. It is a considerable experimental, theoretical, modeling, and computational challenge to capture and represent turbulent mixing which, for high Reynolds number (Re) flows, occurs across a spectrum of scales of considerable span along HCCI engine.

Computations of the flow in a HCCI engine intake manifold with generic boundary conditions indicate, that inlet pulsations are important for the mixing process and that the smoothing effect of URANS is not adequate for accurate mixing computations. LES, on the other hand, is more promising, since it is able to capture the physics of pulsating flows much better.

Exhaust gas recirculation device (EGRD) is an emission control technology allowing significant NOx emission reductions from most types of HCCI and other types of engines. It is used to recycle and trapping the burnt gases within the cylinder by substantial charge dilution for control of heat releasing rates and to initiate the chemical reactions leading to auto-ignition process.

While the application of EGR for NOx reduction is the most common reason for applying EGR to modern commercial HCCI engines, its potential application extents to other purposes as well. Some of these include: imparting knock resistance and reducing the need for high load fuel enrichment in SI engines, aiding vaporization of liquid fuels in SI engines, as an enabler for closed cycle diesel engines or for improving the ignition quality of difficult-to-ignite fuels in diesel engines. While NOx reductions had been reported with EGR as early as 1940, the first engine experiments to investigate the NOx reduction potential of EGR appeared to be carried out in the late 1950s in SI engines. By the 1970s, EGR was being seriously considered as a NOx control measure for diesel engines. [5]

The NOx emission benefit of EGR comes at a cost: other measures are usually required to avoid unacceptable increases in fuel consumption, emissions of PM, HC, and CO, engine wear and reductions in engine durability.

Generally, recently models with different resolution have been developed as a means to understand fundamental concepts underlying HCCI combustion in real engine geometries. The simplest approach to model HCCI follows a thermo-kinetic, zero-dimensional formulation in a single homogeneous zone. Najt & Foster first developed this type of model to help analyze experiment work on a premixed-charge, compression-ignited CFR engine.

A brief summary of the differences between Spark Ignition engine, Compression Ignition engine and HCCI engine technologies is presented in the following table

Table 1.1 Comparison between HCCI engine, CI and SI engine

	Spark ignition Engine	**Compression ignition engine**	**HCCI engine**
Air/ Fuel ratio	Premixed	Non premixed	Premixed
Ignition type	Spark ignited	Compression ignited	Compression ignited
Power output control	Airflow control, with stoichiometric air-fuel ratio	Fuel flow control, with lean air-fuel ratio	Fuel flow control, with lean air-fuel ratio
Mechanism controlling fuel burning rate	Flame propagation speed	Time for fuel vaporization and mixing	Chemical kinetics
Emission characteristics	Cleaner with 3-way catalyst. Higher CO_2	Higher particulate matter, soot, NOx and relatively lower CO_2	Higher unburned hydrocarbons, CO. Lower NOx, soot, particulates, and CO_2 than SI and CI engines

1.2 Statement of Problem

There is currently a great deal of interest in the homogeneous-charge compression-ignition (HCCI) engine concept since it allows good fuel economy with very low emissions of NOx and particulate matter. However, there is no direct control over the ignition timing, and the viable operating range appears to be undesirably small. Incomplete combustion or misfire can occur under very lean conditions imposing a minimum load at which the engine can operate. It has different limitations over control of combustion timing, limited power output, homogeneous mixture preparation, limitations on operating load, speed and cold start.

This research work provided detailed information about HCCI engines, to develop and assess methods suited for the computation of turbulent mixing processes in ethanol fueled HCCI engine conditions and homogeneous mixture preparation method. The knowledge of Ethanol fuel behavior and a way to model it to reach to the needed auto-ignition by studying parameters such as increased turbulent kinetic energy for better turbulence, low temperature heat release, auto-ignition temperatures, the effect of use of exhaust gas recirculation (EGR) has been done.

1.3 Objectives

1.3.1 General Objective

The general objective of this research work is CFD modeling of fast turbulent mixing process of Ethanol fuel in HCCI engine with the application of Exhaust Gas Recirculation (EGR) to minimize fuel consumption, emissions and to increase the thermal efficiency of the engine.

1.3.2 Specific Objectives

- To review HCCI engine related literature, to find research gap.
- To collect primary and secondary data from Automotive Companies
- To develop HCCI engine Geometries on ANSYS Workbench and Solid Works software to operate at different design parameters
- To develop CFD analysis model for combustion in HCCI mode of operation with ethanol fuel
- To study the nature of fuel preparation and turbulent mixing challenges and solutions for ethanol fueled HCCI engine modelling
- To evaluate the performance and emission of ethanol fuel on HCCI mode of operation under different operating conditions with and without EGR
- To study the effect of variation of EGR on the performance of turbulent mixing and emissions of the engine running with Ethanol on HCCI engine.
- To increase the effect of in-cylinder Swirl and Tumble to increase turbulence in combustion chamber for burning of ethanol-air mixture.

- To make a comparative analysis of the HCCI engine performance, efficiency and emissions (pollution aspects) with experimental results of HCCI engine at Lawrence Livermore National Laboratory and other researchers work for validation.

1.4 Delimitations

This research work was intended to find ethanol fueled HCCI engine simulation that was prepared according to the ethanol fueled WO4D HCCI engine that operated at a constant speed of 2000 RPM for purpose of increases in fuel injection pressure, use of ethanol oxidation catalysts, and increased intake manifold boost pressure.

The research limited to theoretical analysis using CFD software simulation results. Finally, the result was compared for validation with other research works including the light duty HCCI engine specifications of the WO4D. This experimental HCCI engine test has been developed at Lawrence Livermore National Laboratory. [17]

1.5 Methodology

First all engine geometry parameters have been collected from MOENCO (Toyota) Addis Ababa, Bishoftu Automotive Industry and other Companies. The HCCI engine geometries have been drawn using SOLIDWORK software and ASYS Workbench for analysis.

After geometry is completed and decomposed correctly, using proper Initial and Boundary conditions, mesh size has been fixed. Lastly, the simulation processes done with 0% - 30% EGR and without the EGR using Laboratory computer.

ANSYS-ICE is used to run a 3D CFD port, cold and combustion flow of the engine simulation according to ethanol fueled HCCI engine geometry design. The progressive results the turbulent mixing and turbulent kinetic energy during the combustion period with and without EGR has been recorded.

Finally, the simulation result has been obtained exactly for all cases and comparison to the existing engine is done for validation. After the final result has compared to the existing literatures and simulation post analysis by the extracting results from ANSYS-ICE, the final report data is prepared.

Chapter Two

Literature review

Amongst the numerous research works published over the last decade, the Homogeneous Charge Compression Ignition engine (HCCI) has often been considered a new combustion process in reciprocating IC engine. Although it is known as a new combustion concept for internal combustion engines in many papers, HCCI has also known as Controlled Auto-Ignition (CAI) has been around over hundred years. [2]

HCCI combustion was discovered as an alternative way for two stroke engines. A first study on such type of combustion process was made by Onishi et al. in 1979 [24]. This completely new type of combustion adopted to the piston engines has been called Active Thermo Atmosphere Combustion as a promising alternative for existing spark and diesel engines. The drawbacks of two stroke engines are high residuals emissions at low and partially loads, and the tendency to run on (knock effect) when the engine is stopped. Onishi and coworkers turned these deficiencies into strengths by devising a combustion mode that relied on both high levels of internal residuals and high initial charge temperature. By creating conditions that led to spontaneous ignition of charge they obtained significant reduction in emissions and an improvement in fuel economy. Not long after Onishi presentation the same combustion process was demonstrated at Toyota [24].

HCCI engines typically operate at compression ratios higher than spark-ignited engines. Depending on the intake conditions and the fuel type, HCCI compression ratios can range from 14:1 to 22:1 [17,18], however lower compression ratios can be used in spark-assisted HCCI implementations. Fuel-air equivalence ratios in HCCI range between 0.20 and 0.55 for implementations without exhaust gas recirculation [17], but can go as high as 1.0 (stoichiometric) for implementations that use extensive dilution with exhaust gas recirculation [14].

Given that the HCCI engine can be approximated with the Otto cycle, the thermal efficiency limits can be estimated using the Otto cycle efficiency relationship. The higher compression ratios of HCCI compared with spark-ignited engines is one reason for their ability to achieve higher thermal efficiencies (similar to Diesel). Another factor contributing to the high efficiency of HCCI is that the intake air is not throttled for power output control. As a result, HCCI does not suffer from the throttling losses that affect part-load operating conditions in spark-ignited engines.

Ethanol is used as a fuels besides gasoline and diesel for HCCI engines. Since natural gas is the second most abundant fuel, many researchers studied the feasibility of using natural gas as a fuel in HCCI engines. Due to high octane rating of natural gas (on the order of methane which has an Octane Rating of 107), high compression ratio, high intake temperatures or additives promoting auto-ignition like NOx, dimethyl ether are required in natural gas fueled HCCI engines. Alcohols exhibit good auto-ignition properties and hence are excellent HCCI fuels with significantly larger operating range than most of the other fuels.

Research Gap

With projected increasing flexibility in both engines hard-ware and control system in long term, the development of a full HCCI engine is possible. Hence, for future long term development of HCCI combustion systems, the key issues will be more flexible injection strategies and EGR control for better mixture formation and control as well as high boost to extend the upper load limits. Whilst HCCI remains the realistic alternative to existing engine combustion technologies to improve emissions, a parametric study can be useful in order to gain more understanding in the emission and fuel consumption reduction possibilities through this new combustion technology for long term viability of both light-duty and heavy-duty vehicles.

2.1 Working Principles of HCCI Engines

In an HCCI engine, the formation of the air-fuel mixture is similar to that of an SI engine (homogeneous mixture) and initiation of combustion is similar to a CI engine (auto ignition at the end of the compression stroke). Therefore, it is reasonable to define an HCCI engine as a hybrid of SI and CI engines. For combustion to happen in an HCCI engine, it is important that during the compression stroke the mean temperature of the charge mixture reaches auto ignition temperature or the engine will misfire. This temperature criterion is achieved either by constraining hot residual gas or by heating intake air.

In an HCCI engine, auto ignition happens throughout the combustion chamber. That is, combustion happens at multiple points throughout the combustion chamber, resulting in simultaneous heat release events without any flame propagation. This process was verified through spectroscopic and imaging investigations by the Lund Institute of Technology. [7], [8].

Multiple parallel auto ignition points in an HCCI engine lead to rapid heat release rates for a shorter combustion duration when compared to SI and CI engines. There are two main controls which have to be satisfied in order to attain proper HCCI combustion: (1) control of combustion near the vicinity of top dead center (TDC), and (2) control of the heat release rate during high load and high speed operating conditions. Failure may lead to improper combustion and knocking effects [9]. To avoid failure during high load and high speed conditions, an HCCI engine should run either in lean conditions or incorporate high amounts of dilute residual gases.

2.2 Ethanol Combustion in HCCI engine

Combustion or burning is the sequence of exothermic (a process or reaction that releases energy from the system, usually in the form of heat, but also in the form of light) chemical reactions between a fuel (ethanol) and air accompanied by the production of heat and conversion of chemical species.

Ethanol and oxygen (air) combine in a chemical reaction with the help of a little bit of energy. The reaction results in a significant release of energy in the form of heat and light, as well as the formation of carbon dioxide and water. Complete combustion of ethanol forms carbon dioxide and water vapor with a specific heat of 2.44 kJ. The chemical reaction of combustion of Ethanol is given as below:

$$C_2H_5OH\ (l) + 3\ O_2\ (g) \dashrightarrow 2\ CO_2\ (g) + 3\ H_2O\ (g);$$

where, l, g stands for liquid and gaseous phases.

With the help of molecular formulas, Ethanol combustion can be characterized chemically. Ethanol, represented by C_2H_5OH, combines with six oxygen atoms denoted as ‘$3O_2$’. When the reaction is commenced through the addition of energy in the form of heat or a spark, $2CO_2$ and $3H_2O$ (two carbon dioxides and three water molecules) are formed. Energy is also released when the reaction occurs.

The Negative aspects of Ethanol combustion is that it produces a quiet flame that gives off few major pollutants when compared to petroleum-based fuels and Ethanol is a central nervous system depressant. Pure ethanol will irritate the skin and eyes.

2.2.1 Global reactions and combustion stoichiometry for Ethanol fuel

The global reaction for the oxidation of a fuel with air can be expressed as:

$$Fuel + x(O_2 + 3.76N_2) \rightarrow yCO_2 + zH_2O + kN_2 \quad (2.1)$$

where (O_2 + 3.76N_2) represents air, which consists roughly of 21% Oxygen and 79% Nitrogen. The coefficients x, y, k and z depend on the particular fuel and the fuel-air equivalence ratio of the reaction.

When the fuel contains oxygen (e.g., with alcohols), the procedure for determining the overall combustion equation is the same except that fuel oxygen is included in the oxygen balance between reactants and products. For ethyl alcohol (ethanol), C_2H_5OH, the stoichiometric combustion equation is

$$C_2H_5OH + 3(O_2 + 3.76N_2) = 2CO_2 + 3H_2O\ 11.28N_2 \quad (2.2)$$

The equivalence ratio (φ) is defined as

$$\varphi = \frac{FAR}{FAR(stoich)} \quad (2.3)$$

where *FAR* is the fuel to air ratio and *FAR(stoich.)* is stoichiometric fuel to air ratio

When the right proportion of both are available to completely consume all fuel and oxygen molecules. $\Phi = 1$ corresponds to a stoichiometric ratio, $\phi<1$ is lean (excess air), and $\phi>1$ is rich (excess fuel). In cases of lean combustion, the above equation must also include unconsumed O_2 as a product on the right-hand-side of the equation. The stoichiometric air-fuel ratio for several common fuels is listed in the following table.

Table 2.2 Stoichiometric air-fuel ratios (by mass) for common fuels

Fuel	**(AFR)***stoich*
Methane	17.2
Propane	15.7
Butane	15.5
Gasoline	14.5-14.7
Ethanol	9.0

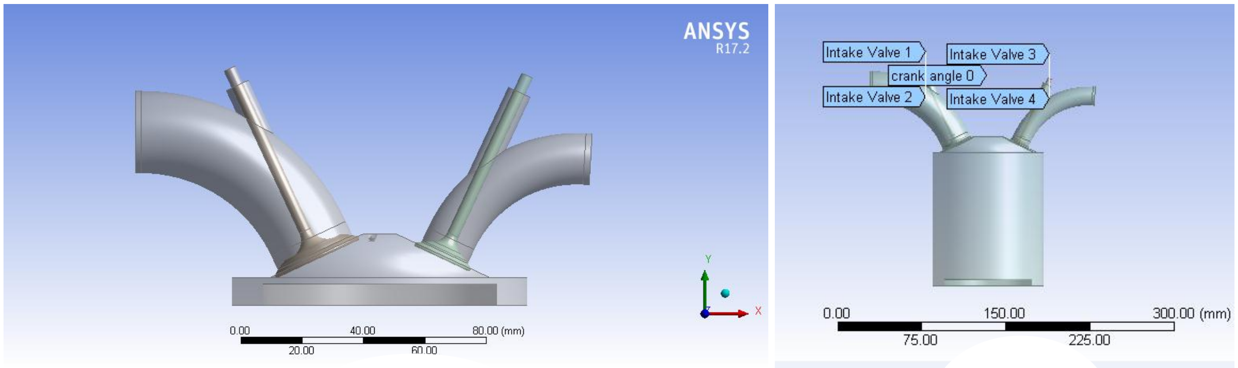
Chapter Three

CFD Modeling of HCCI engine

The HCCI engine parameters and technical specifications for the simulations are prepared accordingly and given in Table 3.1. An inlet and outlet manifold of the engine has sketched as shown in Figure 3.1. Individual control of the intake charge temperature for each cylinder is provided. For validation purpose, the experimental results of HCCI engine of Lawrence Livermore has been taken.

Table 3.1. Technical specifications of the model HCCI engine

Engine input	**Definition**	**Value(if constant)**
α	**Crank radius**	**55mm**
B	**Cylinder bore**	**98mm**
l	**Connecting rod length**	**144.3**
L	**Stroke**	**90mm**
V_l	**Minimum lift**	**2mm**
ω	**Engine speed**	**2000 RPM**
IVC	**Inlet Valve Close**	**577^{O}**
EVO	**Exhaust Valve Open**	**833^{O}**
CR	**Compression Ratio**	**11.96:1**
SOFI	**Start of fuel injection**	**721^{o} aBDC**



(a)

(b)

Figure 3.1: (a) Normal geometry and (b) decomposed geometry of HCCI engine

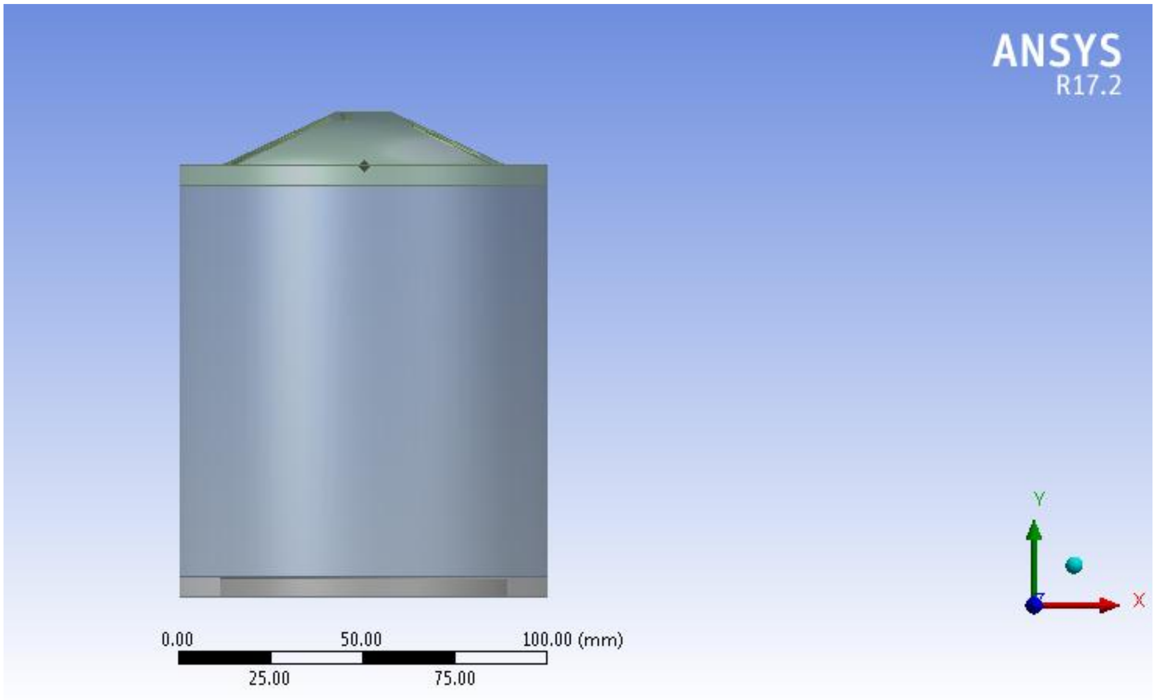


Figure 3.2: Geometry of combustion chamber after decomposition

3.1 Simulation Setting

The CFD simulation model is prepared according to WO4D HCCI engine that operates at the constant speed of 2000 RPM. ANSYS 17.2 ICE was utilized to draw the engine components. Port flow, Cold flow and Combustion are the simulation types done according to the pre-conditioned input Initial and Boundary conditions. When starting the modeling processes with the ANSYS ICE software, the following steps are followed.

- Launch IC Engine system.
- Read an existing geometry into IC Engine.
- Decompose the geometry.
- Define the mesh setup and mesh the geometry.
- Run the simulation.

- ➢ Examine the results in the report.
- ➢ Perform additional post-processing in CFD-Post.

The following settings have been used for simulation purpose in ANSYS 17.2 Fluent:

Mixture material: Ethanol and Air

Fuel species: C_2H_5OH

Solver: ANYSYS 17.2 FLUENT

Start of fuel injection: at CA721

End of fuel injection: at CA743

Cone fuel spray angle: 7^O

Soot model: Mass- Brooks

Post processing quantities are Velocity, Pressure, Temperature, TKE, turbulent dissipation rate, turbulent viscosity, Discrete phase mass of fuel and Phi.

The normal full geometry of the designed combustion chamber has a displacement volume of 793.8 cm^3, but to eliminate long computational time for the ANSYS ICE, the geometry is reduced to one-sixth portion of combustion chamber called sector as shown in figure 5 below.

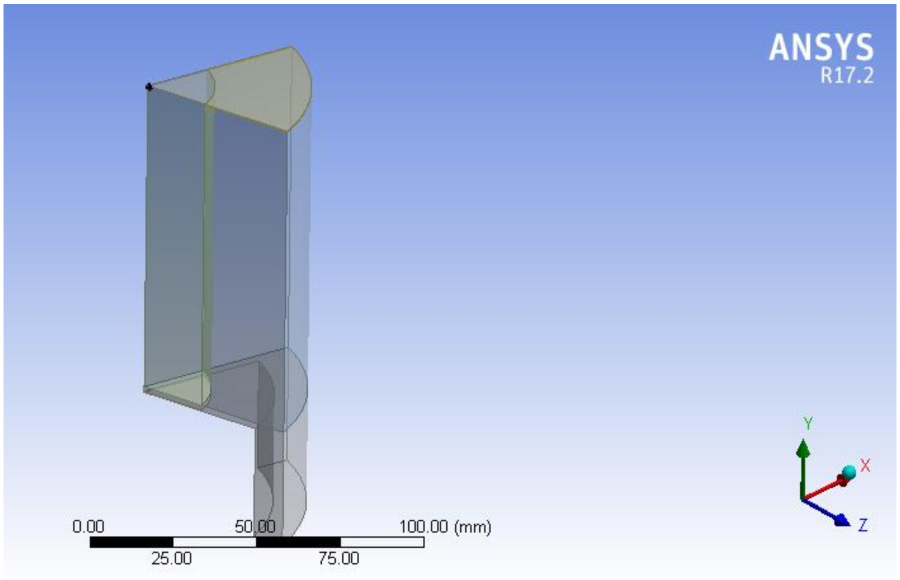


Figure 3.3: Sector portion the geometry of the combustion chamber

3.2 HCCI Engine Combustion Cycle Model

The HCCI engine model satisfy the complete engine power cycles having suction, compression, expansion and exhaust strokes. However, to decrease the computation time, the input option for intake valve closing (IVC) and intake valve opening (EV0) from (IVC) at CA570 to (EVO) at CA833, i.e. describing the properties of air-fuel mixture in a combustion chamber along with in-cylinder temperature and pressure throughout the cycle is used for this research. Here the cycle started after the homogeneous air-ethanol mixture enters the combustion chamber when intake valve is closed until the exhaust valve opens for discharge of exhaust gas and combustion byproducts. It is noted that the cycle takes 263 number of crank angle (CA) to finish the cycle.

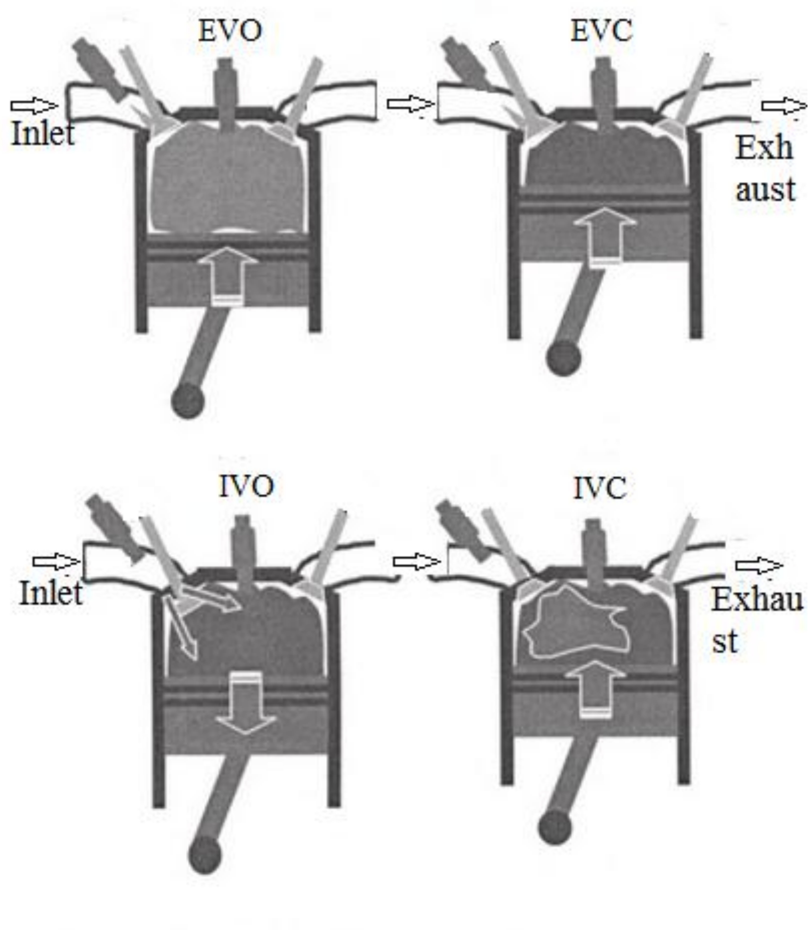


Figure 3.4: HCCI engine operating cycle between IVC and EVO

Chapter Four

Turbulent mixing and Combustion in HCCI Engine

Turbulent mixing designates the mass transport due to turbulence. Turbulence characterizes the chaotic and unsteady motion found in most technical fluid flow applications. Turbulence occurs when the inertial forces are much greater as compared to the viscous ones. Thus, the most important parameter of turbulence is the Reynolds number giving the ratio of the inertial forces to the viscous forces,

$$\mathbf{Re} = \frac{\boldsymbol{uL}}{\boldsymbol{v}} \qquad (4.1)$$

where $\boldsymbol{u}$ is a characteristic velocity and $\boldsymbol{L}$ a characteristic length of the flow and $\boldsymbol{v}$ is kinematic viscosity. $\boldsymbol{L}$ corresponds to the largest scales of the flow. If the Reynolds number is high enough, the flow is turbulent, i.e. even in simple flow situations, as pipe flow, the velocity field can be highly unsteady and chaotic.

In general, reactive mixing can be distinguished from passive mixing. In reactive mixing the mass transport influences the flow properties, whereas in passive mixing, as the name indicates, the transport is passive, i.e. it does not influence the flow field.

This thesis will only consider passive mixing. The mechanisms governing the passive mixing are advection and molecular diffusion. Advection is the transport of mass by the flow and particularly by turbulence. Molecular diffusion is the process caused by motions on the molecular level (Brownian motion). In fluids, molecules are constantly moving in all directions and interacting with other molecules. [3]

In the presence of two species this motion gives a net transport from one species to the other one. In the absence of high temperature and pressure gradients, molecular diffusion acts against the gradient of the transport quantity and the resulting flux is proportional to the gradient of the transport quantity (concentration). Thus, the flux Ji can be expressed by Fick's law,

$$\mathbf{J_i} = -\,\boldsymbol{\kappa}\,\frac{\boldsymbol{\partial \emptyset}}{\boldsymbol{\partial xi}} \qquad (4.2)$$

where $\boldsymbol{\kappa}$ is the diffusion coefficient and φ is some transported scalar (e.g. a concentration). For high Reynolds numbers, molecular diffusion is much slower than advection.

Turbulence can be defined as fluctuations in fluid flow which is used to enhance the air-fuel mixture. A steady flow of air-fuel would have low turbulence while an unsteady flow of air-fuel would have higher turbulence. A uniform measurement scale is needed to measure the magnitude of turbulence and is called Turbulence Intensity. Turbulence Intensity is a scale characterizing turbulence expressed as a percent.

$$\textbf{Turbulence Intensity (T.I.)} = \frac{\mathbf{u}'}{\boldsymbol{U}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.3)$$

u' = *the Root-Mean-Square (RMS), or Standard Deviation, of the turbulent velocity fluctuations at a particular location over a specified period of time*

U = *the average velocity at the same location over same time period*

An idealized flow of fluid with absolutely no fluctuations in air speed or direction would have a Turbulence Intensity value of 0%. This idealized case never occurs on earth. However, due to how Turbulence Intensity is calculated, values greater than 100% are possible. This can happen, for example, when the average air speed is small and there are large fluctuations present.

In order to compute turbulent mixing process, the equations governing the flow (and the turbulence) have to be solved. Additionally, to the flow equations, an equation for the mixing scalar is solved. Several approaches to the numerical solution of these equations have been proposed. The approaches can be categorized into three groups; Direct numerical simulation (DNS), Large eddy simulations (LES) and Reynolds averaged Navier-Stokes (RANS) computations. [10]

The flow processes in the engine cylinder are turbulent. In turbulent flows, the rates of transfer and mixing are several times greater than the rates due to molecular diffusion. This turbulent "diffusion" results from the local fluctuations in the flow field. It leads to increased rates of momentum and heat and mass transfer, and is essential to the satisfactory operation of spark-ignition and diesel engine & Turbulent flows are always dissipative.

4.1. Turbulent Combustion in HCCI engine

Combustion requires that fuel and oxidizer be mixed at the molecular level. How this takes place in turbulent combustion depends on the turbulent mixing process. The general view is that once a range of different size eddies has developed, strain and shear at the interface between the eddies enhance the mixing.

During the eddy break-up process and the formation of smaller eddies, strain and shear will increase and thereby steepen the concentration gradients at the interface between reactants, which in turn enhances their molecular inter diffusion. Molecular mixing of fuel and oxidizer, as a prerequisite of combustion, therefore takes place at the interface between small eddies. Similar considerations apply, once a flame has developed, to the conduction of heat and the diffusion of radicals out of the reaction zone at the interface.

HCCI combustion differs from isothermal mixing in chemically reacting flows by two specific features:

- heat release by combustion induces an increase of temperature, which in turn
- accelerates combustion chemistry. Because of the competition between chain branching and chain breaking reactions this process is very sensitive to temperature changes.

Heat release combined with temperature sensitive chemistry leads to typical combustion phenomena, such as ignition and extinction. This is illustrated in Figure 4.1 where the maximum temperature in a homogeneous flow combustor is plotted as a function of the Damkohler number, which here represents the ratio of the residence time to the chemical time. This is called the S-shaped curve in the combustion literature. [18]

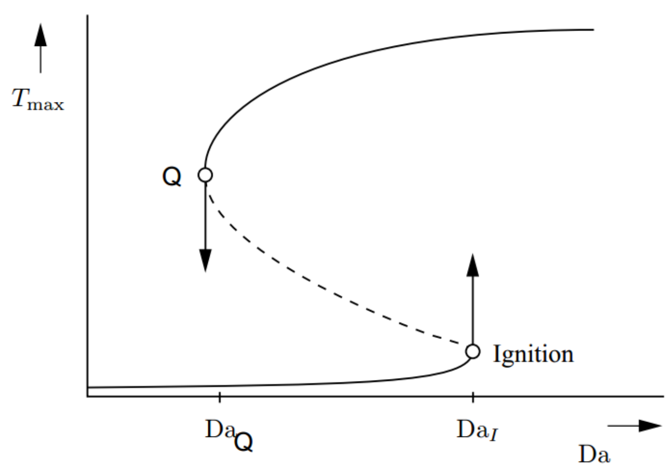


Figure 4.1: The S-shaped curve showing the maximum temperature in a well-stirred reactor as a function of the Damkohler number. [3]

The lower branch of this curve corresponds to a slowly reacting state of the combustor prior to ignition, where the short residence times prevent a thermal runaway. If the residence time is increased by lowering the flow velocity, for example, the Damkohler number increases until the ignition point ***I*** is reached. For values larger than DaI thermal runaway leads to a rapid unsteady transition to the upper close-to-equilibrium branch.

If one starts on that branch and decreases the Damkohler number, thereby moving to the left in Figure 4.1, one reaches the point Q where extinction occurs. This is equivalent to a rapid transition to the lower branch. The middle branch between the point I and Q is unstable.

4.2 Modeling Turbulence by ANSYS software

Turbulence is unsteady, irregular (aperiodic) motion in which transported quantities (mass, momentum, scalar species) fluctuate in time and space through identifiable swirling patterns. Turbulence enhances mixing (matter, momentum, energy, etc.) results.

Direct numerical simulation (DNS) is the solution of the time-dependent Navier-Stokes equations without recourse to modeling. Mesh size must be fine enough to resolve smallest eddies, yet sufficiently large to encompass complete model.

- Solution is inherently unsteady to capture convecting eddies.
- DNS is only practical for simple Low-Reynold flows such as ethanol- air mixture flow.
- Mean flow properties are generally sufficient; most turbulence models resolve the mean flow.
- There is no single, universally reliable engineering turbulence model for wide class of flows.
- Certain models contain more physics that may be better capable of predicting more complex flows including separation, swirl, etc.

The RANS based turbulence models calculate the Reynolds Stresses by one of two methods:
Using the Boussinesq assumption, the Reynolds stresses are related to the mean flow by turbulent viscosity, μ_t:

$$R_{ij} = -\rho\overline{u_i'u_j'} = \mu_t\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)-\frac{2}{3}\mu_t\frac{\partial U_k}{\partial x_k}\delta_{ij}-\frac{2}{3}\rho k\delta_{ij} \quad \text{....................................(4.4)}$$

ANSYS facilitates solving individual transport equations for the Reynolds stresses. For this research works, since turbulent viscosity is not employed, no assumption of isotropy contains more "physics" more complex and computationally expensive.

4.2.1 Navier–Stokes Equations and Turbulence Models

The classical approach to model turbulent flows are based on single point averages of the Navier–Stokes equations. These are commonly called Reynolds averaged Navier–Stokes equations (RANS). For this research work, let use the simplest model for turbulent flows, the k–ε model. Even though it certainly is the best compromise for engineering design using RANS, the predictive power of the k–ε model is, except for simple shear flows, often found to be disappointing. I will present it here, mainly to help us define turbulent length and time scales.

This can formally extend to formulation to non-constant density by introducing Favre averages. In addition, for non-constant density flows the Navier–Stokes equations are written in conservative form:

Continuity Equation: $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$……………………………………..…………………….(4.5)

Momentum Equation: $\frac{\partial \rho v}{\partial t} + \nabla \cdot (\rho v v) = -\nabla p + \nabla \cdot \tau + \rho g$…………………………………….(4.6)

In the two terms on the left-hand side of the above two equations represent the local rate of change and convection of momentum, respectively, while the first term on the right-hand side is the pressure gradient and the second term on the represents molecular transport due to viscosity. Here τ is the viscous stress tensor.

4.3 ANSYS Fluent's Standard *k-e* Model

Transport equation for *k*:

$$\rho \frac{Dk}{Dt} = \mu_t \left(\frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) \frac{\partial U_j}{\partial x_i} + \frac{\partial}{\partial x_i} \left\{ (\mu + \mu_t / \sigma_k) \frac{\partial k}{\partial x_i} \right\} - \rho \varepsilon + G_b - Y_M + S_k \quad \text{...............................(4.7)}$$

Transport equation for ε:

$$\rho \frac{D\varepsilon}{Dt} = C_{1\varepsilon}\left(\frac{\varepsilon}{k}\right)\left[\mu_t\left(\frac{\partial U_j}{\partial x_i}+\frac{\partial U_i}{\partial x_j}\right)\frac{\partial U_j}{\partial x_i}+C_{3\varepsilon}G_b\right]+\frac{\partial}{\partial x_i}\left\{(\mu+\mu_t/\sigma_\varepsilon)\frac{\partial \varepsilon}{\partial x_i}\right\}-C_{2\varepsilon}\rho\left(\frac{\varepsilon^2}{k}\right)+S_\varepsilon$$

Fluent's Standard *k-ε* Model

Transport equation for *k*:

$$\rho \frac{Dk}{Dt} = \mu_t\left(\frac{\partial U_j}{\partial x_i}+\frac{\partial U_i}{\partial x_j}\right)\frac{\partial U_j}{\partial x_i}+\frac{\partial}{\partial x_i}\left\{(\mu+\mu_t/\sigma_k)\frac{\partial k}{\partial x_i}\right\}-\rho\varepsilon+G_b-Y_M+S_k$$
..............................(4.8)

Transport equation for ε:

$$\rho \frac{D\varepsilon}{Dt} = C_{1\varepsilon}\left(\frac{\varepsilon}{k}\right)\left[\mu_t\left(\frac{\partial U_j}{\partial x_i}+\frac{\partial U_i}{\partial x_j}\right)\frac{\partial U_j}{\partial x_i}+C_{3\varepsilon}G_b\right]+\frac{\partial}{\partial x_i}\left\{(\mu+\mu_t/\sigma_\varepsilon)\frac{\partial \varepsilon}{\partial x_i}\right\}-C_{2\varepsilon}\rho\left(\frac{\varepsilon^2}{k}\right)+S_\varepsilon$$

Where, Turbulent viscosity: $\mu_t \equiv \rho C_\mu k^2/\varepsilon$

$\sigma_{k,}\sigma_\varepsilon, C_{1\varepsilon}, C_{2\varepsilon}, C_{3\varepsilon}, C_\mu$ are empirically defined constants.

Y_M compressibility effects (activated when ideal gas is used)

G_b is buoyancy,

S_k and S_ε user defined sources

ANSYS uses two equation turbulent models: Kinetic energy and Energy dissipation

$$\mu_t = \rho\, C_\mu \frac{k^2}{\varepsilon}$$
....(4.9)

We need to model k and ε Two additional equations kinetic energy and dissipation respectively.

$$\rho\left(\frac{\partial k}{\partial \tau}+\mathrm{div}(k\vec{V})\right) = \mathrm{div}\left[(\mu+\mu_t/\sigma_\mu)\mathrm{grad}\ k\right]+2\mu_t E_{ij}E_{ij} - \rho\varepsilon$$

$$\rho\left(\frac{\partial \varepsilon}{\partial \tau}+\mathrm{div}(\varepsilon\vec{V})\right) = \mathrm{div}\left[(\mu+\mu_t/\sigma_\varepsilon)\mathrm{grad}\ \varepsilon\right]+C_{1\varepsilon} f_1 2\mu_t E_{ij}E_{ij} - C_{2\varepsilon} f_2 2\rho\frac{\varepsilon^2}{k}$$

Reynolds Averaged Navier Stokes equations

Continuity Equation: $\frac{\partial V_x}{\partial x}+\frac{\partial V_y}{\partial y}+\frac{\partial V_z}{\partial z}=0$ ....(4.10)

Momentum Equation for x,y,z respectively:

$$\rho(\frac{\partial V_x}{\partial \tau}+V_x\frac{\partial V_x}{\partial x}+V_y\frac{\partial V_x}{\partial y}+V_z\frac{\partial V_x}{\partial z})=-\frac{\partial P}{\partial x}+\frac{\partial}{\partial x}[(\mu+\mu_t)\frac{\partial V_y}{\partial x}]+\frac{\partial}{\partial y}[(\mu+\mu_t)\frac{\partial V_y}{\partial y}]+\frac{\partial}{\partial z}[(\mu+\mu_t)\frac{\partial V_y}{\partial z}]+S_x$$

$$\rho(\frac{\partial V_y}{\partial \tau}+V_x\frac{\partial V_y}{\partial x}+V_y\frac{\partial V_y}{\partial y}+V_z\frac{\partial V_y}{\partial z})=-\frac{\partial P}{\partial y}+\frac{\partial}{\partial x}[(\mu+\mu_t)\frac{\partial V_y}{\partial x}]+\frac{\partial}{\partial y}[(\mu+\mu_t)\frac{\partial V_y}{\partial y}]+\frac{\partial}{\partial z}[(\mu+\mu_t)\frac{\partial V_y}{\partial z}]+S_y$$

$$\rho(\frac{\partial V_z}{\partial \tau}+V_x\frac{\partial V_z}{\partial x}+V_y\frac{\partial V_z}{\partial y}+V_z\frac{\partial V_z}{\partial z})=-\frac{\partial P}{\partial z}+\frac{\partial}{\partial x}[(\mu+\mu_t)\frac{\partial V_z}{\partial x}]+\frac{\partial}{\partial y}[(\mu+\mu_t)\frac{\partial V_z}{\partial y}]+\frac{\partial}{\partial z}[(\mu+\mu_t)\frac{\partial V_z}{\partial z}]+S_z$$

ANSYS software uses the following General CFD Equations to compute turbulence:

$\rho\frac{\partial \Phi}{\partial \tau}+\rho\,\mathrm{div}\overset{\vee}{V}\Phi=\mathrm{div}(\Gamma_{\Phi,eff}\ \mathrm{grad}\ \Phi)+S_\Phi$ ....(4.11)

Equation	**Φ**	$\Gamma_{\Phi,eff}$	S_Φ
Continuity	1	0	0
x-momentum	V_1	$\mu+\mu_t$	$-\partial P/\partial x+Sx$
y-momentum	V_2	$\mu+\mu_t$	$-\partial P/\partial y-\rho g\beta(T_\infty-T_{wall})+Sy$
z-momentum	V_3	$\mu+\mu_t$	$-\partial P/\partial z+Sz$
T-equation	T	$\mu/\sigma_l+\mu_t/\sigma_t$	S_T
k-equation	k	$(\mu+\mu_t)/\sigma_k$	$G-\rho\varepsilon+G_B$
ε-equation	ε	$(\mu+\mu_t)/\sigma_\varepsilon$	$[\varepsilon(C_{\varepsilon1}G-C_{\varepsilon2}\rho\varepsilon)/k]+C_{\varepsilon3}G_B(\varepsilon/k)$
Species	C	$(\mu+\mu_t)/\sigma_c$	S_C

Age of air	τ	$\mu + \mu_t$	ρ
$\mu_t = \rho C_\mu k^2/\varepsilon$, $G = \mu_t (\partial U_i/\partial x_j + \partial U_j/\partial x_i)\, \partial U_i/\partial x_j$, $G_B = -g(\beta/C_p)(\mu_t/\sigma_{T,t})\, \partial T/\partial x_i$			
$C_{\varepsilon 1}=1.44$, $C_{\varepsilon 2}=1.92$, $C_{\varepsilon 3}=1.44$, $C_\mu=0.09$, $\sigma_t=0.9$, $\sigma_k=1.0$, $\sigma_\varepsilon=1.3$, $\sigma_C=1.0$			

4.4 Ethanol–air mixing length

Ethanol and air experience a velocity difference which can be approximated as:

$$\Delta U = l_m \frac{\Delta U}{\Delta y} \approx l_m \frac{dU}{dy} \quad \text{...(4.12)}$$

The distance between the two layers l_m is called mixing length. Since ΔU has the same order of magnitude as u', Prandtl arrived at

$$|u'| = l_m \left|\frac{dU}{dy}\right|$$

By virtue of the Prandtl hypothesis, the longitudinal fluctuation component u' was brought about by the impact of the lateral component v', it seems reasonable to assume that

$$|u'| \propto |v'| \quad \therefore \quad |v'| = C_1 l_m \left|\frac{dU}{dy}\right| \quad \text{...(4.13)}$$

Prandtl Mixing Length Model

Thus, the component of the Reynolds stress tensor becomes

$$\overline{u'v'} = -C_2 l_m^2 \left(\frac{dU}{dy}\right)^2$$

The turbulent shear stress component becomes:

$$\tau_{turbulent,xy} = -\rho \overline{u'v'} = \rho C_2 l_m^2 \left[\frac{dU}{dy}\right]^2 \quad \text{....................(4.14)}$$

Prandtl define *wall friction velocity* using the wall shear stress by the relation

$$u_\tau = \sqrt{\frac{\tau_{wall}}{\rho}} \quad \text{...(4.15)}$$

4.5 Ethanol Premixed turbulent combustion in HCCI Engine

Premixed combustion requires that fuel (Ethanol) and oxidizer (air) be completely mixed before combustion is allowed to take place in combustion chamber. In this research case ethanol and air are mixed before they enter into the combustion chamber. Such a premixing is only possible at sufficiently low temperatures where the chain-branching mechanism that drives the reaction chain in hydrogen and hydrocarbon oxidation is unable to compete with the effect of three-body chain-breaking reactions. Under such low temperature conditions combustion reactions are said to be "frozen." At ambient pressures the crossover from chain-branching to chain-breaking happens when the temperature decreases to values lower than approximately 1,000 K for hydrogen flames or lower than approximately 1,300 K for hydrocarbon flames. The frozen state is metastable, because a sufficiently strong heat source, a spark for example, can raise the temperature beyond the crossover temperature and initiate combustion.

Once ethanol and air have homogeneously been mixed and a heat source is supplied it becomes possible for a flame front to propagate through the mixture. This will happen if the fuel-to-air ratio lies between the flammability limits: Flammable mixtures range typically from approximately $\varphi = 0.5$ to $\varphi = 1.5$, where φ is the fuel-air-equivalence ratio for ethanol fuel.

Owing to the temperature sensitivity of the reaction rates the gas behind the flame front rapidly approaches the burnt gas state close to chemical equilibrium, while the mixture in front of the flame typically remains in the unburnt state. Therefore, the combustion system on the whole contains two stable states, the unburnt and the burnt gas state. In premixed combustion both states exist in the system at the same time; they are spatially separated by the flame front where the transition from one to the other takes place. [19]

4.6 HCCI Emissions Formation

Because ethanol fueled HCCI operates on lean mixtures, the peak temperatures are lower in comparison to spark ignition (SI) and Diesel engines. The low peak temperatures prevent the formation of NOx. This leads to NOx emissions at levels far less than those found in traditional engines.

As mentioned, no fuel-rich zones should exist in ethanol HCCI combustion, and therefore the soot emissions should be low. This theory is supported by reference [21], where soot measurements for HCCI combustion is discussed, both measured particulate matter (PM) and with a Bosch Smoke

Number (BSN). They found that when the engine was operated in HCCI mode the soot emissions were always near zero.

NOx emissions are generally very low for HCCI combustion due to the low combustion temperature. NOx formation is generally governed by the very temperature sensitive Zeldovich mechanism, which implies that the NOx formation has a very high activation energy, and is only sufficiently fast at higher temperatures (above 1700 K) [2]. One of the drawbacks for HCCI combustion are the HC and CO emissions, which are relatively high compared to SI and CI engines, due to the low combustion temperature. The low combustion temperature also leads to lower exhaust gas temperatures, especially near the walls of the combustion chamber. This leads to high carbon monoxide and hydrocarbon emissions. An oxidizing catalyst would be effective at removing the regulated species because the exhaust is still oxygen rich.

Generally, the following are some of the commonly known emissions and their effects on HCCI engines:

NOx Emission - Some of the important mechanisms for formation of NOx in IC engines are: thermal or zeldovich mechanism, Fenimore or promote mechanism, N_2O-intermediate mechanism, NNH mechanism. The minimum activation temperature required for breaking the N_2 bond is approximately 1800K. In the case of an ethanol fueled HCCI engine, the peak temperature of combustion remains below 800K due to the lean and dilute mixture. This inhibits breaking the N_2 triple bonds and therefore avoids NOx formation. SI and CI engines temperature can go as high as 2500K, which exponentially increases formation of NOx during exhaust. Hence NOx emission in an HCCI engine is significantly smaller compared to their counterpart SI and CI engines.

Soot - The main factor for soot formation in an IC engine is because of the rich mixture region which lacks a complete breakdown of hydrocarbon due to insufficient availability of oxygen at the time of combustion.

But in the case of ethanol HCCI engines, the charge inducted in the combustion chamber is leaner and well mixed (homogeneously mixture), which inhibits the formation of pockets of the hydrocarbon chains, thus removing the cause for soot formation.

HC/CO emission - In-cylinder peak temperature is an important factor in deciding the HC/CO emission from an IC engine. Lower in-cylinder temperatures result in increased emissions. The low peak in-cylinder temperature of an ethanol HCCI engine creates a major challenge to limit these emissions.

4.7 Parameters Affecting Ethanol HCCI Combustion

4.7.1 In-homogeneities

Basically two types of in-homogeneities considered inside the cylinder temperature & mixture (air-fuel) in-homogeneity & that would have certain effects on combustion. For a perfectly homogeneous mixture the thermal efficiency is quite high with significantly low NOx, also the combustion duration would be short. But in case of temperature in-homogeneity combustion duration become longer at the expense of lower thermal efficiency & higher NOx emission.

The temperature In-homogeneity mainly originates from the mixing of the fresh charge with exhaust gas (EGR) & wall heat transfer. If temperature in homogeneity become significant, then combustion is likely to be incomplete since colder parts of the mixture probably would not burn. Thus it is important to control the temperature In-homogeneity & intake temperature to achieve proper combustion without degrading thermal efficiency & without higher NOx. As far as combustible mixture is concerned higher the fuel in-homogeneity lengthens combustion. In-homogeneity in cylinder may have an ability of reducing pressure increase rate, maximize pressure & consequently knocking intensity, which means certain control can be established by introducing appropriate in- homogeneities to the in-cylinder mixture.

4.7.2 Equivalence (A/F) Ratio

If the cylinder is hypothetically meshed into zones as function of temperature, high temperature zones ignite before low temperature zones. Among zones within the same temperature range, secondary effect then appears to be the equivalence ratio (a zone with higher F/A ignites before even if its Temperature is slightly lower). Furthermore, equivalence ratio influences the combustion rate as well. The higher this ratio, the higher will be the rate at which temperature increases & the higher will be the peak value of temperature. Thereby combustion proceeds more rapidly.

4.7.3 Temperature & pressure

A] Temperature:

A reduction in initial temperature delays the ignition tie significantly, slowing down the overall oxidation process. The higher the intake temperature, the sooner will be the combustion. For low octane number fuels, first-stage heat release is high, ignition is attained before TDC & increasing the intake charge temperature advances the ignition gradually; whereas for high octane number fuels first stage heat release is low, hence the temperature rises mainly because of compression work. Thus effect of intake temperature on phasing becomes more significant for these kinds of fuels.

B] Pressure:

For fixed intake charge temperature, boosting the charge the effect of advancing the ignition; in other words, boosting reduces the need for higher temperature at the BDC.

4.7.4 Exhaust Gas Recirculation (EGR)

Exhaust gas re-circulation is a method of reducing peak combustion temperature which in turn reduces oxygen available for combustion. It essentially consists of a reaction chamber in the immediate vicinity of exhaust manifold. EGR can be considered as an inert gas that absorbs heat during his combustion reducing the combustion rate. It increases the inlet temperature when mixed with the fresh charge, decreases the O_2 concentration, increases the heat capacity of the mixture owing to the high heat capacities of CO_2 & water vapors (which reduces the temperature at the end of the compression) & introduces chemical species into fresh charge that will take part in chemical reactions.

Air is injected to the exhaust in this chamber and makes it inert. A part of this exhaust sample is re-circulated back to the engine combustion chamber. EGR considerably minimizes emissions of oxides of nitrogen, carbon monoxides and unburnt hydrocarbons so that fuel economy is achieved.

4.8 Fuel composition/ octane number

Start of ignition is very sensitive to the fuel octane number; Ignition delay increases with increasing octane number generally it is observed that ignition delay becomes shorter as the first stage is greater & this is highly dependent on the concentration of the fuel with low octane number. Latent heat of vaporization appears to influence auto ignition as well. Molecules with heat of vaporization absorbs a great quantity of energy during vaporization & therefore decrease the temperature of the mixture, this makes ignition more difficult & narrows the operating range at low loads, the effect inverses for high loads.

4.9 Compression ratio

It is observed that the effect of compression ratio on HCCI combustion that decreasing the compression ratio delays the ignition process. Another thing is that at higher compression ratio HC emission increases. Two compression ratios are significant. The geometric compression ratio can be changed with a movable plunger at the top of the cylinder head. This system is used in diesel model aircraft engines. The effective compression ratio can be reduced from the geometric ratio by closing the intake valve either very late or very early with variable valve actuation (variable valve timing that enables the Miller cycle). Both approaches require energy to achieve fast response. Additionally, implementation is expensive, but is effective.

4.9.1 Raising the Compression Level:

If mileage and power are a concern, there are ways to get it back. The octane rating of ethanol is much higher than gasoline and typical resides in the 100 to 105 range. For this reason, the compression ratio of an engine can be raised without fear of detonation (a symptom where multiple flame fronts appear during ignition and the collisions cause high mechanical stresses on engine parts).

Before ethanol, most engines ran an 8:1 compression ratio but today's engines are running to 10:1 compression ratios. On ethanol this ratio could be increased to 12:5 to 14:1. This property may tend itself well to a super or turbo charged engine, where the compression can be raised by merely changing a pulley or impeller speed to cause a higher boost ratio.

Another method is to mill-the-head, lowering it closer to the piston and reducing the clearance volume but this requires major engine modifications and may preclude the engine from running on regular unleaded fuels. Thus, accordingly, for this project the compression ratio is 11.96:1

4.10 Challenges facing ethanol HCCI combustion

Although ethanol fueled HCCI combustion engine can be achieved using the methods such as using EGR as described above, it presents several hurdles and challenges which need to be overcome before commercial application can be considered.

The first is to control the phasing and rate of combustion for best fuel economy and lowest pollutant emissions. Unlike SI combustion, HCCI combustion is achieved by controlling the temperature, pressure and composition of the in-cylinder mixture through the following parameters:

- EGR or residual rate
- Air/fuel ratio
- Compression ratio (CR)
- Inlet mixture temperature
- Inlet manifold pressure
- Fuel properties or fuel blends
- Injection timing and
- Coolant temperature.

Another major challenge blocking progression to commercial production of HCCI engines is the limited operating boundary compared with traditional SI operation. Knocking or violent combustion at high load and partial-burn or misfire at low load are the two main limiting regions in ethanol fueled HCCI combustion engine.

Generally, the attainable ethanol HCCI region is limited by three boundaries:

- misfire
- partial burn
- knock limit.

The first boundary defines the misfire region. At higher EGR rates, the CO_2 and H_2O content of the intake charge is raised significantly, causing the occasional failure of ignition. Higher EGR rates are obtainable as lambda is increased because there is increasingly more O_2 and less CO_2 and H_2O content in the intake charge, leading to more stable ignition and subsequent combustion.

As fuel flow-rate is decreased (lambda increase), the net heat-release is also decreased. The resulting gradual lowering of average combustion temperature leads to more unburned charge, characterized by high CO and unburned HC emissions, and by an increase in cycle-to-cycle variations. Knocking combustion occurs at the lower boundary (high-load) of the region. At the knock boundary, if no EGR is used, the richest lambda attainable is approximately 3.15. As EGR is increased, the knock limit is brought closer to lambda 1.0, with 43% EGR.

4.10.1 Cold Weather Starting

In colder climates, starting may be a concerned when using ethanol fueled HCCI engines. Alcohol contains much less explosion potential and has a lower heating point than regular gasoline, which prevents it from exploding well in a sub-freezing engine. Potential solutions to this are block and radiator heaters, running regular fuels during this time, starter fluid, raising the compression of the engine (to aid in explosion), or having a separate fuel tank with regular gas (and a switching valve).

Chapter Five

Results and Discussions

The turbulent mixing, performance, combustion and emission characteristics of the ethanol fuel in HCCI engine depend heavily on the thermo-physical properties of the ethanol. However, the instantaneous heat release rate, ignition delay, particulate matters and smoke emission are found to be more with ethanol fuel HCCI engine and can be controlled by turbulence mixing and addition of 0-30% EGR. Combustion behavior investigation is carried out on varied temperatures 0% to 30%. Emission test are done at 570CA and 833CA for air-fuel ratio of $\lambda = 3.0$ and 3.5 with EGR 0% and 30% respectively.

5.1 Turbulent Kinetic Energy

In this research, it is found that in order to increase the in-cylinder combustion in ethanol HCCI engine, a rich air-fuel mixture is required at the beginning (start) of combustion but the overall mixture needs to lean. Even though preparation of pre-mixed ethanol-air mixture is somehow difficult, increasing the turbulent kinetic energy will facilitate rapid combustion in the combustion chamber.

It is found that in cylinder increased swirl and tumble, by means of selecting appropriate engine design, will increase turbulent kinetic energy to burn the molecules of ethanol completely in combustion chamber which leads to improvements in the combustion efficiency.

As flow into the cylinder is turbulent and the mean velocity is often smaller than the turbulent velocities, high turbulence levels at ignition produce higher effective flame speeds, and more reliable combustion at very lean air-ethanol ratios, or with addition of EGR. Hence, in this research work, one possible reason for increasing swirl or tumble to promote high turbulence levels at ignition stage.

The in-cylinder turbulence during the intake and the early part of the compression stroke is noted as anisotropic. However, turbulence has been noted to become approximately homogeneous and isotropic in both swirling and tumbling flows as top dead center (TDC) is approached.

The turbulence model has been used in 'lumped mass' form in this research. The instantaneous values of turbulence kinetic energy and the turbulent eddy dissipation rate averaged over the entire combustion chamber volume are evaluated on the assumption that the in-cylinder turbulence is approximately homogeneous.

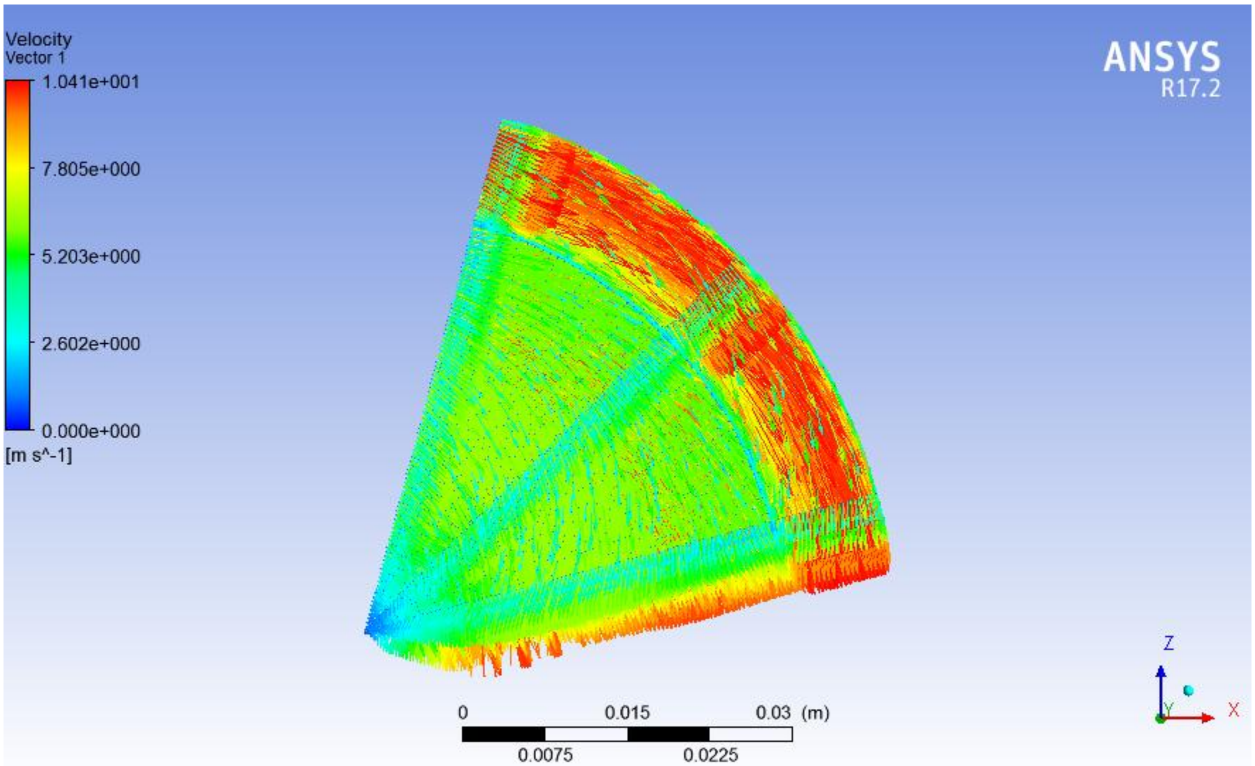


Figure 5.1: Velocity streamlines in sector combustion chamber, with 0% EGR

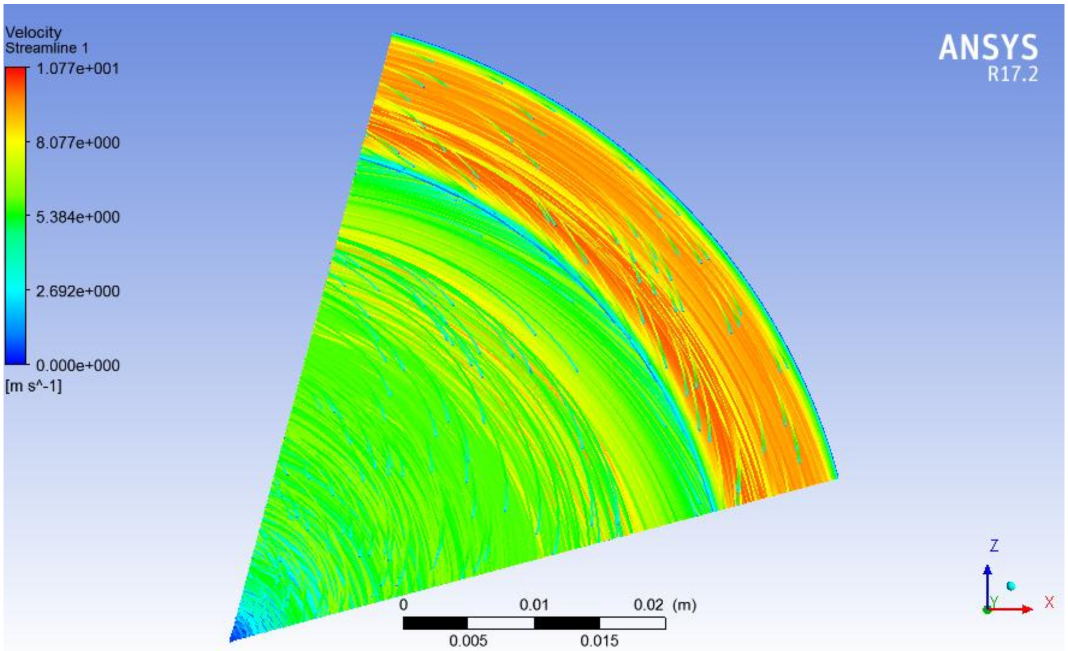


Figure 5.2: Velocity streamlines in sector combustion chamber, with 20% EGR

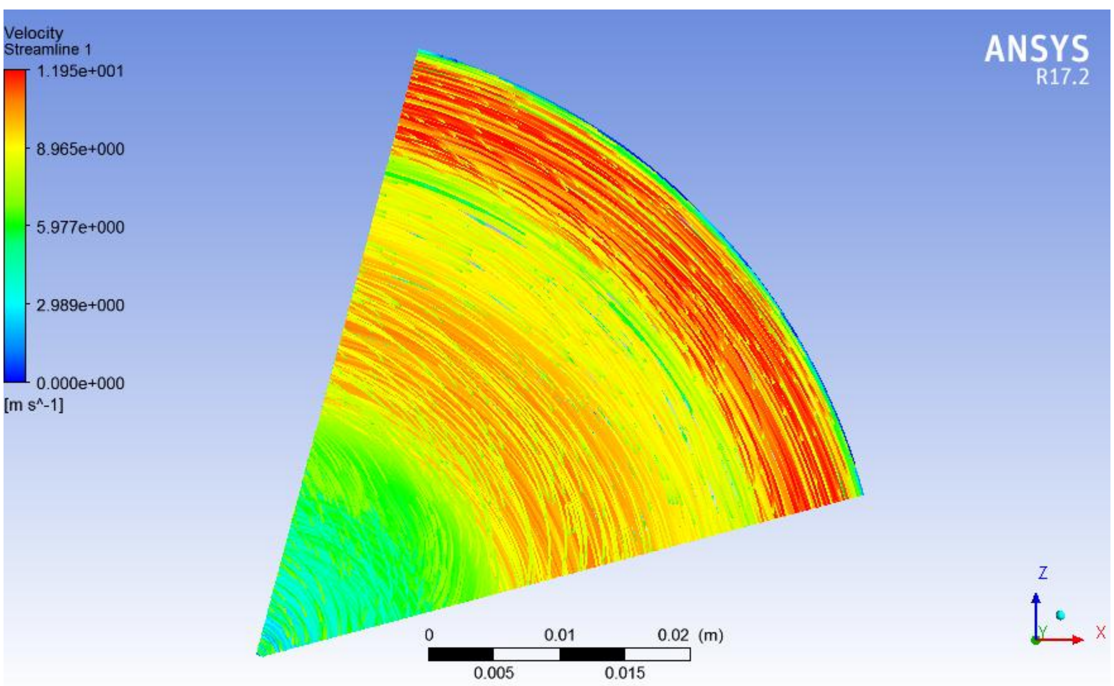


Figure 5.3: Velocity streamlines in sector combustion chamber, with 30% EGR

Since the flow of ethanol-air lean mixture in the HCCI engine cylinder is turbulent, viscous shear stresses perform deformation work on the fluid which increases its internal energy at the expense of its turbulence kinetic energy. A common source of energy for turbulent velocity fluctuations is shear in the mean flow. And this turbulent flows are always dissipative.

From simulation results, it seen that high turbulence levels facilitate rapid flame propagation and complete combustion during the power stroke in ethanol fueled HCCI engine. A well-mixed and highly turbulent air flow is critical to ensure the right air/fuel ratio throughout the combustion.

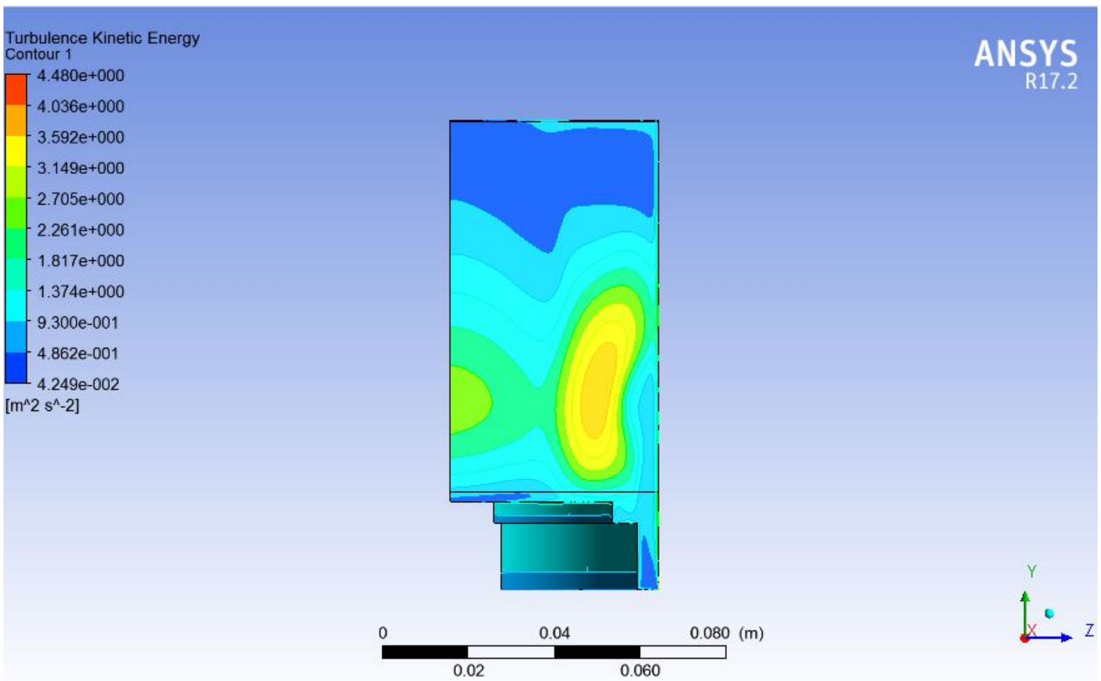


Figure 5.4: Turbulent Kinetic Energy contour in sector combustion chamber, 0%EGR

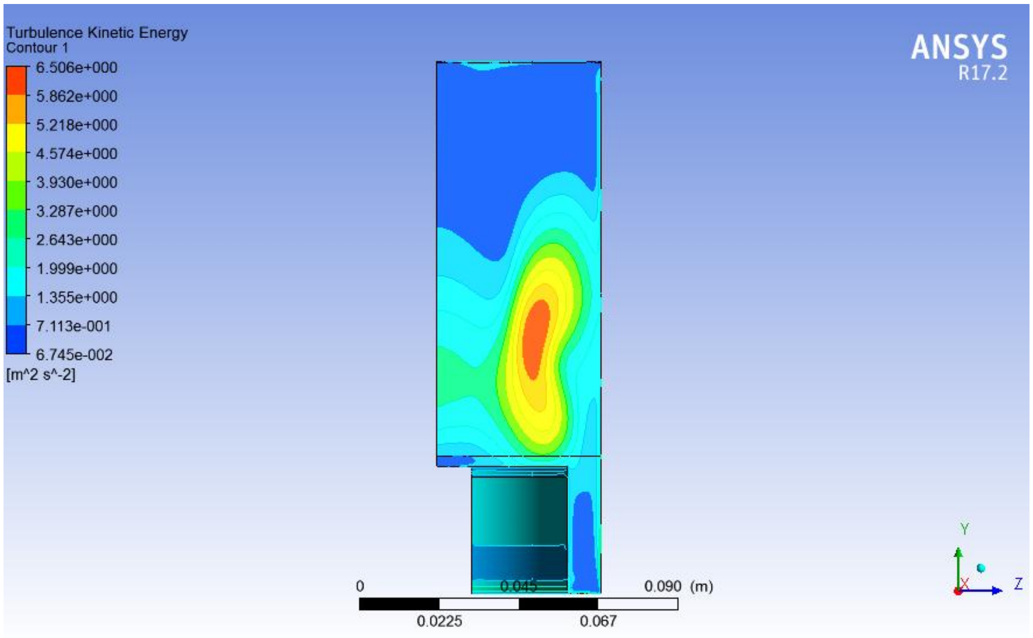


Figure 5.5: Turbulent Kinetic Energy contour in sector combustion chamber, 10%EGR

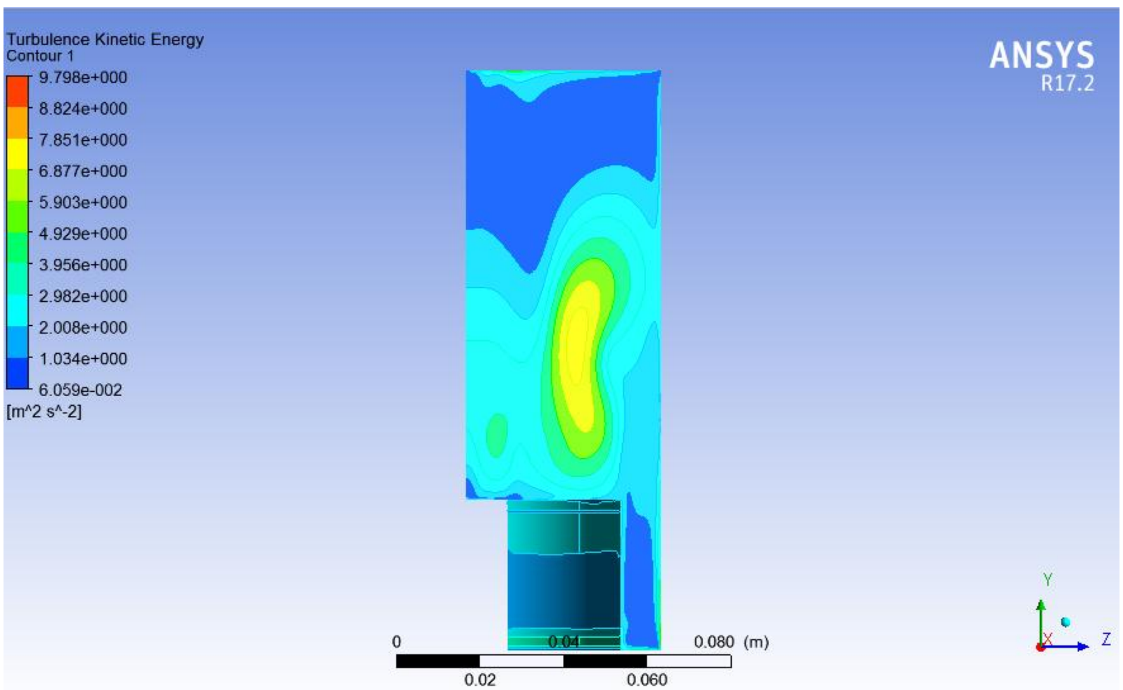


Figure 5.6: Turbulent Kinetic Energy contour in sector combustion chamber with 20% EGR

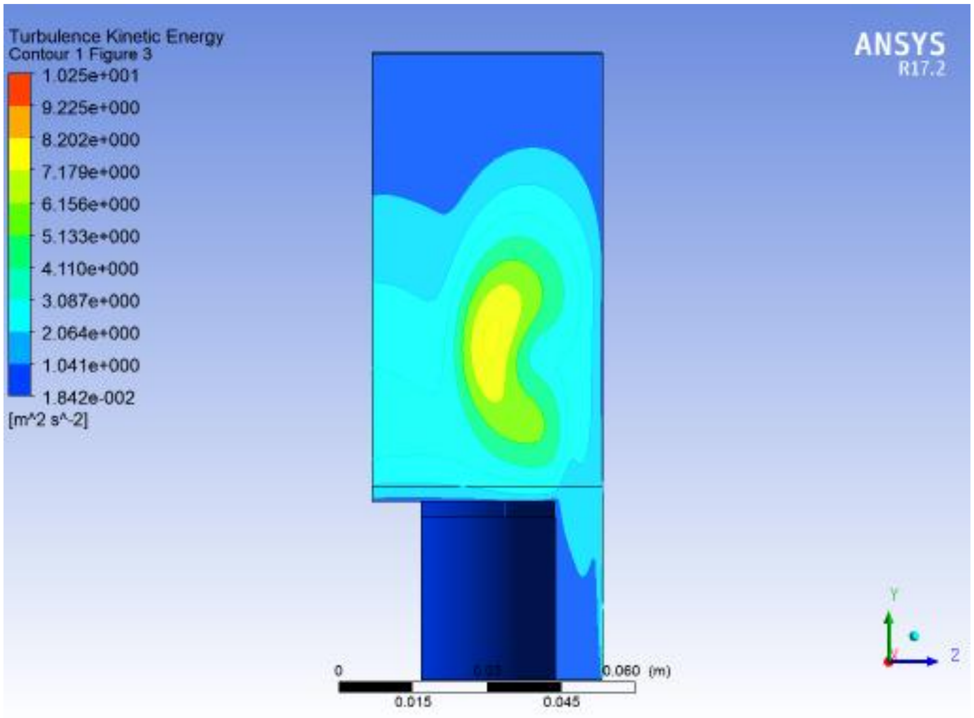


Figure 5.7: Turbulent Kinetic Energy contour in sector combustion chamber with 30% EGR

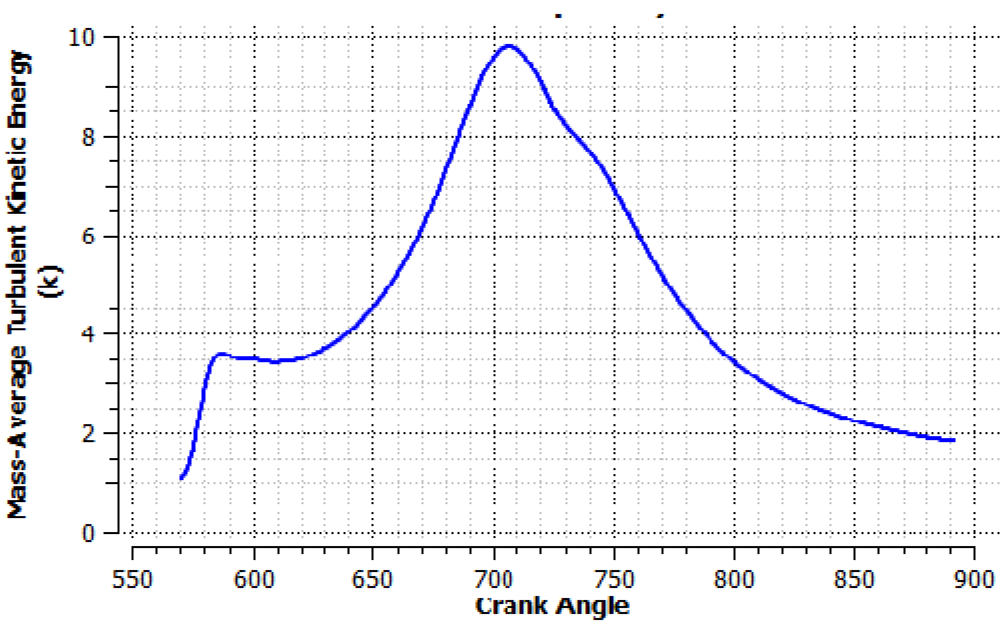


Figure 5.8: Mass average TKE versus Crank angle graph with 30% EGR

Generally, it is founded that the improved turbulence kinetic energy (TKE) in HCCI engine ensures higher turbulence which allows better mixing of Ethanol and air to create homogeneous mixture which will eventually improves the combustion efficiency.

5.2 Effect of use of hot EGR in Ethanol HCCI engine

In this research work, in order to achieve HCCI combustion fueled by ethanol, high intake charge temperatures and a copious amount of charge dilution must be utilized. In-cylinder gas temperature must have been sufficiently high to initiate and sustain the chemical reactions leading to auto ignition processes. Substantial charge dilution is necessary to control runaway rates of heat releasing reactions. Both of this requirements can be realized by recycling or trapping the burnt gases (EGR) within the cylinder.

In practice, hot burned gases (EGR) are preferred in most cases in order to increase cylinder charge temperature without external heating source. In order to study the effect of hot burned gases, the initial temperature of air-fuel mixture was assumed to at 400K and the burned gases temperature was between 700K and 1300K.

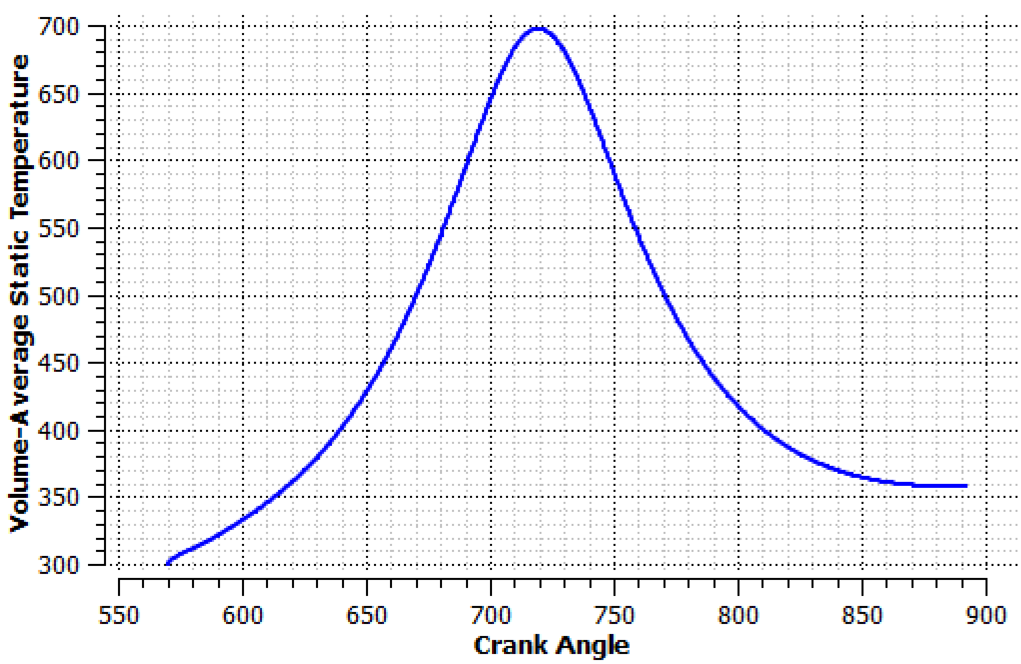


Figure 5.9: Combustion chamber's static temperature versus crank angle, 0%EGR

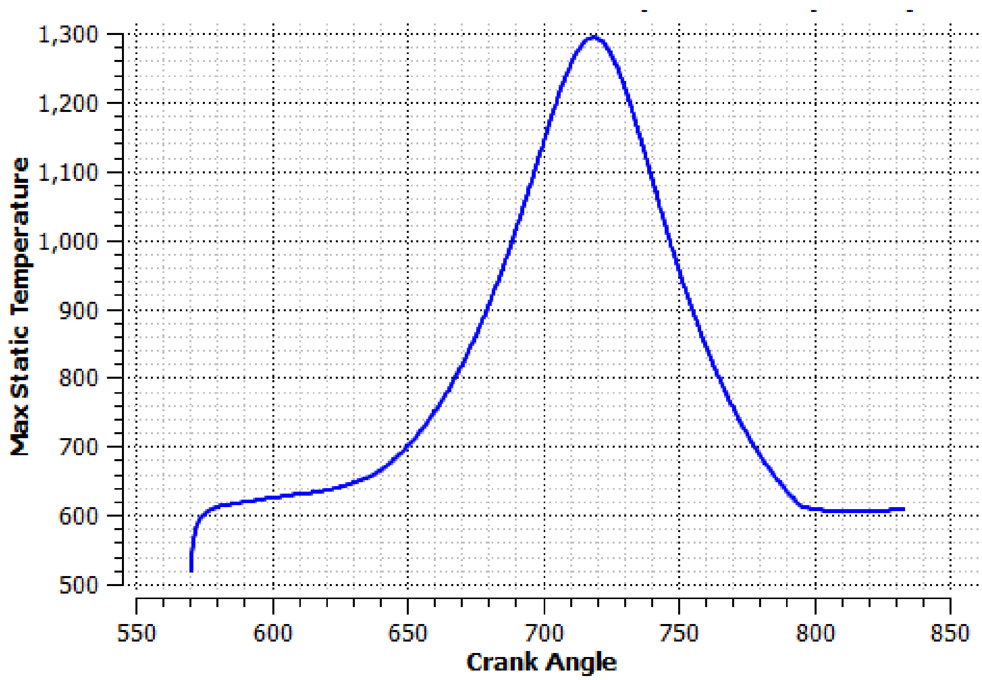


Figure 5.10: Maximum static temperature vs crank angle graph with 30% EGR

The addition of the EGR has brought a number of effects on HCCI combustion and emission processes within the cylinder. Firstly, if hot burned gases are mixed with the cooler inlet mixture of ethanol and air, the temperature of the intake charge increases resulting in heating effect of hot burnt gases of combustion of high octane ethanol. Secondly, the introduction of EGR in cylinder replaces some of the inlet air and hence causes a substantial reduction in the oxygen concentration. The reduction of air/oxygen due to the presence of EGR is called the dilution effect. Thirdly, the total heat capacity of the in-cylinder charge will be higher with burnt gases, mainly owing to higher specific heat capacity values of carbo dioxide and water vapor.

It is found here that if continued to add percentage of EGR more than 30%, the engine will misfire prior to the charge mixture reaches auto ignition temperature. This temperature criterion is achieved either by constraining hot residual gas or by heating intake air. This situation is shown in figure 5.11 when intake temperature is raised to 700K by addition of 40% EGR.

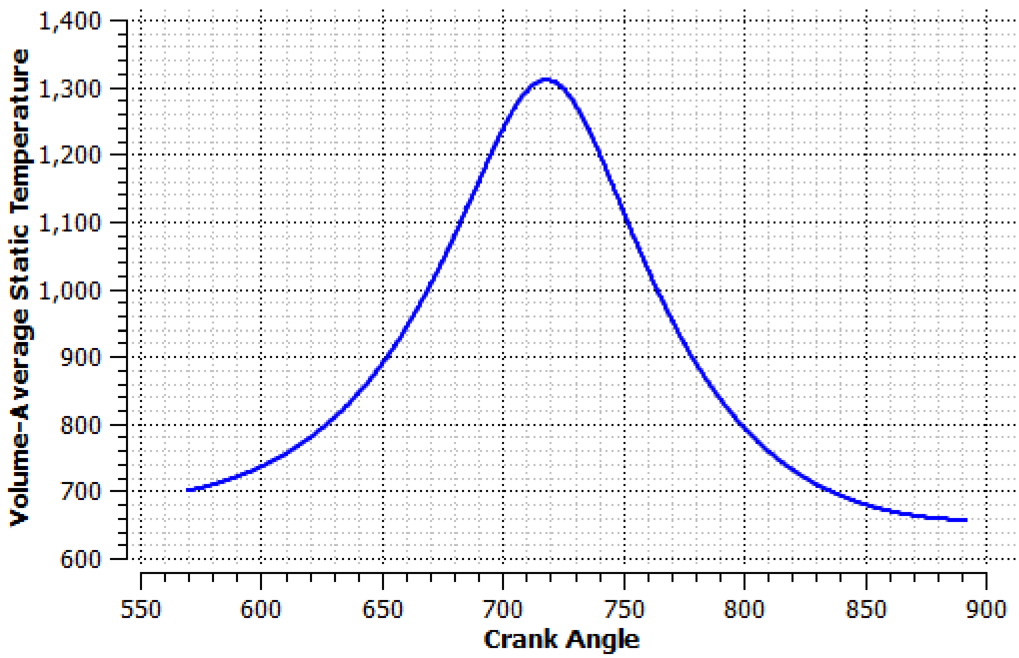


Figure 5.11 Volume average static temperature vs crank angle graph with 40% EGR

It is founded that the addition of EGR for oxygen rich air reduces the proportion of the cylinder contents available for combustion. This causes a correspondingly lower heat release and peak cylinder temperature, and reduces the formation of NOx. It is founded that because the required NOx reduction was quite modest, the allowed EGR back into the cylinder was no need for EGR cooling in this work.

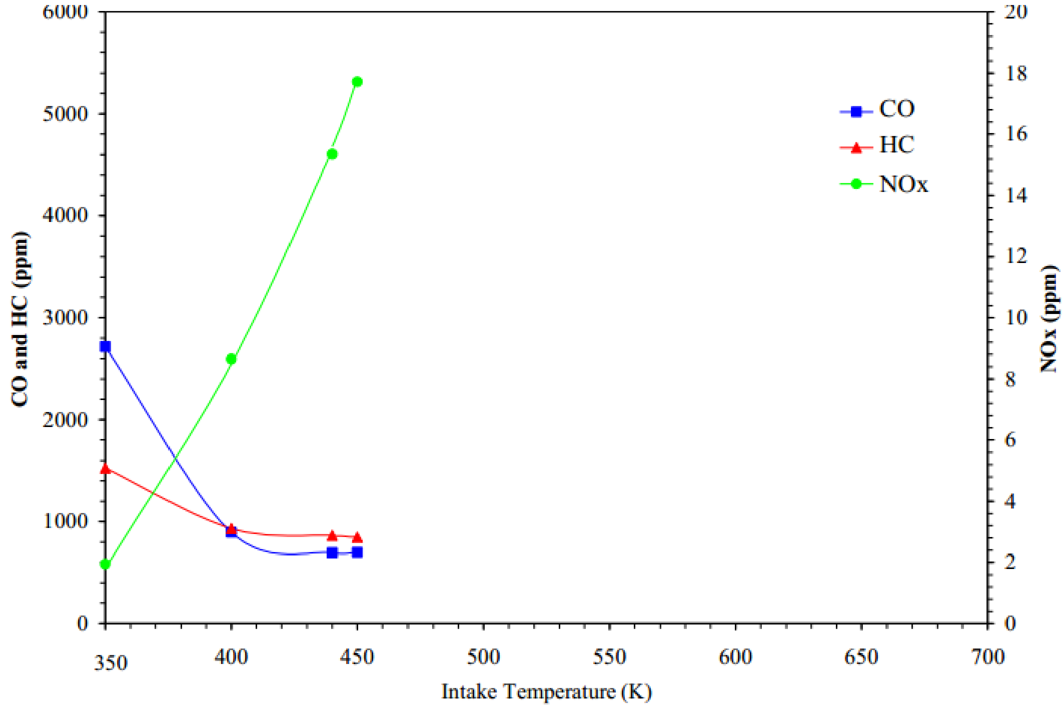


Figure 5.12: Ethanol HCCI with varying Intake Temperature, λ~3.0, 2000 RPM

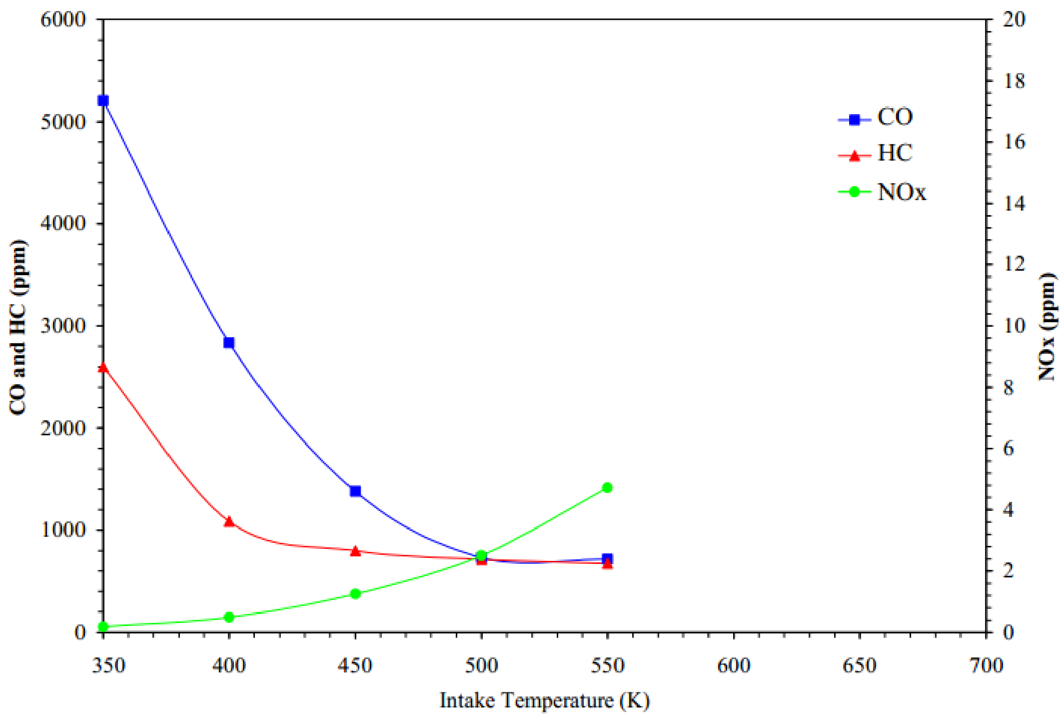


Figure 5.13: Ethanol HCCI with varying Intake Temperature, λ~3.5, 2000 RPM

At start of each simulation, hot EGR and ethanol –air mixture was assumed to be completely mixed and the intake charge temperature was then calculated assuming isentropic mixing. As expected, the initial charge temperature of the total in-cylinder charge was increased owing the heating effect of hot EGR, the relative air-fuel ratio was reduced as EGR replaced some of the air.

It is concluded that ethanol HCCI engine combustion can be controlled by varying the relative air-fuel ratio of the cylinder charge. Here the range of the burned gas concentration was limited by misfire at low concentration due to insufficient heating for auto-ignition to start and high concentration by incomplete combustion due to too much dilution.

As obtained from the simulation results shown in figure 19 above, during the compression stroke, the temperature of the premixed charge increases and reaches the point of auto- ignition; i.e. the mixture burns without the help of any ignition system. It is found that in this research, ethanol HCCI combustion starts at intake air temperature of approximately between 400K and 450K.

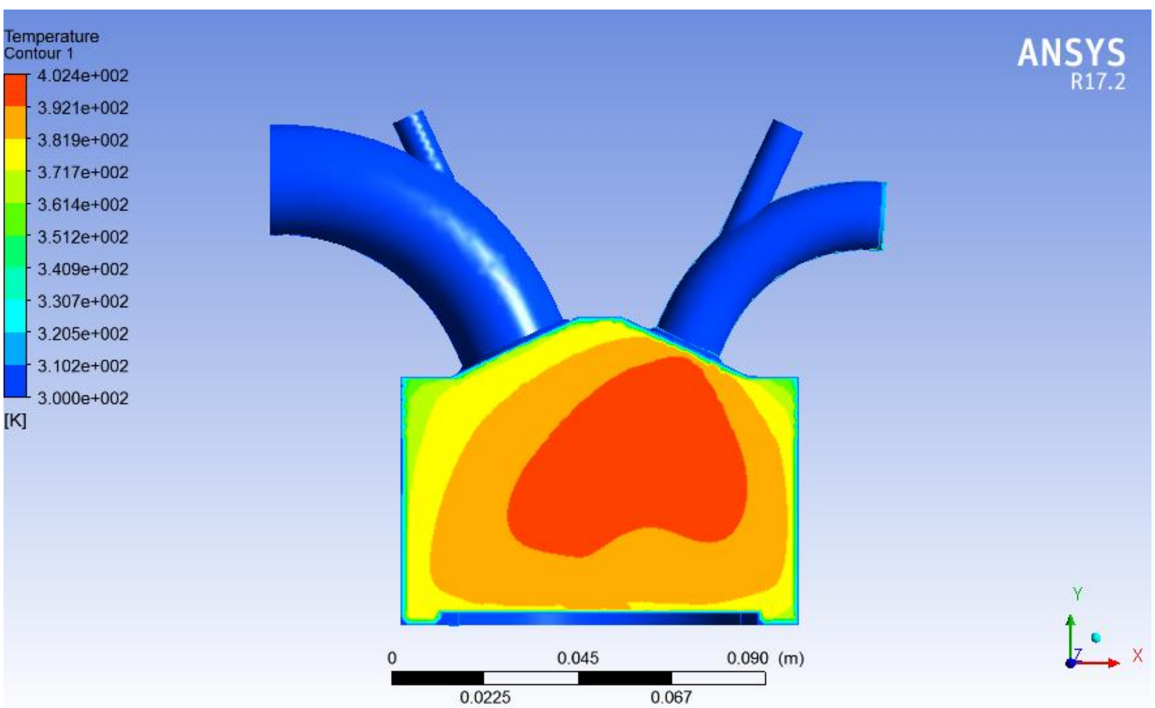


Figure 5.14: Temperature contour after addition of 30% EGR

Again, it is founded that in-cylinder temperatures are typically sufficiently need to be low to avoid significant NOx (nitric oxide) formation, and the premixed nature of ethanol HCCI allows very low soot and particulate matter emissions in this research work. The low in-cylinder temperatures, however, also cause higher emissions of unburned hydrocarbons and carbon monoxide. As detailed plots of the emissions characteristics in ethanol fueled HCCI are shown in figure 5.12 and 5.13 above, one principle benefit from the high-efficiency operation of HCCI is that carbon dioxide emissions are lower when compared to that of the conventional spark-ignited engines.

Supercharging can deliver increased charge density and pressure at all engine speeds while turbo charging depends upon the speed of the engine. The in- cylinder density and volumetric efficiency can be increased using a high boost pressure. The evaporation of the fuel increases with a high intake pressure of 321255 Pa because of high in-cylinder temperatures. The mixing time decreased with the boost pressure is beneficial in all early injection systems. The combustion efficiency can be increased slightly at high boost levels, and hot EGR rates were introduced.

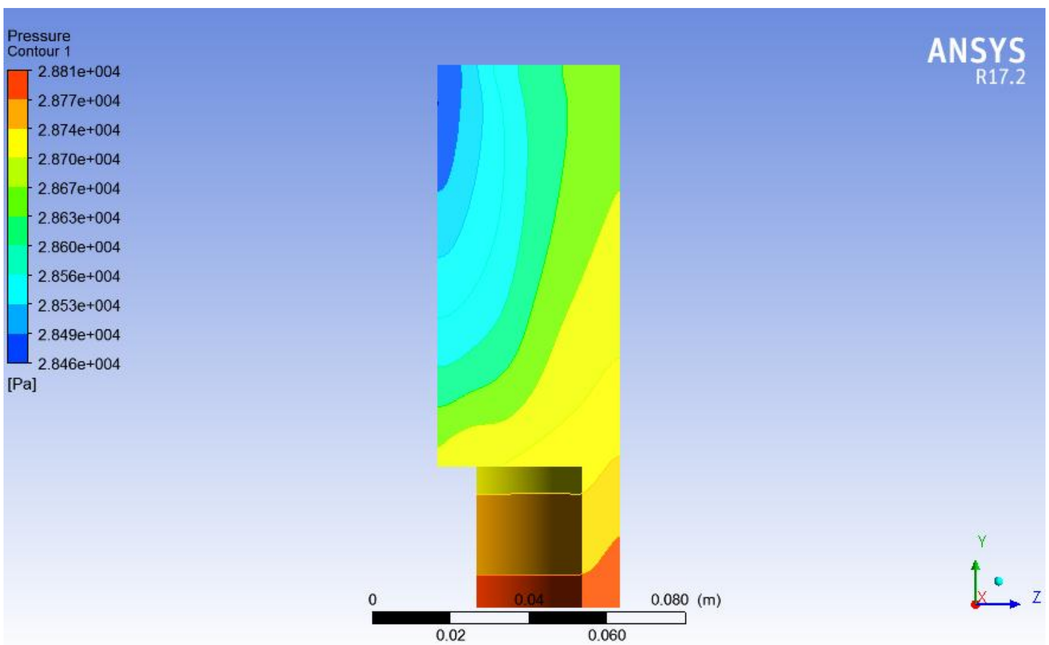


Figure 5.15: Pressure contour simulation Results of sector cylinder, 10%EGR

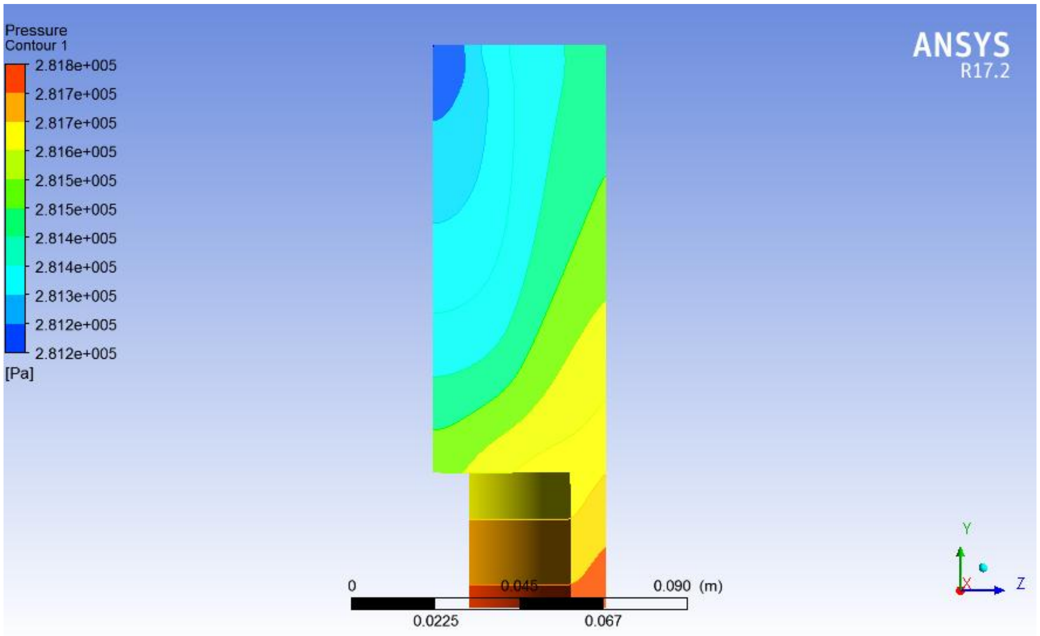


Figure 5.16: Pressure contour simulation Results of sector cylinder, 20%EGR

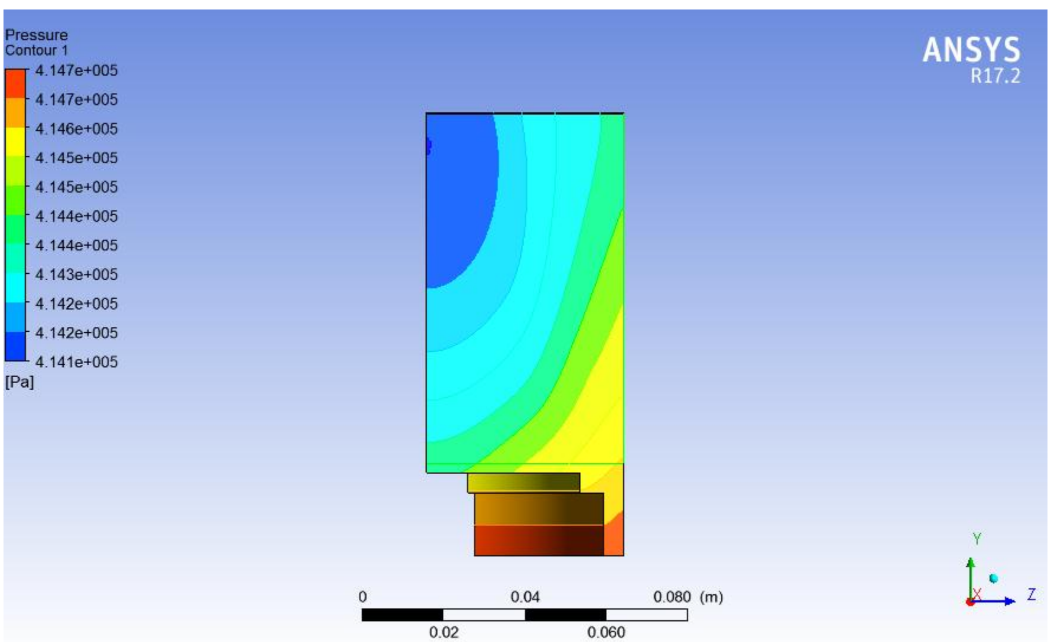


Figure 5.17: Maximum Pressure contour simulation Results of sector cylinder, with 30%EGR

5.3 Control strategies to improve the mixing rate of Ethanol and air

5.3.1 Ultra high injection pressure with small nozzle holes

The atomization of the fuel inside the combustion chamber can be enhanced significantly by using high injection pressures (high velocity of the jet) and by reducing the nozzle hole diameter. Xiangang et al. studied the effects of ultra-high injection pressure (300MPa) and micro-hole nozzle (d =0.08 mm) on the flame structure and the soot formation of impinging diesel spray. [13]

A bigger flame structure and weak soot formation was identified with a micro- hole nozzle at the injection pressures of 200 and 300 MPa. No liquid wetting was found for micro-hole nozzle. The fuel–air mixture homogeneity can be improved by increasing the injection pressures and by reducing the diameter of the nozzle hole.

5.3.2 Inducing high Swirl and Tumble

Swirl is defined as the large scale vortex in the in-cylinder fluid with the axis of rotation parallel to the cylinder axis. It is an organized rotation of the air flow about the HCCI engine cylindrical axis helps in the combustion chamber to improve the mixing rate between the ethanol and air which leads to improved combustion efficiency. Swirl can be generated by constructing the intake system to give a tangential component to the intake flow as it enters the cylinder. This is done by shaping and contouring intake manifolds, valve ports and piston faces.

The radially inward or transverse gas motion that occurs towards the end of compression stroke when the portion of the piston face and cylinder head approach each other closely is called Squish. As the piston reaches TDC, the squish motion generates a secondary flow called tumble, where the rotation occurs about a circumferential axis near the outer edge of the cavity or piston bowl. The necessity of tumble motion is to increase the turbulence level which favors proper and quick mixing of fresh charge which leads to effective combustion with reduced emission. Again The introduction of tumble into the combustion chamber is an effective method of enhancing turbulence intensity prior to ignition, thereby accelerating the burn rates, stabilizing the combustion, and extending the dilution limit.

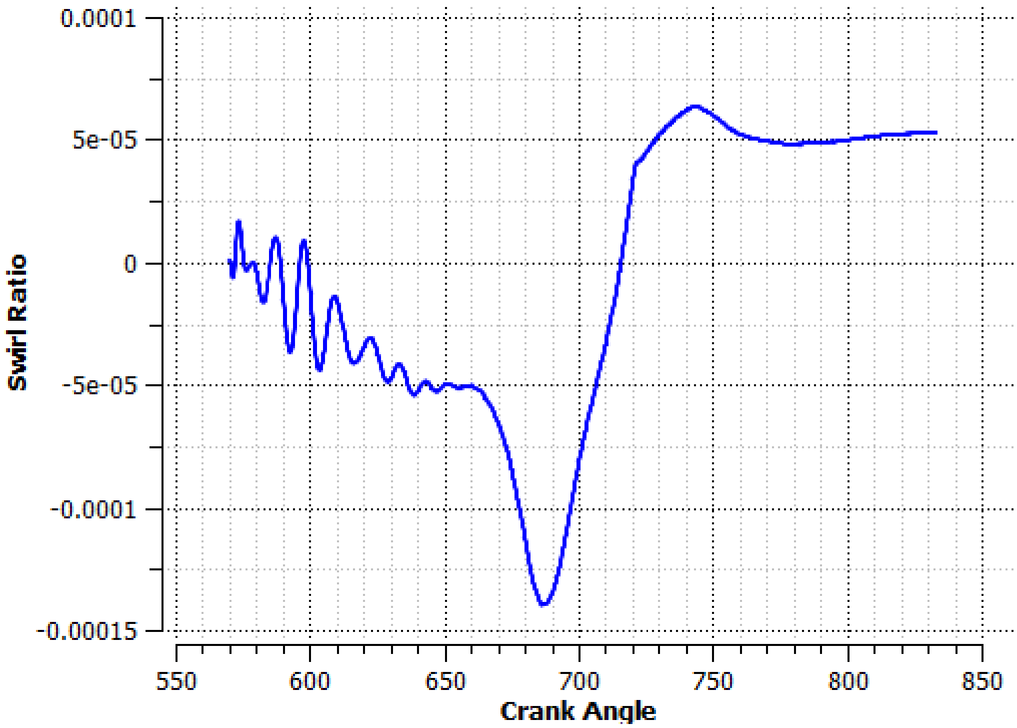


Figure 5.18: Swirl ratio versus CA with 0% EGR

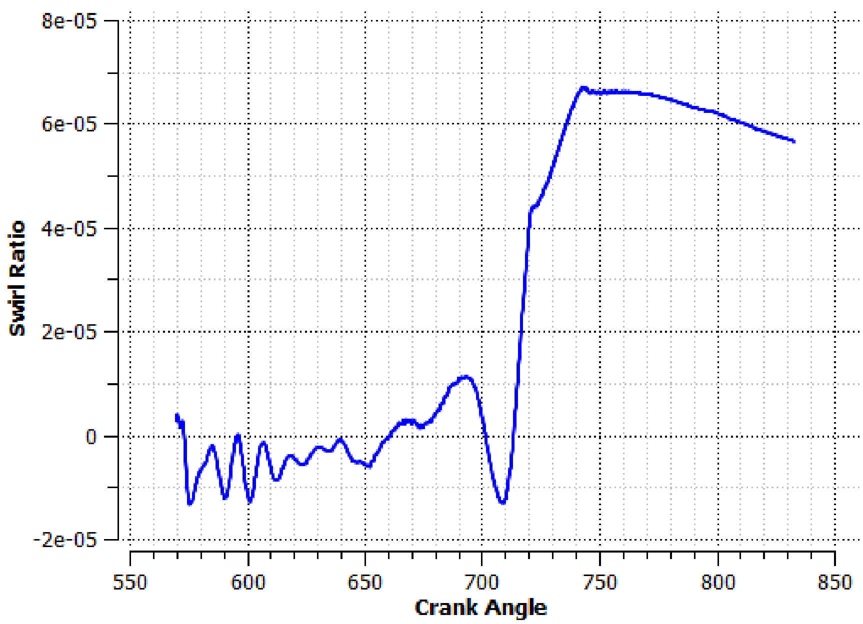


Figure 5.19: Swirl ratio versus CA with 30% EGR

Tumble appears always to break down to turbulence, because as the piston approaches TDC, there is not room between the piston crown and the cylinder head for a vortex. Since combustion chamber is with squish providing the transition from cylinder to head, and/or with the piston crown protruding into the head, the swirl must accommodate itself to the changing shape of the space available to it (from circular to rectangular, and increasingly narrow), and will also break up into turbulence.

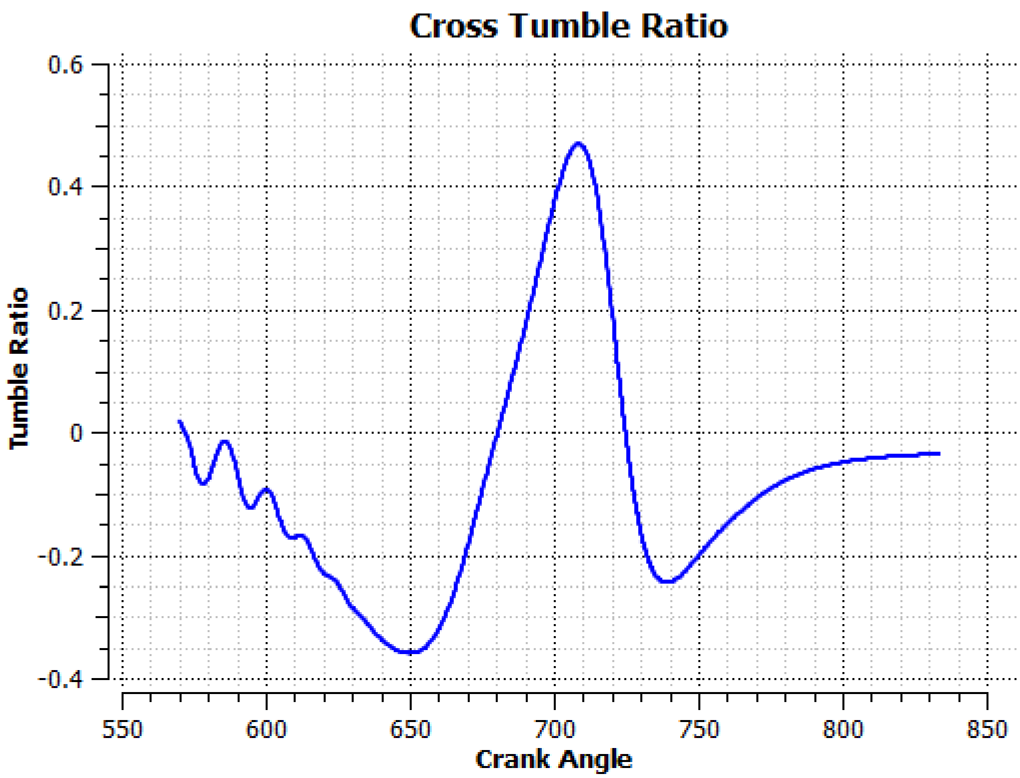


Figure 5.20: Tumble ratio versus crank angle simulation graph

For validation, the BUMP combustion chamber incorporated with the bump rings, used in MULINBUMP combustion system applies a high swirl ratio (3–5) increasing the mixing rate of fuel and air and a high swirl is necessary for the quick homogeneous mixture preparation for combustion. [13]

5.3.3 Pulsed fuel injection

The in-cylinder fuel injection requires multi-pulse injections of the total amount of the fuel to be inducted in the cylinder. The lower air density during injection in the compression stroke results in over penetration of the fuel. In other combustion system, which applies a two stage fuel injection, the first injection is used for premixed lean combustion, while the second injection is used for diffusion combustion. In this research, fuel injection during early compression stroke, used by the HCCI combustion systems, fuel–air mixing is increased.

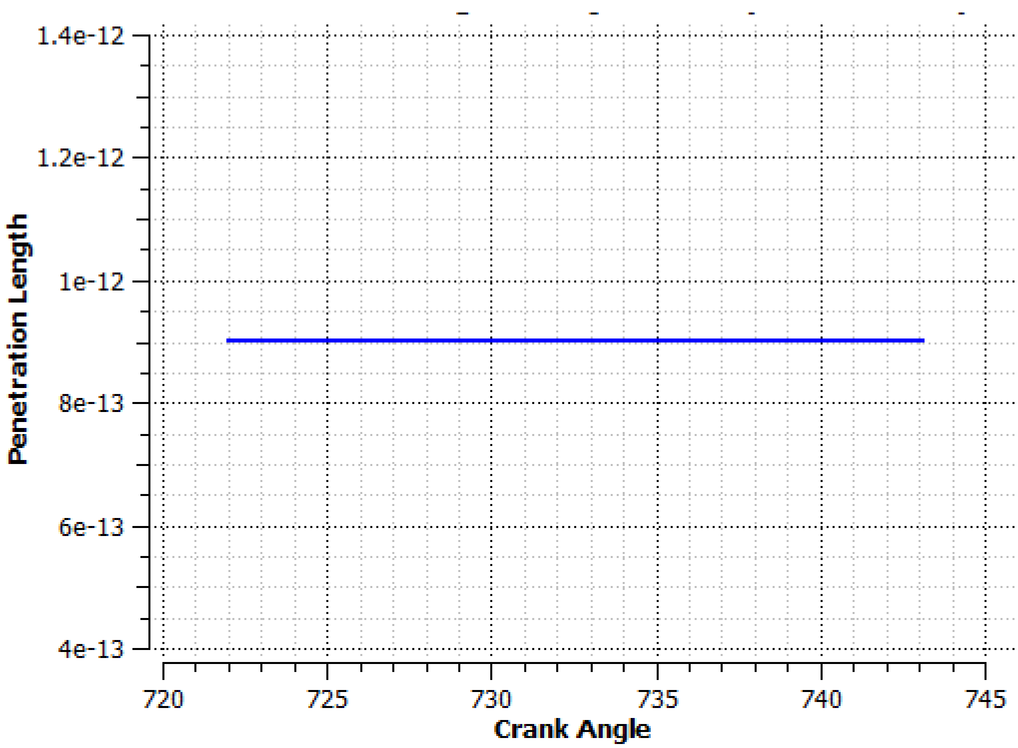


Figure 5.21: Penetration length in injection vs crank angle graph

5.4 Heat Release in Ethanol HCCI engine

The heat release characteristics of the HCCI engine combustion can be compared with those of SI and CI combustion engines in different ways. In the case of SI engine combustion, a thin reaction zone or flame front separates the cylinder charge into burned and unburned regions and heat release is confined to the reaction zone. The cumulative heat released in SI engine is therefore the sum of heat released by certain mass, dm_i, in the reaction zone and it can be expressed as

$$Q = \int_0^N q \, . \, dmi \ldots\ldots(4.6)$$

where q is the heating value per unit mass of fuel and air mixture, N is the number of reaction zone.

In idealized HCCI engine combustion process, combustion reaction takes place simultaneously in the cylinder and all the mixture participates in the heat release process at any instant of the combustion process. The cumulative heat release in such case engine is therefore the sum of the heat released from each combustion reaction, dq_i, of the complete mixture in the cylinder, *m*, i.e

$$Q = \int_1^K m \,.\, dqi \quad \text{...(4.7)}$$

where *K* is the total number of heat release reactions, and q_i is the heat released from the *i*th heat release reaction involving per unit mass of fuel and air mixture.

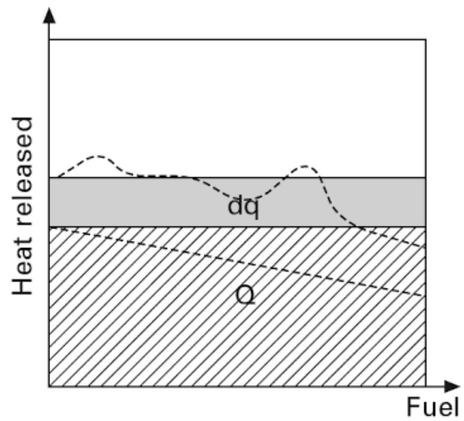


Figure 5.22: Heat release characteristics of HCCI engine [2]

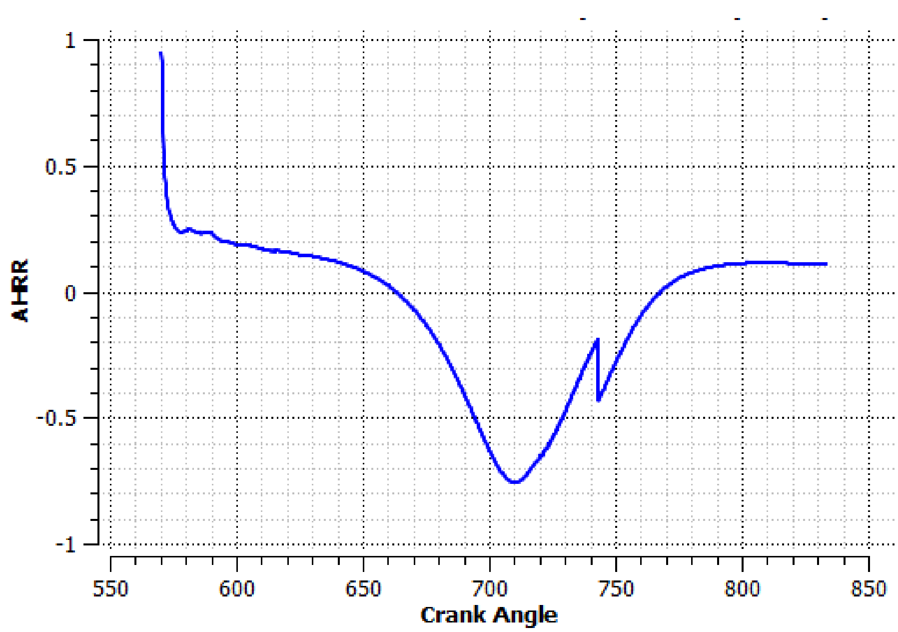
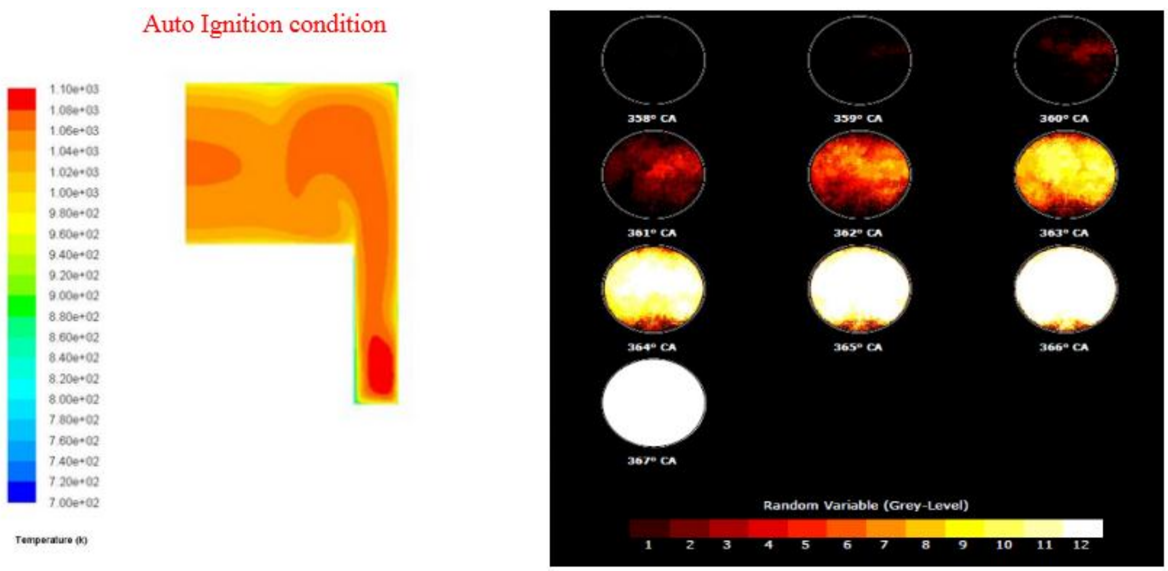


Figure 5.23: Apparent heat release rate in combustion chamber vs crank angle graph

Heat release takes place uniformly across the entire charge in idealized HCCI engine combustion. However, in practice, due to in-homogeneities in the mixture composition and temperature distributions in a real engine, the heat release process will not be uniform throughout the mixture. Faster heat release process can take place in the less diluted mixture and high temperature region, resulting in a non-uniform heat release pattern as indicated by the dashed lines in figure below.

5.5 Ethanol HCCI engine Model Validation

This research is validated based on the same engine test in the laboratory that has been developed at Lawrence Livermore National Laboratory.

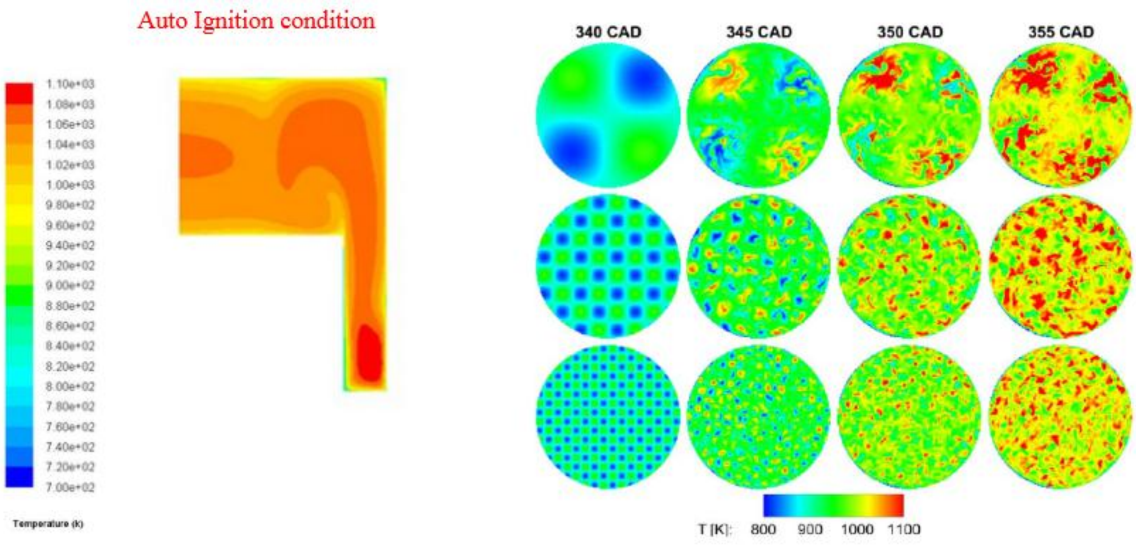


(a)

(b)

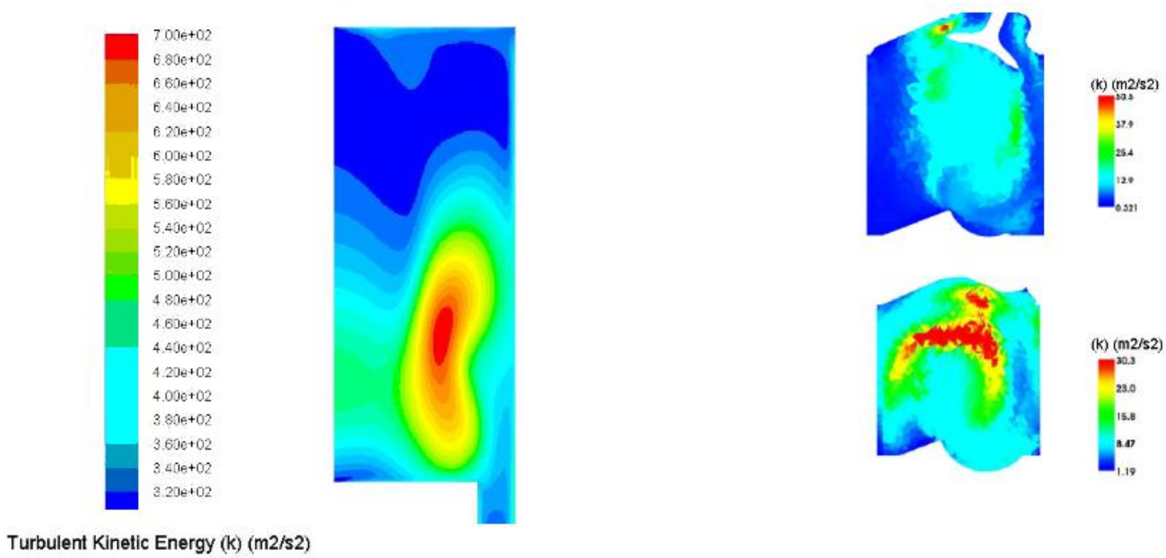
Figure 5.24: Auto ignition condition; (a) simulation result (b) Lab test

Because of a homogeneous charge at reasonable air-fuel ratio was prepared in all cases, the level of smoke emitted gives an indication of the quality of mixture preparation under HCCI conditions. Since the smoke levels were near-zero it can be concluded that the fuel was well vaporized and mixed in the ethanol HCCI engines. It seems likely that the presence of high proportions of hot EGR at the time of injection would be beneficial in this respect.



(a) (b)

Figure 5.25: Auto ignition condition; (a) simulation result (b) Lab test simulation result



(a) (b)

Figure 5.26: Turbulent Kinetic Energy; (a) simulation result (b) Lab test simulation result

Chapter Six

Conclusions

Based on this research work, HCCI is characterized by the fact that the ethanol and air are mixed before entering to the engine's cylinder, the mixture auto-ignites as a result of the temperature increase in the compression stroke and combustion starts in the combustion chamber. Uniform combustion throughout the combustion chamber is achieved when air-ethanol mixture is sufficiently prepared through fast turbulent mixing mechanism. This technique has been improved turbulence kinetic energy (TKE) in the engine which ensures higher turbulence that allows better mixing of ethanol and air to increase combustion efficiency up to 15%. Hence, HCCI is an engine that could be controlled kinetically by ignition and combustion of the air-fuel mixture.

EGR was primarily used to control combustion by means of regulating the initial mixture temperature, to control the heat release rate because of its impact on chemical reaction which can delay the auto-ignition timing and lower peak cylinder pressure. It is founded that the examined effects of 0% to 30% exhaust recirculation gas on ethanol HCCI, showed the increments of temperature of the intake mixture from 400K to 1350K.

Since the effect of ethanol volatility is primarily on the ethanol and air mixture, Ignition temperature is reached by the charge heating through addition of EGR. Again the combustion duration is dominated by the dilution of charge by displacing excess oxygen, thereby increasing the in-cylinder equivalence ratio. This is what makes the HCCI combustion concept thermodynamically favorable, reducing the heat losses and therefore giving an increased engine efficiency.

The delivery ratio has brought effect on the combustion process through changes in the concentrations of ethanol and air in the reacting mixture. Therefore, at high delivery ratios the heat release became violent and for a CR of 11.96:1, in this research case, it was found that a delivery ratio was acceptable for efficient heat release. From obtained simulation results, NOx emissions increased with increased ethanol flow rate and increased intake gas temperature. CO and HC emissions decreased with increased ethanol flow rate and increased intake gas temperature through EGR.

Recommendations for future works

As concluded from the simulation results, based on the findings made, ethanol HCCI engine could be controlled by combustion of the air-fuel mixture, addition of exhaust gas recirculation (EGR) and kinetically by ignition. It is recommended that super computer need to be used to perform the simulation to decrease computation time and effort.

Since the ethanol's auto ignition reactivity is one of the most important parameter that affects HCCI combustion characteristics, the engine must be investigated in laboratory by rapid compression machine (RCM) at the condition of auto-ignition to occur in the cylinder to generate power before going to be applied to light duty vehicles.

As ethanol fueled HCCI engine is more difficult to control than other popular modern combustion engines, the air-ethanol mixture before injected to the cylinder, needs to be mixed carefully to create the homogeneous charge prior to entering to the combustion chamber for proper combustion. This need be done using fumigation devices for the introduction of ethanol to the HCCI engine.

At the time of addition of EGR, the heat release rate decrease because of the burnt gas in the EGR. In this case it is recommended that the peroxide additives need to be added to the fuel to increase the auto ignition property and reaction rate for proper combustion. Though EGR facility is quite common nowadays in an engine system, care should be taken in the addition of EGR to ethanol fueled HCCI engine which otherwise may seriously affect the engine performance and lead to misfire.

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