EFFECT OF CONSTANT AND VARYING MIXTURE PROPERTIES IN SPARK IGNITION ENGINE COMBUSTION PROCESS USING COMPUTATIONAL FLUID DYNAMICS (CFD)

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BORANG PENGESAHAN STATUS TESIS

JUDUL: **EFFECT OF CONSTANT AND VARYING MIXTURE PROPERTIES IN SPARK IGNITION ENGINE COMBUSTION PROCESS USING COMPUTATIONAL FLUID DYNAMICS (CFD)**

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OMAR BIN ARSHAD

Report submitted in fulfillment of the requirements
for the award of the degree of
Bachelor of Mechanical Engineering with Automotive Engineering

Faculty of Mechanical Engineering
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JANUARY 2012

SUPERVISOR'S DECLARATION

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STUDENT'S DECLARATION

I hereby declare that the work in this project is my own except for quotations and summaries which have been duly acknowledged. The project has not been accepted for any degree and is not concurrently submitted for award of other degree.

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Date : 16 JANUARY 2012

Dedicated to my beloved family and friends

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ABSTRACT

This project deals with the numerical setup about the effect of different mixture properties of premixed combustion material using Computational Fluid Dynamic (CFD). Mitsubishi Magma 4G15 is used as the base line engine design for the simulation model. 2000 revolution per minute (rpm) and 1000 iterations are set as the tested speed and the number of iterations per time step respectively. The simulation is started right before the spark ignited and when both valves are closed. The model is simulated at different mixture properties which are constant and varying mixture properties. The constant mixture properties value is taken from previous study. While the varying mixture properties is simulated using kinetic theory where only specific heat, thermal conductivity, and viscosity are varied. Case 1 is set as the constant mixture properties and also as the benchmark case. Case 2 until case 5 is the varying mixture properties with different value of L-J parameters. Case 1 gives only 2.19% of deviation from the experimental result on the peak pressure value and 25% deviation on the peak pressure timing. Meanwhile, for case 2 until case 5, they give as much as 22.34% until 45% deviation on peak pressure value and 100% until 162.5% deviations on the peak pressure timing. The key parameter that caused the results are the L-J parameters, mass fraction burned, and turbulence flame speed. The inaccuracy of the turbulence speed is mostly based on laminar flame speed, thermal conductivity, and specific heat. So, the study of L-J parameter is needed to ensure the perfect result in using kinetic theory approach.

ABSTRAK

Projek ini berkaitan dengan kajian berangka tentang kesan sifat-sifat campuran bahan pembakaran pracampuran yang berlainan menggunakan Perkomputeran Dinamik Bendalir (CFD). Mitsubishi Magma 4G15 digunakan sebagai reka bentuk asas enjin bagi model simulasi. 2000 revulasi per minit (rpm) dan 1000 iterasi ditetapkan sebagai kelajuan enjin dan bilangan iterasi setiap satu langkah. Simulasi bermula sejurus sebelum percikan api dinyalakan dan apabila kedua-dua injap ditutup. Model disimulasikan pada sifat-sifat campuran yang berbeza iaitu malar dan berbeza sifat-sifat campurannya. Nilai untuk sifat-sifat campuran yang malar diambil daripada hasil kajian terdahulu. Manakala sifat-sifat campuran yang berbeza-beza disimulasikan menggunakan teori kinetik di mana hanya haba tentu, kekonduksian terma, dan kelikatan sahaja yang berbeza-beza. Kes 1 ditetapkan sebagai sifat-sifat campuran yang malar dan juga dijadikan sebagai penanda aras. Kes 2 sehingga kes 5 pula adalah sifat-sifat campuran yang berbeza-beza dengan nilai parameter L-J yang berbeza-beza. Kes 1 hanya memberikan sebanyak 2.19% sisihan daripada nilai hasil eksperimen pada tekanan tertinggi dan sisihan sebanyak 25% ke atas masa tekanan tertinggi. Sementara itu, untuk kes 2 sehingga kes 5, mereka memberi sebanyak 22.34% sehingga 45% sisihan pada nilai tekanan tertinggi dan 100% sehingga 162.5% sisihan untuk masa tekanan tertinggi. Parameter utama yang mempengaruhi keputusan adalah parameter L-J, pecahan jisim dibakar, dan kelajuan nyalaan gelora. Ketidaktepatan kelajuan nyalaan gelora disebabkan oleh kelajuan nyalaan lamina, kekonduksian terma, dan haba tentu. Oleh yang demikian, kajian mendalam mengenai parameter L-J diperlukan untuk mendapatkan hasil yang sempurna dengan menggunakan pendekatan teori kinetik.

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LIST OF SYMBOLS

A	Cross sectional area of conducting surface
A_f	Flame area
C_p	Specific Heat
$D_{i,m}$	Diffusion coefficient for species *I* in the mixture
e	Energy
F_i	External body force from interaction with dispersed phase in *i* direction
f_i	Number of modes of energy storage (DOF)
h	Enthalpy
$J_{i,i}$	Diffusion flux of species
k	Thermal conductivity
k_{th}	Laminar thermal conductivity
K_{eff}	Effective conductivity
l_T	Turbulent length scale
m	Mass
$\dot{m}$	Mass rate
m_a	Mass of air
$\dot{m}_a$	Mass flow rate of air
m_f	Mass of fuel
$\dot{m}_f$	Mass flow rate of fuel
M_w	Molecular weight
N	Number of mol
P	Pressure corresponding to burn fraction
P_o	Pressure at start of combustion
P_f	Pressure at end of combustion
Q_{cond}	Constant thickness
R_i	Net of production of species *i* by chemical reaction
S_i	Rate of creation by addition from the dispersed phase
S_L	Laminar flame speed
T	Temperature
ΔT	Temperature difference
u	Displacement in *x* direction

u'	Root mean square (RMS) velocity
u_j	The *jth* Cartesian component of instantaneous velocity
V	Volume
ν	Kinematic viscosity
v_x	Velocity in direction *x*
V_o	Volume at start of combustion
V_f	Volume at end of combustion
Δx	Constant thickness
α_L	Laminar thermal diffusivity
Φ	Equivalence ratio
σ	L-J characteristic length
δ_{ij}	Kronecker delta
τ	Shear stress
τ_T	Turbulent time scale
τ_C	Chemical time scale
ρ	Density
μ	Dynamic viscosity
$\dot{\gamma}$	Strain rate
$\in/k_g$	L-J energy parameter

LIST OF ABBREVIATIONS

AF	Air-Fuel ratio
BDC	Bottom Dead Center
^{o}CA	Crank Angle Degree
CA	Crank Angle
CO_2	Carbon dioxide
CO	Carbon Monoxide
CFD	Computational Fluid Dynamics
DOF	Degree of Freedom
FA	Fuel –Air ratio
H_2O	Water
RMS	Root Mean Square
rpm	Revolution per minute
SI	Spark Ignition
TFSC	Turbulent Flame Speed Closure
3D	Three dimensional

CHAPTER 1

INTRODUCTION

1.1 Project Background

The spark ignition engine is a system that mixed air and fuel together in the intake system prior to entry the engine cylinder. While the both intake and exhaust valve are closed, the piston will move to the top dead center to make a compression. The compression will decreased the volume and in the same time the pressure will increase. Combustion of this mixture inside the engine cylinder is one of the processes that control engine power, efficiency, and emission (Heywood, 1988). Inside the combustion chamber, the oxidation of fuels can releases thermal energy. Then, this energy will be converted into mechanical energy or electrical energy (Razali, 2008). The burned products after combustions are the actual working fluids. The work transfers which provide the desired power output occur directly between these working fluids and the mechanical components of the engine (Heywood, 1988).

From previous experimental method, it is understandable that in-cylinder flow analysis caused high cost and technologies. So that, many engineers invent software to prevent this problem. By doing the simulation of the experiment in the software, the result produced will not affect any cost. Same as Computational Fluid Dynamics (CFD) software, they can represent the model or system in computational model. The software will predict what will happen due to the input parameter. Mixture properties is one of the important parameter that need to be known. By using constant mixture properties, the result is predicted has less than 5% deviation from the experiment. And, by using varying mixture properties, which has different value each crank angle, it is predicted the result is more accurate compared to constant properties. Normally, when each crank

angle increase, the temperature will also increase due to the decreasing the volume. Increasing of the temperature will affect the properties value.

1.2 Problem Statement

The study is carried out with purpose to analyze the different of constant and varying mixture properties using CFD method. The stability of the model is difficult to predict. The varying properties approach is rarely done by previous researcher. It is tough to choose the approach to ensure the model has perfect stability. It is expected that more realistic mixture definition will resulted with more accurate results.

1.3 Scope of Study

The analysis of spark ignition engine combustion with constant and variable dependence mixture properties are carried out in the framework of Turbulent Flame Speed Closure (TFSC) model of Zimont. Single operating point at 2000 RPM is simulated to study the feasibility of variable dependence mixture setup. Model is simulated using 1000 number of iteration due to get acceptable result.

1.4 Objectives of the Project

The objective of this research is to study the effect of different mixture properties of premixed combustion material on combustion pressure.

1.5 Flow Chart of the Study

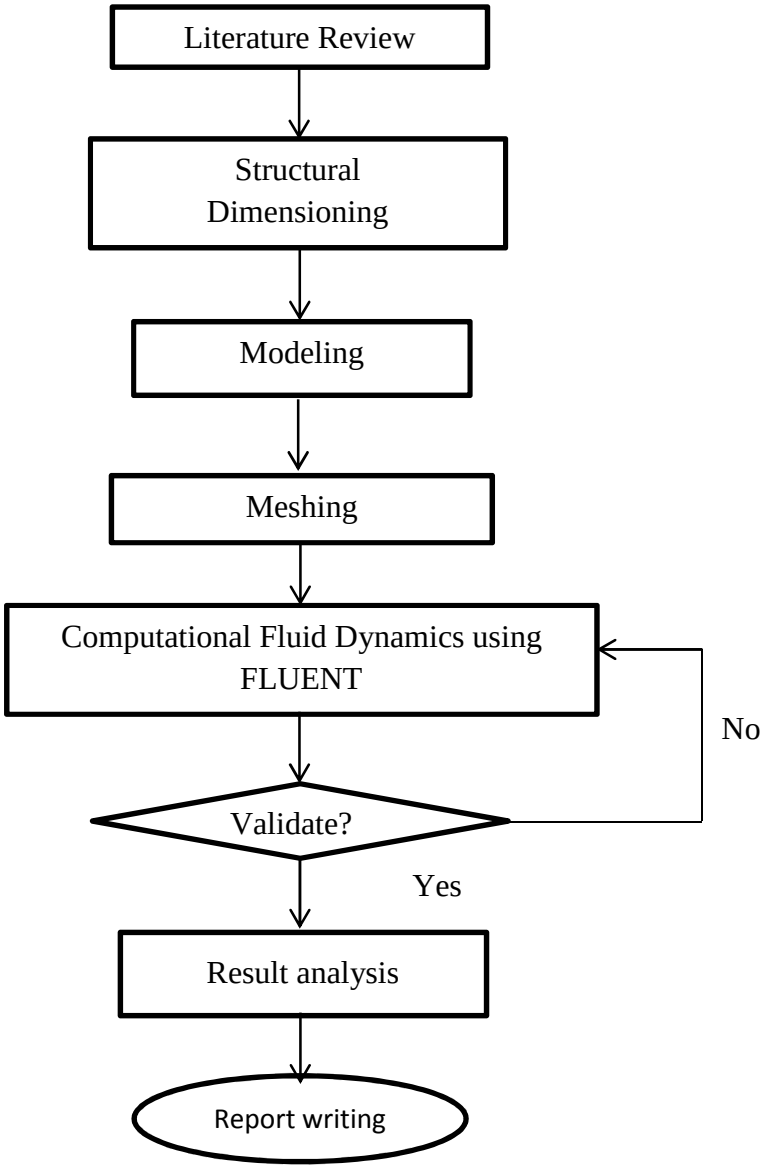

Figure 1.1: Project flow chart

1.6 Organization of Thesis

This thesis consists of five main chapter, introduction, literature review, methodology, result and discussion and the last part is conclusion and recommendation. For Chapter 1 presents some findings that lead to problems statement, objective, scopes and flow chart of work. Chapter 2 is literatures that related to the study and become basic of study framework. Chapter 3 presents the dimensioning work on Mitsubishi Magma 4G15 engine, development of 3D model and generation of computational model. The pre-processing setup is presented in order make the mesh for the model and imported to the solver to analyze. Chapter 4 addresses the validation of the predicted results against experimental results of the cylinder pressure. Chapter 5 presents the important findings of the study and recommendation for future study.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

This chapter deals with definition and characteristics of internal combustion engine. Then, the chapter continues with SI engine model which contain (i) intake, (ii) compression, (iii) combustion, (iv) expansion, and (v) exhaust. After that, discussion continues with chemical reaction between isooctane as the fuel and air. Then, discussion continue with fundamental of thermodynamics properties which are (i) density, (ii) specific heat, (iii) thermal conductivity, (iv) viscosity, (v) molecular weight, (vi) laminar flame speed, and (vii) critical rate of strain. Lastly, CFD approach for in-cylinder modelling and effect of constant and variable mixture properties are discussed.

2.2 Internal Combustion Engine

Internal combustion engine is a heat engine that converts chemical energy in fuel into mechanical energy. Chemical energy from fuel will converted into thermal energy from process of combustion or oxidation with air inside the cylinder. This thermal energy will increased the temperature and pressure of gases inside the engine. The high pressure gases will operate the piston downward and moved the mechanical system. The crankshaft will rotate cause of the high pressure of the gas. The crankshaft is connected with the transmission and power train and will transfer the rotating motian into final use (Heywood, 1988).

The internal combustion engine is a system that mixed air and fuel together in the intake system before entering the engine cylinder. After both intake and exhaust

valve are closed, the piston will move to top dead center to completing compression. The compression will decreased the volume and in the same time the pressure will increase. Combustion of this mixture inside the engine cylinder is one of the processes that control engine power, efficiency, and emission (Heywood, 1988). Inside the combustion chamber, the oxidation of fuels released thermal energy. Then, this energy is converted into mechanical energy or electrical energy (Razali, 2008). The mechanical energy transfers which provide the desired power output occur directly between these working fluids and the mechanical components of the engine. After the combustion process end, the burned product will be exhausted to the surrounding.

2.3 Principal Operation

The model, which can be programmed in CFD, predicts the cylinder pressure throughout the intake, compression, combustion, expansion and exhaust processes that make up the engine operating cycle. Pressure will be modeled as a function of the crank angle which ran for 720 degrees per cycle or two revolutions because the crank completed two rotations per cycle. The valve and spark timings, engine geometry, engine speed and inlet pressure data will be input into the model (Kuo, 1986).

The individual processes of the engine cycle, intake, compression, combustion, expansion and exhaust, are discussed below in order of occurrence (Kuo, 1986).

2.3.1 Intake

Intake occurs between exhaust valve closing and the start of compression. The intake valve opens before the exhaust valve closes. This period of during both valves are open is called overlapping (Kuo, 1986).

During the overlapping, the model used an s-curve to describe the gradual transition between exhaust pressure and intake or inlet pressure. When the intake valve closes, compression process will occur. The engine speed will determines the time for intake valve closing which fluid will stops flowing into the cylinder (Kuo, 1986).

2.3.2 Compression

During the compression process, both intake and exhaust valves are closed, so that the gases can neither enter nor exit the cylinder. When the piston is moving upward and cylinder volume will be decreases. Which will increase the pressure automatically due to the compression of the fluid.

2.3.3 Combustion

There are three major combustion processes of SI engines namely; ignition and flame development, flame propagation, and flame termination as shown in Figure 2.1. Flame development is generally considered the consumption of the first 5% of the air-fuel mixture. During the flame development period, ignition occurs and the combustion process starts, but only a very little pressure rise occurs. Most of the work produced in an engine cycle is the result of the flame propagation period of the combustion process which the period when the bulk of the fuel and air mass is burned. During this period, pressure in the cylinder is greatly increased, providing force to produce work in the expansion stroke (Pulkrabek 1997).

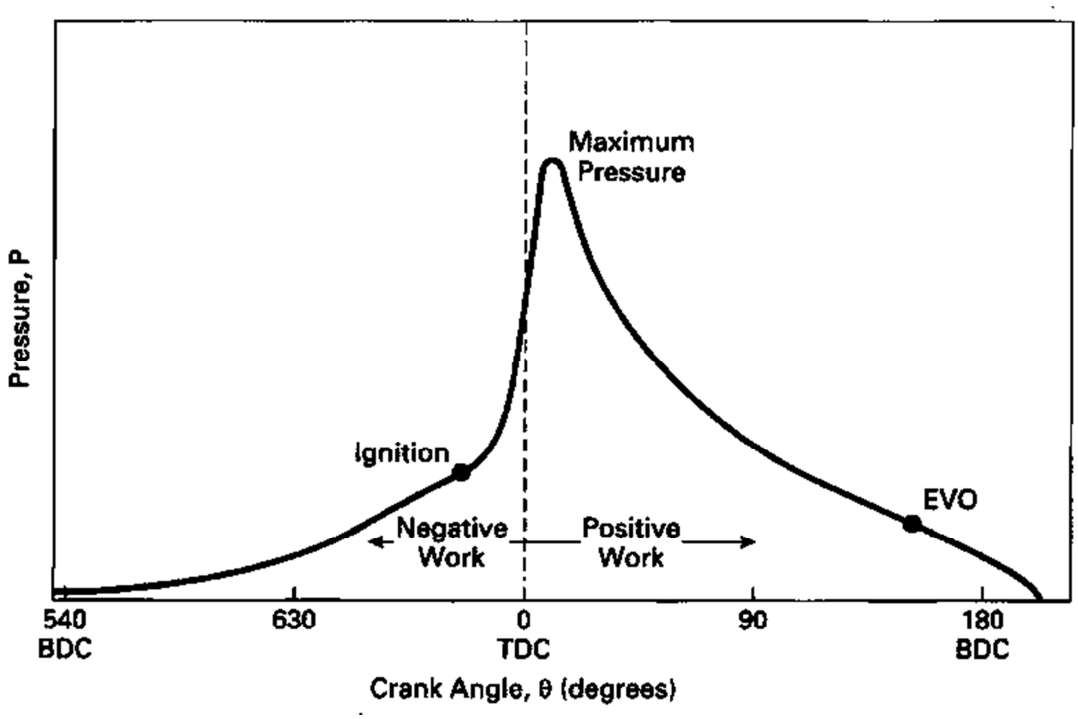

Figure 2.1: In-cylinder pressure profile of SI engine.

Source: Pulkrabek (1997)

2.3.4 Expansion

Expansion process will begin slightly after Top Dead Center (TDC) which is the end of combustion process. The pressure of the burned gases drives the piston down. Work done by turning the crank-shaft will provides power to the car. During expansion, the heat transferred to the cylinder liner is small compared to the work done and the energy lost to internal friction of the gas is also minimum (Kuo, 1986).

2.3.5 Exhaust

Exhaust valve opening occurs before the crank reaches Bottom Dead Center (BDC). At this point, the pressure in the cylinder is much greater than the exhaust system pressure which is around 4-5 atmosphere and the temperature is above 1000 K. The higher pressure in the cylinder will cause a rapid flow of burnt gases going out of the cylinder (Pulkrabek, 1997).

The flow of the gases going out of the cylinder is depends on the area of the opening exhaust valve. The small area of the opening valve will increase the flow. Same goes when the valve is closing. It increases quickly to a maximum, and falls off again as the valve closes. Pressure in the cylinder settles down to the exhaust system pressure as the exhaust valve remains open. The valve closes after TDC, which mean after the overlapping on the next engine cycle (Kuo, 1986).

2.4 Chemical Reaction of Fuel

Most of internal combustion engine gain their energy from combustion of fuel with air. The maximum amount of energy that can be released is when the fuel reacts with a stoichiometric amount of oxygen. Stoichiometric oxygen itself is enough to convert all the carbon in the fuel to CO_2, and all hydrogen to H_2O with no carbon or oxygen left over. The balanced chemical equation of the fuel component, C_8H_{18} burning with stoichiometric oxygen would be (Pulkrabek, 1997):

$$C_8H_{18} + 12.5\ O_2 \rightarrow 8\ CO_2 + 9\ H_2O$$

The component on the left side of the chemical reaction equation is called reactant, while the right side of the equation is called products or exhaust (Pulkrabek, 1997).

A small powerful engine could be built if fuel were burned with pure oxygen. However, the cost that needed to use pure oxygen is very expensive. Usually, air is used as the source of oxygen to react with fuel (Pulkrabek, 1997). Atmospheric air is made up of about 78% of nitrogen, 21% of oxygen, and 1% of argon. Thus, the chemical reaction of fuel and atmospheric air is:

$$C_8H_{18} + 12.5\ O_2 + 12.5(3.76)\ N_2 \rightarrow 3\ CO_2 + 9\ H_2O + 10(3.76)\ N_2 + 5\ CO$$

2.5 Thermodynamics Properties

In thermal design of the internal combustion engines most researchers use air-standard power cycle models to perform their thermodynamic analyses. They used the air-standard to make the comparison reasons in order to show the effect of varying engine parameters, conditions, fluid properties. But, due to the high rise in combustion temperature this assumption becomes less realistic. Although air-standard power cycle analysis gives only approximation to the actual conditions and outputs (Pulkrabek, 1997).

2.5.1 Density

Density is a property that depends on temperature and pressure. The density of most gases is proportional to pressure and inversely proportional to temperature. Density is defined as mass per unit volume (kg/m^3):

$$\rho = \frac{m}{V} \tag{2.1}$$

where

ρ = Density
m = Mass
V = Volume

The density of liquids and solids depends more strongly on temperature than it does on pressure. This is proved when density of water changes from 998 kg/m^3 at 1 atm to 1003 kg/m^3 at 100 atm. The changes are only 0.5%. And the density of water changes from 998 kg/m3 at 20°C to 975 kg/m3 at 75°C. The changes of the density are 2.3% which is greater than changes to pressure (Cengel, 2007).

2.5.2 Specific Heat

The specific heat is known as the energy required to raise the temperature of a unit mass of a substance by one degree. This energy is depends on how the process is finished. There are two kinds of specific heats which are at constant volume and constant pressure (Cengel, 2007). Since there are no constant volumes in the cylinder when the engine is running, specific heat at constant volume is ignored.

By considering a fixed mass in a stationary closed system undergoing a constant-pressure process, conservation of enthalpy principle for this process can be expressed in the differential form (Cengel, 2007).

$$e_{\text{in}} - e_{\text{out}} = \Delta e_{\text{system}}$$
$$\delta e_{\text{in}} - \delta e_{\text{out}} = dh \qquad (2.2)$$

where

e = Energy

h = Enthalpy

The left-hand site of the differential equation is the amount of enthalpy that transfers to the system. Thus,

$$Cp = \left(\frac{\delta h}{\delta T}\right)_p \qquad (2.3)$$

where

c_p = Specific heat (constant volume)

The values of specific heats are usually used as cold properties. This assumption can be used only for small temperature differences. It will produce greater error in modeling. In order to calculate for the large temperature difference encountered in air-standard power cycles, constant average values of specific heats and specific heat ratios

are sometimes used. These average values are evaluated using the extreme temperatures of the cycle, and are believed to yield better results (Abu-Nada, 2006).

For varying mixture properties, kinetic theory is being used to obtain the value of specific heat since in this simulation the density is set as ideal gas (Fluent Inc, 2004) Thus,

$$C_{p,i} = \frac{1}{2}\frac{R}{M_{W,i}}\left(f_i + 2\right) \tag{2.4}$$

where

f_i = Number of modes of energy storage (DOF)

R = Universal gas constant

2.5.3 Thermal Conductivity

Thermal conductivity is a substance which has an ability to transfer the heat. Usually, a good electric conductor is also a good heat conductor, and therefore they have high value of thermal conductivity, *k*. Material such as rubber and plasticn are not a good conductor. So that, the value of *k* is lower (Cengel, 2007). Based on Fourier's law of conduction.

$$Q_{cond} = kA\frac{\Delta T}{\Delta x}. \tag{2.5}$$

where

Q_{cond} = Heat conductor

k = Thermal conductivity

A = Cross sectional area of conducting surface

ΔT = Temperature difference

Δx = Constant thickness

Thus,

$$k = \frac{Q_{cond}}{A}\frac{\Delta x}{\Delta T} \tag{2.6}$$

By using kinetic theory approach, thermal conductivity can be calculated for the varying thermal conductivity in spark ignition engine simulation (Fluent Inc, 2004). Noted that, the density of the model must be set as ideal gas first. The thermal conductivity using kinetic theory is:

$$k = \frac{15}{4}\frac{R}{M_W}\mu\left[\frac{4}{15}\frac{c_p M_W}{R} + \frac{1}{3}\right] \tag{2.7}$$

where

M_w = Molecular weight

μ = Computed viscosity

c_p = Computed specific heat

2.5.4 Viscosity

Viscosity is a measure of the resistance of a fluid which is being deformed by either shear stress or extensional stress. It is commonly perceived as "thickness", or resistance to flow. Viscosity describes a fluid's internal resistance to flow. Or in other word, viscosity is a measure of fluid friction. Thus, water is "thin", having a lower viscosity, while vegetable oil is "thick" having a higher viscosity. All real fluids (except superfluid) have some resistance to stress, but a fluid which has no resistance to shear stress is known as an ideal fluid or inviscid fluid (Symon 1971). There are two related measure of fluid viscosities namely dynamic viscosity and kinematic viscosity.

(i) Dynamic viscosity which also known as absolute viscosity or the coefficient of absolute viscosity is a measure of the internal resistance. Dynamic viscosity is the tangential force per unit area required to move

one horizontal plane with respect to the other at unit velocity when maintained a unit distance apart by the fluid.

The shearing stress between the layers of non-turbulent fluid moving in straight parallel lines can be defined for a Newtonian fluid as:

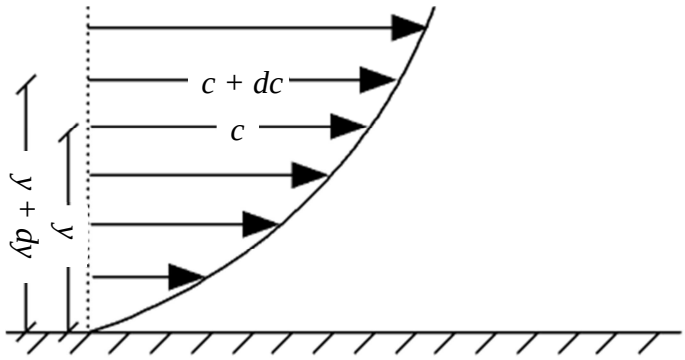

Figure 2.2: Newtonian fluid fundamental.

Source: Symon (1971)

The dynamic viscosity can be expressed like equation below based on Newtons Law of Friction.

$$\tau = \mu \frac{dc}{dy} \tag{2.8}$$

where

τ = Shear stress

μ = Dynamic viscosity

(ii) Kinematic viscosity is the ratio of dynamic viscosity to density (a quantity in which no force is involved). Kinematic viscosity can be obtained by dividing the absolute viscosity of a fluid with its mass density.

$$\nu = \frac{\mu}{\rho} \tag{2.9}$$

where

ν = Kinematic viscosity

For the varying mixture properties, kinetic theory is applied to calculate the value of viscosity since the simulation used ideal gas as the density (Fluent Inc, 2004).

$$\mu = 2.67x10^{-6} \frac{\sqrt{M_W T}}{\sigma_2 \Omega_\mu} \tag{2.10}$$

where μ is in units of kg/m-s, T is in units of Kelvin, σ is in units of Angstroms, and $\Omega_\mu = \Omega_\mu(T^*)$ where

$$T^* = \frac{T}{\in/k_g} \tag{2.11}$$

where

σ = L-J characteristic length

$\in/k_g$ = L-J energy parameter

2.5.5 Molecular Weight

Molecular weight also known as molar mass, *M* which can be defined as the mass of one mole (also called a gram-mole, or gmol) of a substance in grams, or the mass of one kmol (also called a kilogram-mole, or kgmol) in kilograms. Notice that the molar mass of a substance has the same numerical value in both unit systems because of the way it is defined. The mass of a system is equal to the product of its molar mass M and the mole number N (Cengel, 2007).

$$m = MN \tag{2.12}$$

where

M = Molar mass

N = Number of mol

2.5.6 Laminar Flame Speed

Laminar flame speed is an important flame property of fuel and air combustion. This flame speed is a velocity relative to and normal to the flame front which is the unburned gas moves into the front and be heated and transformed to products under laminar flow conditions (Heywood, 1988). The flame front consists of two regions which are (i) a preheat zone (ii) reaction zone.

i. ***Preheat zone.***

Temperature of the unburned mixture is raised mainly by heat conduction from the reaction zone. There are no energy release occurs and the temperature gradient is concave upward ($\delta T/\delta x^2 > 0$).

When reaching a critical temperature, exothermic chemical reaction will begins. The release of the chemical energy is known as heat result in a zone where the temperature gradient is concave downward ($\delta T/\delta x^2 < 0$) (Heywood, 1988).

ii. ***Reaction zone.***

A region between temperature where exothermic chemical reaction begins, and the hot boundary at the downstream equilibrium burned gas temperature

The thickness of the preheat zone in (Heywood, 1988):

$$\delta_{L,ph} = \frac{4.6\bar{k}}{\bar{c}_p \rho_u S_L} \tag{2.13}$$

where

$\bar{k}$ = Thermal conductivity

$\bar{c}_p$ = Specific heat (constant pressure)

S_L = Laminar flame speed

So, the factors which give the laminar flame speed a specific unburned mixture are the temperature and species concentration gradient within the flame, and the mixture transport and thermodynamic properties. Laminar flame speed usually measured in spherical closed vessels which has typical temperature and pressure.by propagating a laminar flame radially outward from the center of the vessel.

$$S_L = \frac{dm_b/d_t}{A_f \rho_u} \tag{2.14}$$

where

dm_b/dt = Mass burning rate (determined from the rate of the pressure rise in the vessel)

A_f = Flame area

The effect of mixture fuel/air equivalent ratio on laminar flame speed for several hydrocarbon and isooctane is shown in Figure 2.3. The flame speed peaks slightly rich of stoichiometric for all fuels shown. Data at higher pressures and temperature have been fitted to a power low of the form (Heywood, 1988):

$$S_L = S_{L,O}\left(\frac{T_u}{T_o}\right)^{\alpha}\left(\frac{\rho}{\rho_o}\right)^{\beta} \tag{2.15}$$

Where, $S_{L,o}$, α, and β are constant for a given fuel, equivalence ratio and burned gas diluent fraction. Constant values for T_o= 298K and p_o= 1 atm are for the reference.

$$S_L = B_m + B_\phi(\phi - \phi_m)^2 \tag{2.16}$$

$$\alpha = 2.18 - 0.8(\phi - 1) \tag{2.17}$$

$$\beta = -0.16 + 0.22(\phi - 1) \tag{2.18}$$

Table 2.1: Parameters ϕ_m B_m B_ϕ

Fuel	ϕ_m	B_m	B_ϕ
Methanol	1.11	36.9	-140.5
Propane	1.08	34.2	-138.7
Isooctane	1.13	26.3	-84.7
Gasoline	1.21	30.5	-54.9

Source: Heywood, (1988)

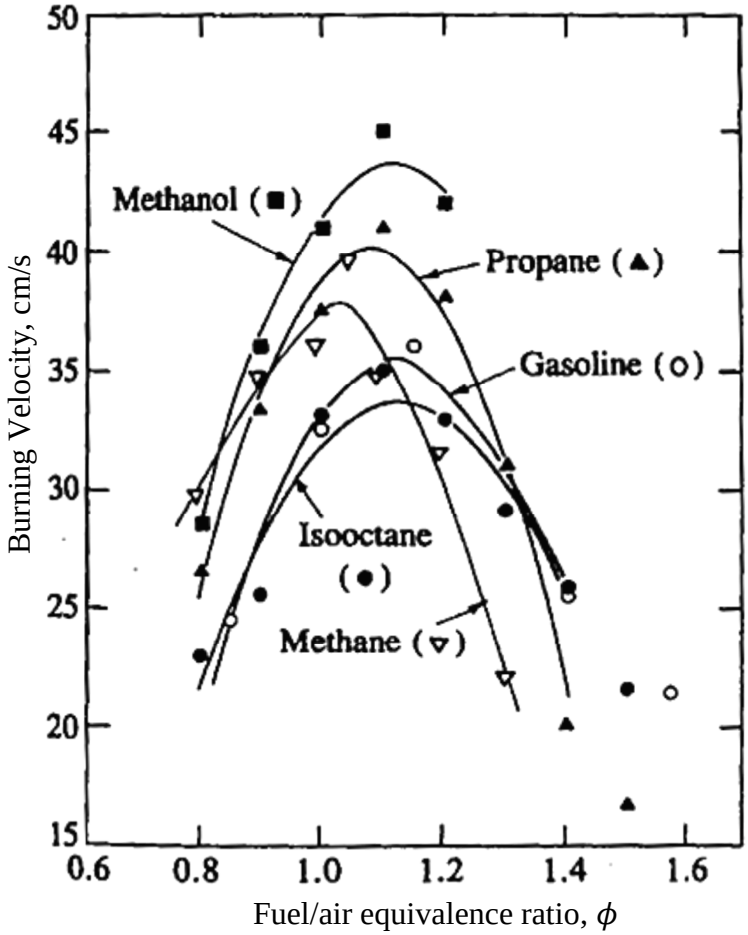

Figure 2.3: Laminar burning velocity for several fuels as function of equivalence ratio, at 1atm and 300K.

Source: Heywood, (1988)

2.5.7 Strain rate

Strain rate can be defined as rate of change of the size and shape of a body under an applied stress. Figure 2.4 shows a piece of a liquid moving at a strain rate $\dot{\gamma}$ under an applied shear stress of τ. The viscosity of the liquid is the ratio of the applied shear stress to the resulting strain rate (or equivalently, the ratio of the shear stress required to move the solution at a fixed strain rate to that strain rate). The shear strain in Figure 2.4 is:

$$\gamma = \frac{d_u}{d_y} \tag{2.19}$$

where

u = Displacement in x direction.

The strain rate is

$$\dot{\gamma} = \frac{d}{dt}\frac{du}{dy} = \frac{d}{dy}\frac{du}{dt} = \frac{dv_x}{dr} \tag{2.20}$$

$$\dot{\gamma} = \frac{dy}{dt} \tag{2.21}$$

where

v_x = Velocity in direction x.

$\dot{\gamma}$ = Strain rate

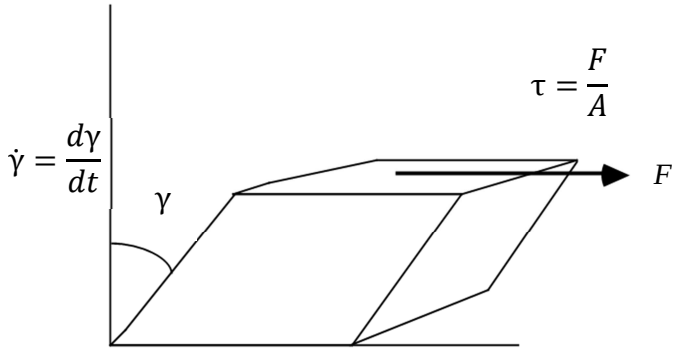

Figure 2.4: A piece of a liquid moving at shear rate $\dot{\gamma}$ under an applied shear stress of τ.

Source: Heywood, (1988)

The relation between viscosity, shear stress, and shear rate is

$$\tau = \mu\dot{\gamma} \tag{2.22}$$

$$\mu = \frac{\tau}{\dot{\gamma}} \tag{2.23}$$

2.6 CFD Modeling Approach

Combustion analysis using CFD software is already applied by many researcher before. CFD approach provides a real insight inside the cylinder to study the fluid flow behavior which is the application of three-dimensional calculation codes by solving the governing flow equation (Payri, 2003).

The result obtained is in form of graph, images and table. CFD approach has an impressive graphic as one of data interpretation. The improvement in graphic, power and speed of modern computer much help in computing the simulation (Payri, 2003). Researcher easily can compared the fluid flow inside the duct, combustion chamber, pipes and few more by observing and differentiate the result appear.

The model meshing process also apart of CFD approach. This task is very important due to the effect of the flow work and the result accuracy. The hexahedral meshes type is useful in this approach. Though a better shape cannot be formed, the deforming process can be much longer than tetrahedral. Finer mesh is needed to make the result more accuracy. As researcher expecting the best outcome, the consideration starts from meshing and grid generation. The good mesh selection is half of the CFD analysis done (Jain, 2008).

2.7 Effect of Constant and Variable Specific Heats in Si Engine.

Based on Abu Nada, 2006, a variation of cylinder pressure versus volume for SI engine using constant-average specific heats running at piston speeds of 2000 and 5000 rpm at a given air–fuel ratio of 15 is shown in Figure 2.5.

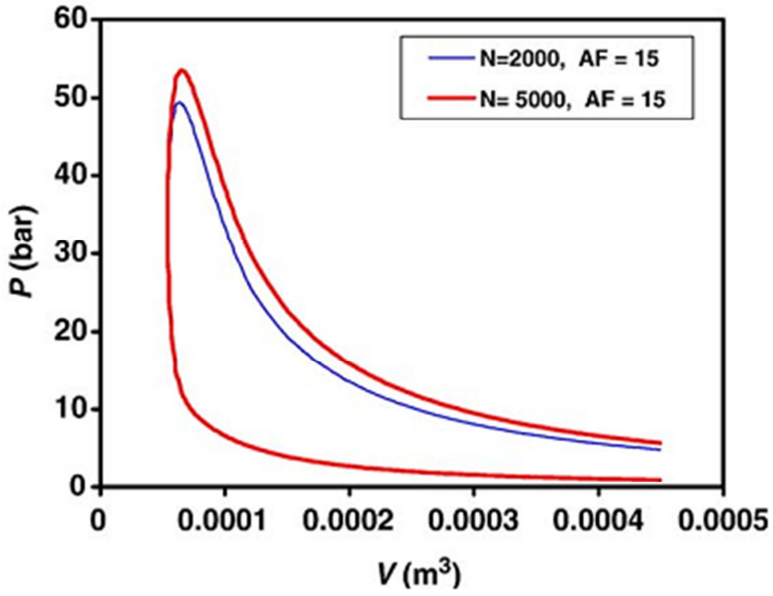

Figure 2.5: Variation of cylinder pressure versus volume for SI engine using constant-specific heats running at 2000 rpm and 5000 rpm

Source: Abu Nada, (2006)

The variation of pressure and gas temperature versus crank angle using variable and constant specific heats running at engine speed of 5000 rpm and in cylinder air–fuel

ratio of 15 presented in Figure 2.6. It is obvious that there is some difference when temperature dependent specific heat is used instead of constant specific heat. Although they have similar trends, the maximum temperature and pressure with constant specific heats are significantly over-estimated in comparison with results obtained with variable specific heats.

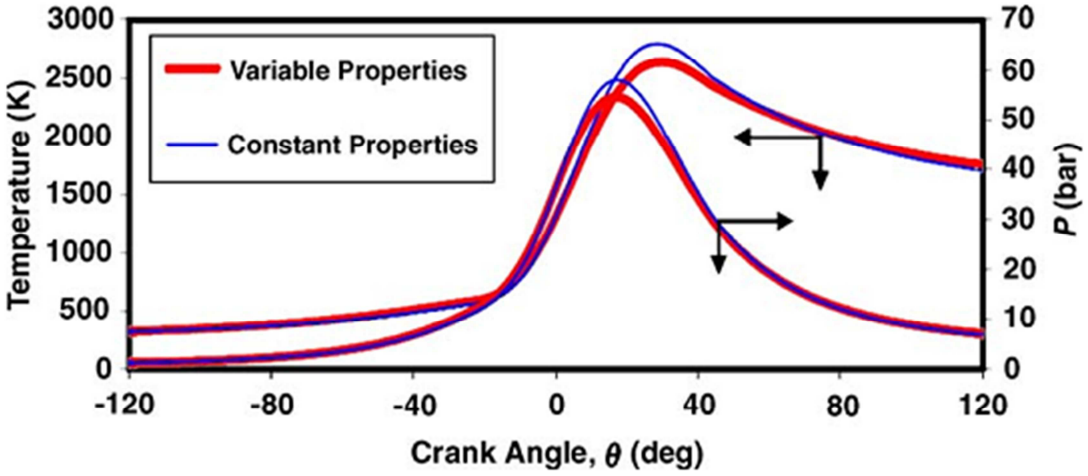

Figure 2.6: Temperature and pressure variation of constant and variable specific heats running at 5000 rpm.

Source: Abu Nada, (2006)

2.8 Summary

The application of CFD is not limited in developing only, but to simulate real cases that may hazardous and dangerous that can take lives such flood, toxic gas, fire, smoke, etc. Focus of this study is on the effect of different mixture properties on in-cylinder flows. The model was meshed based on complexity of design. Then, the numerical model set up for solving the models. Finally, the results produced which the variable mixture properties pressure is predicted to be lower than constant mixture properties. The result must be validated based on previous study and experiment data so that the current study is acceptable.

CHAPTER 3

METHODOLGY

3.1 Introduction

This chapter is present the numerical modelling techniques using CFD approach on reactive flow simulation. These include the baseline of engine specification, governing equation of CFD, model creation and mesh generation. Problem setups which are mixture properties and boundary condition are also described. Solution setup, full crank angle event and validation methods also presented in this chapter.

3.2 Baseline Engine Specification

Table 3.1: Engine specification Mitsubishi Magma 4G15.

Parameter	Size and Feature
Combustion chamber type	Pent-Roof type
Piston bore (mm)	75.5
Piston stroke (mm)	82
Compression ratio	9.2
Intake valve open/closed	150 BTDC/630 ABDC
Exhaust valve open/closed	570 BBDC/130 ATDC

Source: Fadzil, (2008)

From Table 3.1, Mitsubishi magma 4G15 is taken as engine baseline to completing this project. The bore for this engine is 75.5 mm and 82.0 mm as the stroke. Since the engine combustion chamber type is pent-roof type, the development of top of combustion chamber is pent-roof type. From the table, the compression ratio is 9.2. So

that, the model that need to be created must obey the compression ratio to simulating as it is. The connecting rod for the piston is 129 mm.

3.3 Governing Equation For Computational Fluids Dynamics

CFD methodology is using partial differential equations of flow variables to calculate and to simulate numerous kind of analysis concerning the fluid flow. Among them are mass, momentums, energy, species concentration, quantities of turbulence and mixture fractions.

3.3.1 Mass Conservation Equation

The continuity equation or the mass conservation equation for any fluid flow is expressed as below (Fluent Inc, 2004);

$$\frac{\partial}{\partial x} + \frac{\partial}{\partial xj}\left(\rho u_j\right) = \dot{m} \tag{3.1}$$

where

ρ = Fluid density

u_j = The *jth* Cartesian component of instantaneous velocity

$\dot{m}$ = The rate of mass of the object generated in the system

This equation is valid for the incompressible and compressible flow. Moreover, the rate generated in the system, $\dot{m}$ can be defined as the mass added to continues phase from the dispersed second phase such the vaporization of the liquid droplets and any other user-defined sources.

3.3.2 Momentum Conservation Equation

The conservation of momentum in *i* direction for an inertial reference frame can be explained as below (Fluent Inc, 2004):

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial xj}(\rho u_i u_j)=\frac{\partial p}{\partial xi}+\frac{\partial \tau ij}{\partial xj}=\rho gi+F_i \quad (3.2)$$

where

ρ = Fluid density

$u_i \& u_j$ = The *ith* and *jth* Cartesian components of the instantaneous velocity

τij = Stressor pressure

ρgi = Gravitational body force

F_i = External body force from interaction with dispersed phase in *i* direction

The stress tensor in given in Eq. (3.2)is given as below:

$$\tau_{ij}=\mu\left(\frac{\partial ui}{\partial xj}+\frac{\partial uj}{\partial xi}\right)-\frac{2}{3}\mu\left(\frac{\partial uk}{\partial xk}\right)\delta_{ij} \quad (3.3)$$

where

μ = Fluid dynamic viscosity

δ_{ij} = Kronecker delta

Note that the second term on the right hand side of Eq. (3.4) describes the effect of volume dilation. By substituting Eq. (3.4) into Eq. (3.3), another equation is produced that is complete momentum equation.

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial xj}(\rho u_i u_j)=-\frac{\partial p}{\partial xi}+\frac{\partial p}{\partial xj}\left\{\mu\left(\frac{\partial ui}{\partial xj}+\frac{\partial uj}{\partial xi}\right)-\frac{2}{3}\mu\left(\frac{\partial uk}{\partial xk}\right)\partial_{ij}\right\}\rho gi+Fi \quad (3.4)$$

3.3.3 Energy Conservation Equation

$$\frac{\partial}{\partial t}(\rho e)+\frac{\partial}{\partial xi}[u_i(\rho e+P)]=\frac{\partial}{\partial xi}\left[K_{eff}\frac{\partial T}{\partial xi}-\sum_j h_j J_j+u_j\left(\tau_{ij}\right)_{eff}\right]+S_h \tag{3.5}$$

where

K_{eff} = Effective conductivity

= $k + k_i$ (where k_t = turbulent thermal conductivity)

J_j = Diffusion flux of species j

S_h = Additional volumetric heat sources (example: heat of chemical reaction)

h = Sensible enthalpy

e = Specific total energy

The first three terms on the right-hand side of Eq. (3.5) represent the energy transfer due to conduction, species diffusion and viscous dissipation respectively. From Eq. (3.5) also, sensible enthalpy, h and specific total energy, e are defined as below (Fluent Inc, 2004):

$$e=h-\frac{p}{\rho}+\frac{ui^2}{2} \tag{3.6}$$

Sensible enthalpy for ideal gas is defined as:

$$h=\sum_j m_j h_j \tag{3.7}$$

Sensible enthalpy for incompressible flow is defined as:

$$h=\sum_j m_j h_j+\frac{p}{\rho} \tag{3.8}$$

where

m_j = mass fraction of species j

h_j = $\int_{Tref}^{T} c_{p.j}$ dT with T_{ref} = 298.15K

3.3.4 Species Conservation Equation

When choosing to solve conservation equation for chemical species, the prediction of local mass fraction to each species, m_i, through the solution of a convection- diffusion equation for the *ith* species. This conservation equation takes the following general form.

$$\frac{\partial p}{\partial t}(\rho m_i) + \frac{\partial}{\partial xi}(\rho u_i m_i) = -\frac{\partial}{\partial t} J_{i,j} + R_i S_i \qquad (3.9)$$

where

R_i = Net of production of species *i* by chemical reaction.

S_i = Rate of creation by addition from the dispersed phase

$$J_{i,i} = -\rho D_{i,m} \frac{\partial ui}{\partial xj} \qquad (3.10)$$

where

$J_{i,i}$ = Diffusion flux of species *i*

$D_{i,m}$ = Diffusion coefficient for species *I* in the mixture

The reaction rates that appear as source terms in Eq. (3.9) are computed by eddy dissipation model. The reaction rates are assumed to be controlled by the turbulence instead of calculation of Arrhenius chemical kinetics. The net rate of production for species *i* due to reaction *r,* is given by smaller of the two expressions below (Fluent Inc, 2004):

$$R_{i,r} = \nu'_{i,r} M_{W,i} A\rho \frac{\varepsilon}{k} \min\left(\frac{Y_R}{\nu'_{j,r} M_{W,j}}\right) \tag{3.11}$$

where

Y_R = Mass fraction of a particular reactant R

A & B = Empirical constant equal 4.0 & 0.5

3.4 Turbulent Flame Speed Model

The closure for the reaction rate terms in TFSC is closed by the empirically derived turbulent flame speed model. The flame speed value represents the turbulent flame speed normal to the mean surface of the flame. The mathematical expression for the turbulent flame speed model is given as:

$$\begin{aligned} S_T &= A(u')^{\frac{3}{4}} S_L^{\frac{1}{2}} \alpha_L^{-\frac{1}{4}} l_T^{\frac{1}{4}} \\ &= Au' \left(\frac{\tau_T}{\tau_C}\right)^{\frac{3}{4}} \end{aligned} \tag{3.12}$$

where

A = Model constant

u' = Root mean square (RMS) velocity

S_L = Laminar flame speed

α_L = Laminar thermal diffusivity

l_T = Turbulent length scale

τ_T = Turbulent time scale where $\tau_T = l_T/u'$

τ_C = Chemical time scale where $\tau_C = \alpha/S_L^2$

The turbulence parameter required for the model such as turbulent length scale, l_T, and turbulent time scale, τ_T, are mostly calculated using the turbulent model.

3.5 Burning Acceleration Due To Compression

In the case of engine's combustion, the burning process is accelerated due to the compression of the cylinder mixture. This burning acceleration affects the chemical reaction time scale through the so-called laminar thermal diffusivity. In TFSC model of Zimont, the chemical time scale is defined as Eq. (3.13):

$$\tau_c = \frac{\alpha_L}{S_L^{\,2}} \tag{3.13}$$

The reference value of thermal diffusivity α_{ref} is given as Eq. (3.14):

$$\alpha_{ref} = k_{th} / \rho c_p \tag{3.14}$$

where

k_{th} = Laminar thermal conductivity

c_p = Mixture specific heat

3.6 Model Creation and Mesh Generation

The model is created using Solidworks based on the compression ratio of Mitsubishi Magma 4G15 which is 9.2. There are two intake valves, one exhaust valve, a cylinder and a combustion chamber for each cylinder. Every valve has different size. Since this project is based on degree standard, the model was simplified from the actual engine. The manifold is created as a cylinder shape as shown in Figure 3.1 to make the meshing process easier.

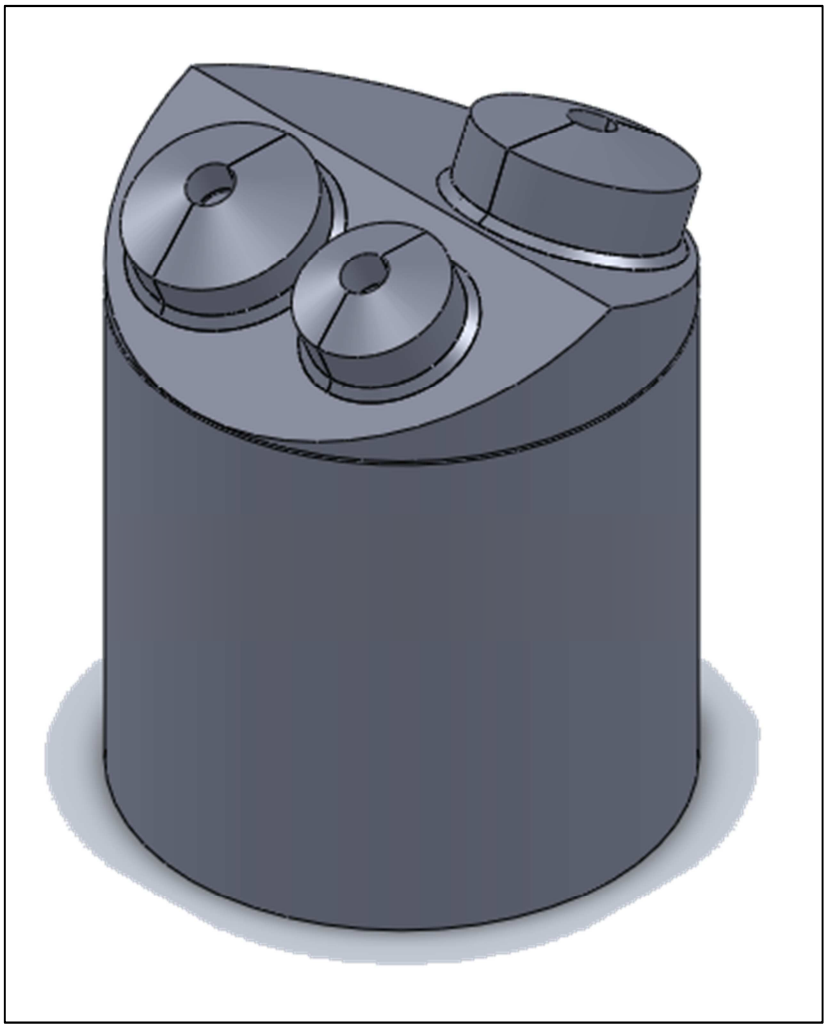

Figure 3.1: Structural model

Then, the model was imported to Design Modeler which is one of the components of Fluid Flow (FLUENT) inside Workbench. The model detail was changed from solid to fluid. Every part of the model was renamed to make the setup process easier.

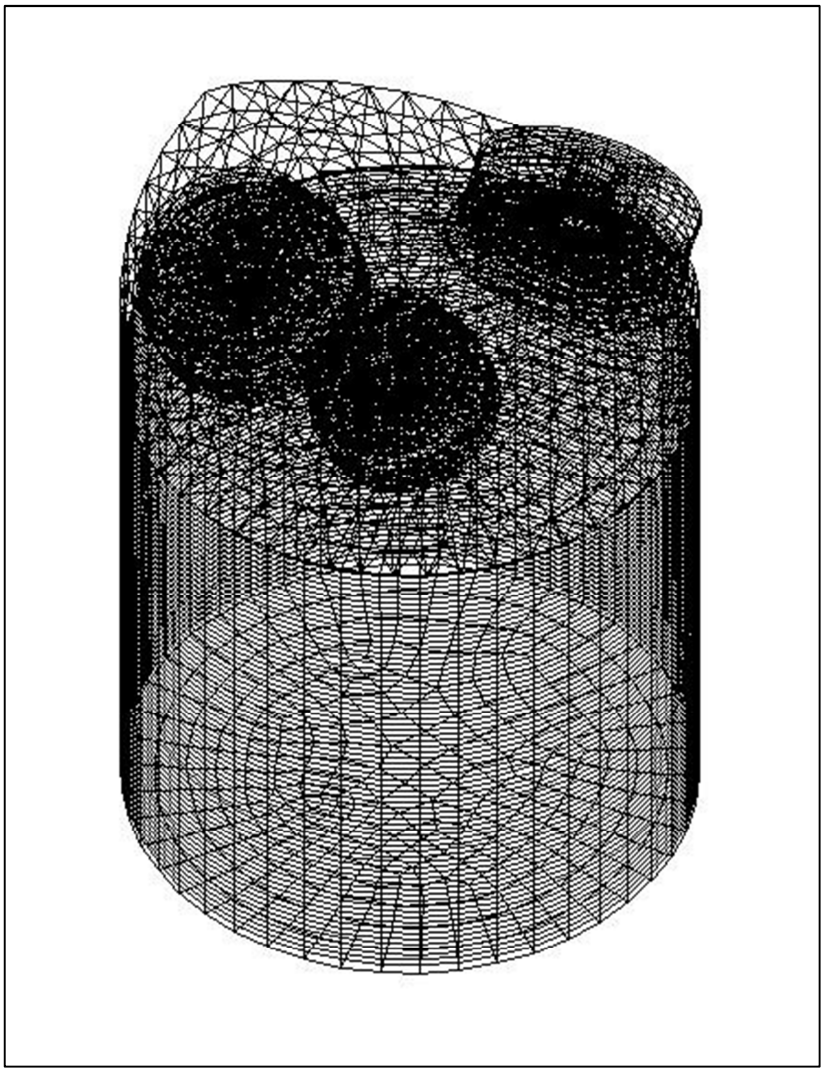

Figure 3.2: Compelete model mesh

Figure 3.2 shows the complete mesh of the baseline engine. The model was meshed using Meshing component of Fluid Flow in Workbench. The tetrahedral mesh was meshed at the combustion chamber volume part and as hexahedral mesh at cylinder volume part, manifold and valve volume part. Mesh of the model part can be seen in Figure 3.3.

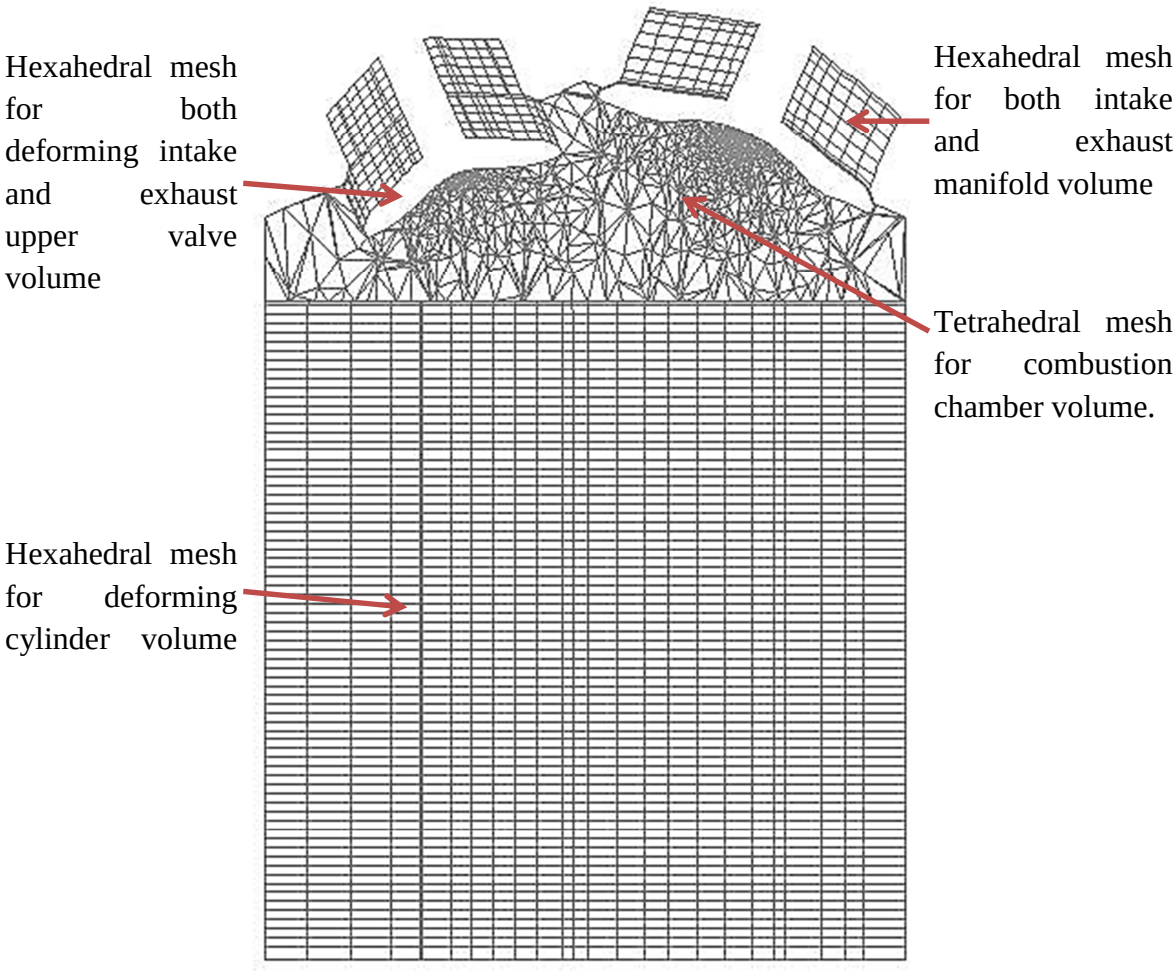

Figure 3.3: Type of mesh for model when piston at BDC.

3.7 Mixture Properties

For this analysis, there are two simulations will be analyzed to achieve the desire result. Even though there are two simulations analyzed, same model will be used. Initial condition and other parameter will be remained equal. The difference between both simulations is their mixture properties. The first simulation utilized the constant mixture properties as the properties for the material and the variable mixture properties will be applied for the second simulation.

A set of numerical input of the model for the constant premixed mixture properties is shown as Table 3.2.

Table 3.2: Input for constant premixed mixture properties at 2000 rpm

Properties	Value	Units
Specific heat	2040	J/kg.K
Thermal Conductivity	0.08207936	W/m.K
Laminar Viscosity	4.10317×10^{-5}	kg/m.s
Molecular Weight	27.4547	kg/kmol
Laminar Flame Speed	0.4762	m/s
Critical Rate of Strain	18563	s^{-1}
Unburned Fuel Mass Fraction	0.07643	-
Lower Heating Value	4.43×10^{7}	J/kg

Source: Fadzil, (2008)

For the variable mixture properties, kinetic theory is been chosen for most of the properties. The properties then will be calculated automatically. Input data for varying mixture properties is shown in Table 3.3.

Table 3.3: Input for varying premixed mixture properties at 2000 rpm

Properties	Input data	Units
Specific heat	$C_{p,i} = \frac{1}{2}\frac{R}{M_{w,i}}(f_i + 2)$	J/kg.K
Thermal Conductivity	$k = \frac{15}{4}\frac{R}{M_w}\mu\left[\frac{4}{15}\frac{c_p M_w}{R} + \frac{1}{3}\right]$	W/m.K
Laminar Viscosity	$\mu = 2.67\ x\ 10^{-6}\frac{\sqrt{M_w T}}{\sigma^2 \Omega_\mu}$	kg/m.s
Laminar Flame Speed	Metghalchi-Keck Law	m/s

Source: Fluent Inc, (2004)

The value from Table 3.2 and Table 3.3 was set as the starting parameter of the simulation for both constant and varying mixture properties. Other parameter in varying mixture properties was set as constant which used the constant mixture properties data.

3.8 Boundary Conditions

The model boundary was sets as walls. The materials for all walls are set as aluminum. The cylinder walls are set as deforming boundary to simulate the compression and power stroke. Deforming boundary will automatically create or delete mesh to make the volume of the engine as calculated. The pent-roof walls are set as stationary walls since they are not moving. The piston face wall was set as moving wall in order to simulate the movement of the piston in combustion chamber from bottom dead center to top dead center. Manifold face was set as pressure inlet and outlet as can be seen in Figure 3.4. In order to make the fluid flow inside the model, pressure inlet has to be set. When exhaust stroke happen, pressure outlet which set at exhaust manifold face will be a medium for the products came out.

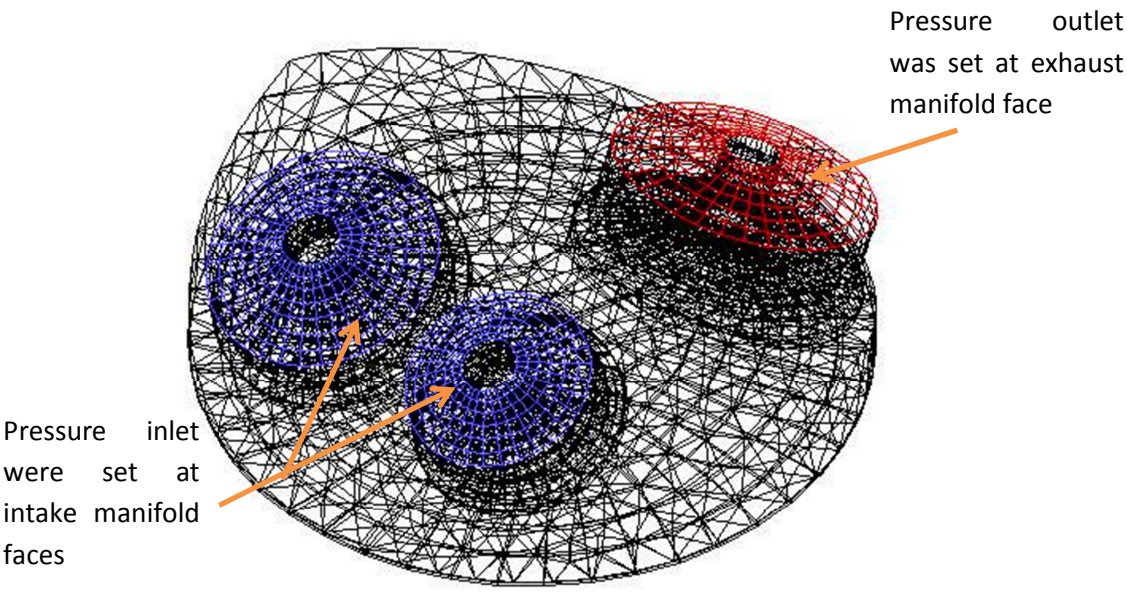

Figure 3.4: Pressure inlet and outlet at manifold face.

Constant engine speed is required for this simulation and 2000 rpm was selected as uniform engine speed for both constant and varying mixture properties models. This is important because to comparing pressure difference of both models need a constant engine speed. The other main part of boundary condition setting is temperature along the walls. The temperature setup followed the actual condition as presented in Table 3.4

Table 3.4: Wall temperature at 2000 rpm

Variables	Value	Units
Cylinder head Temperature	550	K
Piston face temperature	573	K
Cylinder wall temperature	458	K

Source: Fadzil, (2008)

3.9 Full Crank Angle Event

Table 3.5: Full crank angle event

Crank angle (CA)	Events	Process
-360^o	At TDC	Start of intake process
-347^o	Exhaust valves closed & exhaust manifold deactivation	Intake process
-180^o	At BDC	Start of compression process
-117^o	Intake valves closed & intake manifold deactivation	Compression process
-23^o	Timing of ignition (for 2000 rpm)	
0^o	At TDC	Start of power stroke
123^o	Exhaust valves opened & exhaust manifold activation	Power stroke
180^o	At BDC	Start of exhaust stroke
345^o	Intake valves opened & intake manifold activation	Exhaust stroke
360^o	End of single cycle (at TDC)	

Source: Fadzil, (2008)

At TDC (-360^oCA), where the simulation will be started, both valves are already open. The valves overlap when intake valve is opening and the exhaust valve is closing. At -347^oCA, exhaust valve will be closed and the manifold will be deactivated. Deactivating manifold will make the calculation smoother. After BDC (-180^o), the piston will pushed upward and the compression process happened. Before the piston reach TDC, spark will be ignite when crank angle -23^o. The power stroke started right after the piston reach TDC. 57^o before BDC, exhaust valve and exhaust manifold will

start to open and activate. Exhaust stroke will start after BDC. At 345^{o}, intake valves opened and intake manifold will activate. One cycle of the simulation finish when the crank angle reaches 360^{o}CA.

Noted that, the simulation will be started when the ignition occur. Only 50^{o}CA will be simulated which from -23^{o}CA (combustion process) until 27^{o}CA (Power stroke). Pressure of the simulation will be plotted in chapter 4.

3.10 Initial Parameter

The simulating process is focus on the combustion process which started when the spark ignited. The spark will ignite when the crank angle reach -23^{o}CA. In simulating the combustion process, several initial conditions need to be known. The initial conditions are used to make the engine run using the exact parameter of the crank angle degree. Table 3.6 show the initial condition for the simulation at 2000 rpm.

Table 3.6: Initial conditions at 2000 rpm

Variables	Value	Units
Cylinder pressure	1150684	Pa
Cylinder temperature	605.1476	K
Turbulent kinetic energy	22.836	m2/s2
Turbulent dissipation rate	3396.147	m2/s3
Progress variable	0	-

Source: Fadzil, (2008)

3.11 Simulated Problem

To ensure an acceptable result, there are some parameters that need to be adjusted during the simulation. It can be list as (i) L-J characteristic length, (ii) L-J energy parameter, and (iii) number of DOF. By using kinetic theory to vary properties, there are some parameters need to be filled up. To calculate the viscosity value, L-J parameter need to be known. However, by putting the calculated value, the result seems to be unreasonable. Therefore, the study has selected the L-J parameter as the adjustable

parameter based on the realistic method. Case 2 until 5 is the value of L-J parameter that has been adjusted. Noted that, case 1 is selected to be the constant mixture properties and also as the benchmark case for this study. Table 3.7 shows the value of L-J parameter for case 2 until case 5.

Table 3.7: Problem setup for the case study

Case study	L-J characteristic length	L-J energy parameter
Case -1	-	-
Case -2	3.745	80
Case -3	3.766	86.267
Case -4	3.79	90
Case -5	3.90	100

To calculate the variable specific heat, the value of DOF must be known. Since the simulation is done in 3 dimensional model, there are three axis been used. The combustion process is not completed by using only 3 degree of freedom. So that, the additional axis is been added. And by assuming each axis has one rotational axis, there are six axis total. So that, the specific heat for varying properties can be calculated.

3.12 Technical Specification

To perform this simulation, a computer is needed to make the simulation run in 24 hours. The simulating process will make the computer's temperature increase. In order to maintain the temperature, the device must be placed in cool environment. A room with air-conditioning system is highly recommended. For this study, a computer lab is used. The specification for the computer is shown in Table 3.7.

Table 3.8: Computer specification

Parameter	Size and Feature
Operating System	Window 7 Professional
Processor	Intel(R) Xeon(R) CPU X5650 @2.67GHz 2.66GHz (2 processors)
System type	64-bit Operating System
Serial ATA Hard Drives	500GB SAMSUNG HM320JI ATA Device (1 unit)
Installed Memory (RAM)	16.0 GB
Graphics	Intel Standard

3.13 Validation Method

After the simulation done, the graph of both simulations plotted. The result compared with the experimental data for validation purpose. The result of constant mixture properties and variable mixture properties are plotted along with the experimental data. By do so, the graph is studied on pressure different among the properties and experimental data which taken from the previous study.

3.14 Limitation of Study

Since the study is only based on the simulation using CFD approach, some of the parameters have to be assumed due to lack of exact data or event. Besides, the model design has to be simplified because of the limitation of computer processor. The simplified model will reduce the difficulties during problem setup, meshing process, simulation and the computing time.

The mesh size is an important parameter to be considered. The smaller mesh size will produce a better result. Since the computing time is increase once the mesh size decrease, it is acceptable for the mesh size is in average size.

CHAPTER 4

RESULT AND DISCUSSION

4.1 Introduction

This chapter presents the computational result produced by simulating the internal combustion engine modeling. The result composed of simulated cylinder combustion pressures which contain (i) combustion pressure, (ii) mass fraction burned, and (iii) turbulent flame speed. Results are continued with laminar flame speed, thermal conductivity and lastly summary.

4.2 Combustion Pressures

Combustion process in an engine is a very complex process. It is because every crank angle increased has different value of temperature which affects most of the properties in SI engine. In order to validate the result calculated from this simulation, result from experimental data carried out by (Fadzil, 2008) based on the cylinder pressure was used. The total simulation period for this simulation is exactly 50 units of crank angle which is during the combustion process right before the spark plug ignites and result of the cylinder pressure has been plotted according to this period. The spark plug was set to be ignites at 23^{o}CA before TDC. Thus, the simulation start from 337^{o}CA which the spark start to ignite and the start of combustion process until the fuel mixture in cylinder is majorly burned at 27^{o}CA after TDC.

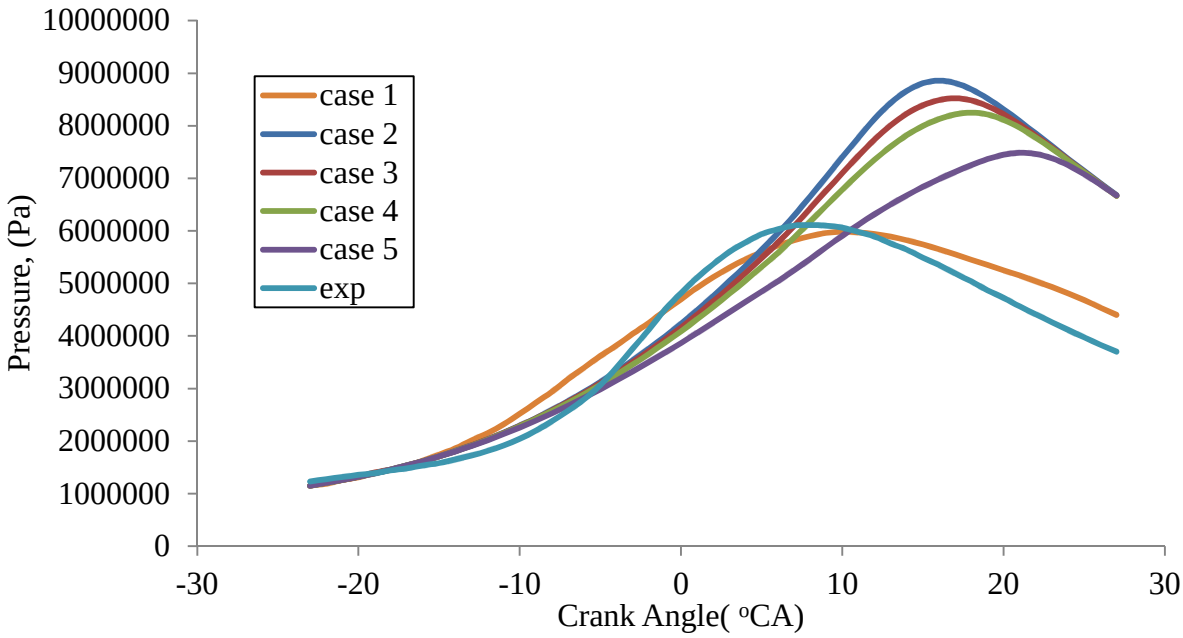

Figure 4.1: Cylinder pressure different for each case.

Figure 4.1 shows a graph of cylinder pressure against crank angle degree for both experimental data and simulation result. From the graph, there is only small pressure rise during the start of the combustion process for all cases, which from 23°CA until about 16°CA. This is because of only small amount of cylinder mixture has been burned. This period is known as the ignition and flame development stage, where about 5-10% of the cylinder mixture is burned and little pressure rise is noticeable. For the experimental data, the cylinder pressure increase greatly from 23°CA before TDC until about 6°CA after TDC. It is different with case 2 until case 5 which their cylinder pressure increased greatly from about 7°CA before TDC until about 12°CA after TDC.

The difference of this stage is basically because of the mass fraction burn of each cases is different. It also caused the peak pressure timing for each case different. The peak pressure value and the timing peak value for each case can be seen in Table 4.1 and Table 4.2. The greatly increased in the pressure is classified as the turbulent flame propagation stage and turbulent flame speed is greatly influenced to the cylinder pressure during this period. About 90-95% of the cylinder mixture is burned during this stage. This stage also provided the force to produced work in the expansion stroke. The final 5-10% of the cylinder mixture is burned in flame termination stage which after the

cylinder reached the peak pressure and during this period, the pressure quickly decrease and the combustion stop.

Table 4.1: Peak pressure predicted for case 1 to 5

Case Number	**Peak Pressure** (bar)	**Deviation from exp** (%)
Exp.	61.19	0%
Case 1	59.85	2.19%
Case 2	88.58	45%
Case 3	85.22	39.27%
Case 4	82.49	34.81%
Case 5	74.86	22.34%

Table 4.2: Peak pressure timing predicted for case 1 to 5

Case Number	**Timing** (^{o}CA after TDC)	**Deviation from exp** (%)
Exp.	8	0%
Case 1	10	25%
Case 2	16	100%
Case 3	17	112.5%
Case 4	18	125%
Case 5	21	162.5%

Based on Table 4.1 and 4.2, in case 2 until case 4, the peak pressure values are 88.58 bar, 85.22 bar, and 83.49 bar. These give deviations as much as 45 %, 39.27% and 34.81% for those cases. The large deviations are shown to be unreasonable for a normal combustion process. On the other hand, the peak pressure timing for those cases are 16^{o}CA, 17^{o}CA and 18^{o}CA respectively. These give about 100%, 112.5% and 125% deviation from the experimental data.

For case 5, the peak pressure is 74.86 bar which give 22.34% of deviation. Although the value of deviation is still large, it is the smallest value among all cases using varying properties in simulation. However, the peak pressure timing for this case is 21^{o}CA after TDC which give deviation as much as 162.5% which is the largest among them.

For case 1 which using constant properties in this simulation, the peak pressure is 59.85 bar respectively. This gives only 2.19% deviation from the experimental data which is the closest value in this simulation. The peak pressure timing in this case is 10^{o}CA after TDC. This give deviation of 25% compared to the experimental data. Thus, case 1 gives the best prediction of the peak pressure and peak pressure timing for all cases.

Among those case using constant and varying mixture properties, the cases used varying mixture properties give finer prediction of cylinder pressure profile than constant mixture properties. Even though their peak pressure and peak pressure timing give large deviation value. Logically, when the temperature increasing in the combustion process, the mixture properties value will also increase and this will cause the mixture properties value become variable. By using varying mixture properties, the result supposedly closed to the experimental result. The lacking of peak pressure timing is mostly caused of the mass fraction burned. Thus, in order for exactly fit the experimental cylinder profile, the simulated models must approximate exact values of mass fraction burned at each time step. However, in TFSC model formulation, the mass fraction burned value is calculated by the conservation equation of progress variable.

4.3 Mass Fraction Burned

In order to understand the variation of cylinder pressure, the results of mass fraction burned has been study. The mass fraction burned value is equivalent to the instantaneous progress variable, calculated by TFSC model. Figure 4.16 presents the comparison of experimental and simulated mass fraction burned for five different cases. The results of mass fraction burned have been plotted from the start of combustion at 23^{o}CA before TDC until the burning complete at 27^{o}CA after TDC. Total simulated period is 50 units crank angle degree. The timing of mass fraction completely burn is presented by Table 4.3.

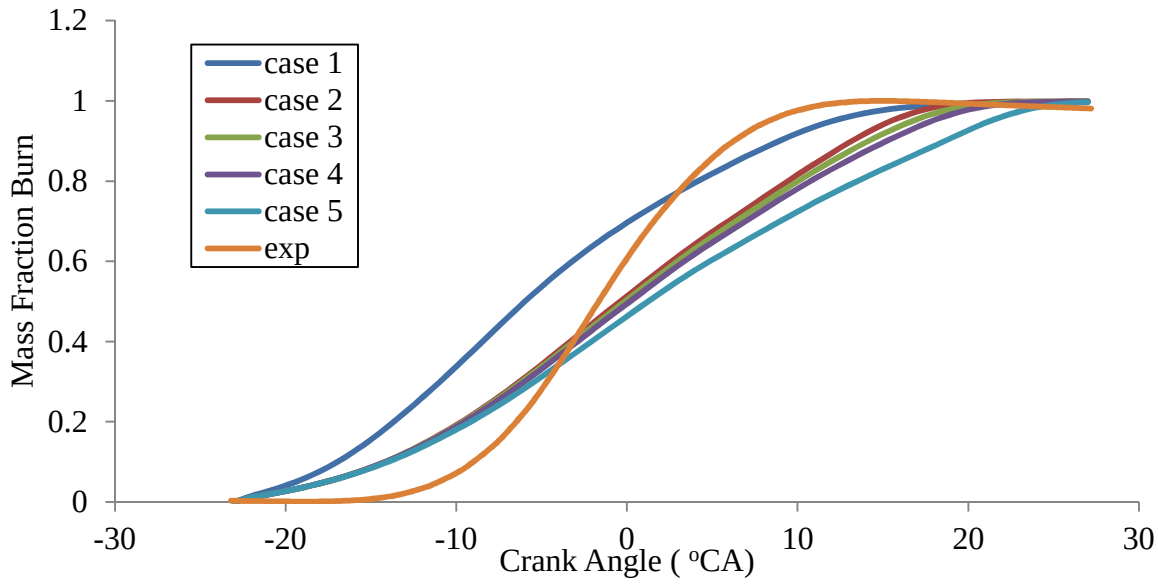

Figure 4.2: Mass fraction different for each case.

Figure 4.2 shows graph of mass fraction burned against crank angle degree during the combustion process for both experimental and simulation result. Based on Figure 4.2, the experimental data of fraction burned give a typical profile of mass fraction burned found in conventional SI engine. As the start, a very small fraction burned causing low heat release and also the cylinder pressure. The rising of mass fraction value in the middle of the process make the cylinder pressure highly raised. After the mass fraction value approximately 1, the cylinder mixtures are fully burned and cause the pressure drop in the cylinder.

Table 4.3: Timing of mass fraction burned predicted for case 1 to 5

Case Number	**Timing** (^{o}CA after TDC)	**Deviation from exp.** (%)
Exp.	10	0%
Case 1	12	20%
Case 2	18	80%
Case 3	19	90%
Case 4	20	100%
Case 5	23	130%

From Table 4.3, the simulated model of case 1 has the smallest value of deviation which is 20% of deviation followed by case 2 with 80% of deviation, case 3 with 90% of deviation, case 4 with 100% of deviation and lastly case 5 with 130% of deviation which the largest value. Small value of deviation in mass fraction burned mean the mass fraction fully burn is closed to the experimental data and will cause the peak pressure timing closest to the experimental peak pressure. For case 2 until case 5, the timing of mass fraction fully burned is very late. This will cause the heat released for the combustion process slower and the cylinder pressure raised slower. Additionally, in TFSC model formulation, the model assumed the instantaneous mass fraction burned is equivalent to the instantaneous progress variable value which is highly affected by the turbulence flame speed.

4.4 Turbulent Flame Speed

The turbulent flame speed is the most important parameter that controls the reaction rate at each stages of engine combustion. The flame speed depends on the turbulence immediately in front of the flame and turbulent flame develops from the spark discharge, spreads across the mixture and extinguishes at the combustion chamber wall.

Based on Figure 4.3, case 1 start with high value of turbulent flame speed and slightly increase before it start to decrease until the end of the process. Different with case 2 until case 5 which they start with low value of turbulent flame speed and it is slightly decrease before it start increasing. When the crank angle degree about 6^{o}CA – 10^{o}CA, the turbulent flame speed for those cases are decreased and had a mirror increased among them. It mean before the turbulent flame speed drop, case 2 has the highest value and case 5 has the lowest value of the flame speed. When they are increased, case 2 has the lowest value while case 5 has the highest value of the turbulent flame speed. Then, about 17^{o}CA – 22^{o}CA, the speeds drop a little before highly increase. Case 4 and 5 are drop right before the end of the combustion process. For case 3 and 4, they might drop in the next process of SI engine.

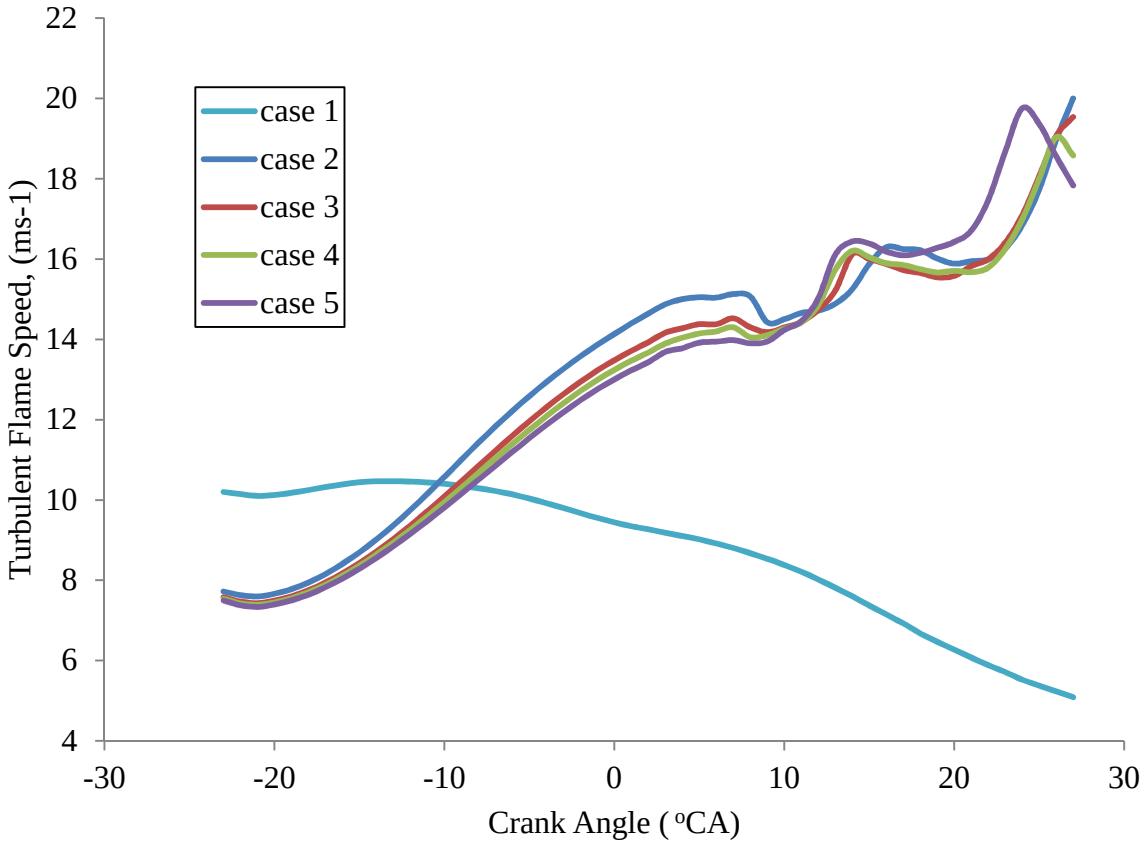

Figure 4.3: Turbulent Flame Speed different for each case

Figure 4.3 shows graph of turbulent flame speed against crank angle degree during combustion process for both constant and varying mixture properties. Constant mixture properties has different trend compare to varying mixture. Which show that, the mass fraction burned and the cylinder pressure graph for both constant and varying mixture properties has different trend.

Based on Eq. (3.12) of Zimont's turbulent flame speed model, the value of turbulent flame speed is influenced by the root mean square (RMS) velocity, laminar flame speed, laminar thermal diffusivity, turbulent length ,time scale and chemical time scale. For current study, the RMS velocity is calculated by the solver based on the prescribed boundary and initial condition. The value of laminar flame speed is calculated using metghalchi-keck law. Then, value of chemical time scale is computed based on the value of laminar thermal diffusivity and laminar flame speed of Eq (3.13). Laminar thermal diffusivity is computed using thermal conductivity and specific heat of

Eq (3.21). So, the calculated value of turbulent flame speed is most influenced by some properties which are 1) laminar flame speed, 2) thermal conductivity and 3) specific heat.

4.4.1 Laminar Flame Speed

Laminar flame speed is calculated using metghalchi-keck law by the TFSC model. The combustion mixture is set as isooctane-air. Thus, the data is plotted in Figure 4.4.

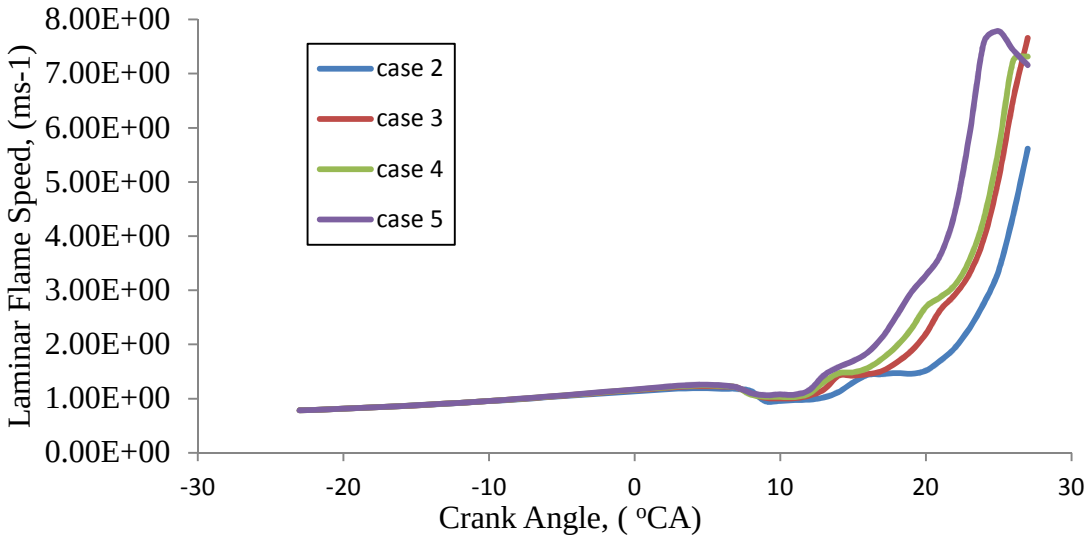

Figure 4.4: Laminar Flame Speed difference for each case.

Figure 4.4 shows graph of laminar flame speed against crank angle degree during combustion process for varying mixture properties. Noted that, the value of laminar flame speed for constant mixture properties was set constant which is 0.4762 ms^{-1}. Based on Figure 4.4, there only small value of increasing from 23^{o}CA before TDC until about 6^{o}CA after TDC for all cases. Their value is approximately same in this stage which in range of ±0.01 ms^{-1} changes. All cases has same trend which increased slowly at the beginning, drop a little, then flat and had sudden increase before they increasing casually.

The value of laminar flame speed is inversely proportional to the chemical reaction time scale of Eq (3.13). And the chemical reaction time scale is also inversely proportional with turbulent flame speed of Eq (3.12). These answer why in Figure 4.3, the turbulent flame speed is decrease slightly around 6^{o}CA after TDC.

4.4.2 Thermal Conductivity

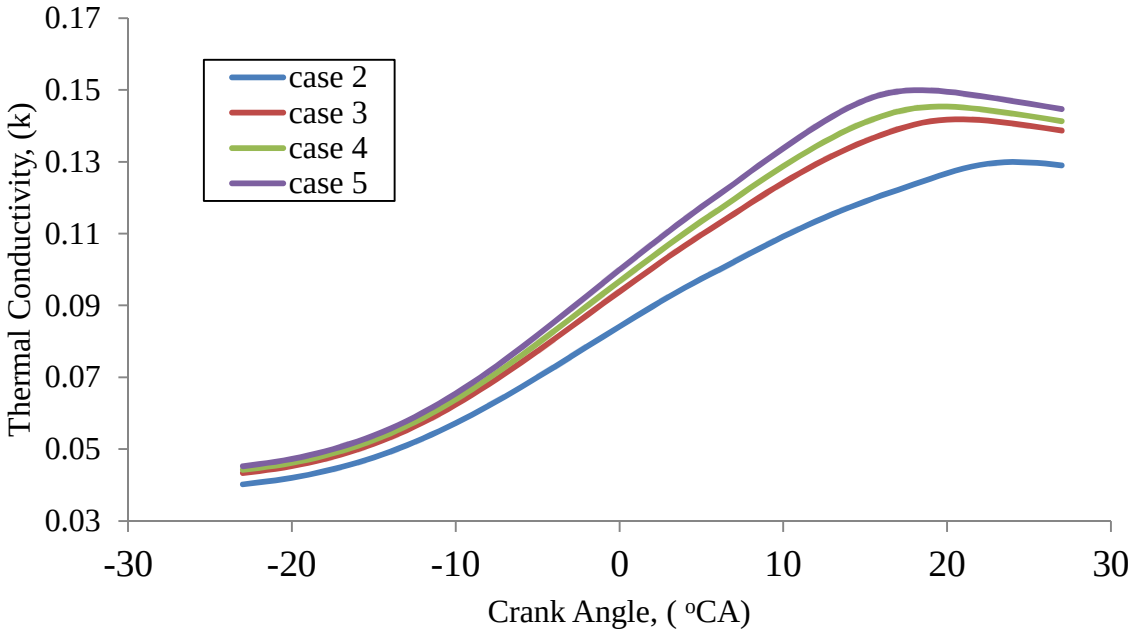

Figure 4.5: Thermal Conductivity difference for each case

Figure 4.5 shows graph of thermal conductivity against crank angle degree in combustion process for varying mixture properties. The value for constant mixture properties was set constant which 0.08207936 W/m.K. Based on Figure 4.5, all cases have the same trend. They increase slowly from 23^{o}CA before TDC until about 15^{o}CA before TDC. Then, the increasing becomes faster before each case closely to their peak. Case 2 has the lowest curve among others. The peak value for case 2 is 0.13 k, followed by case 3, 0.1451 k, then case 4, 0.1453 k and lastly case 5, 0.15 k.

4.5 Summary

This chapter has presented the simulation data and the experimental result. The simulation data have been validated with the experimental result. Combustion pressure analysis using CFD prediction is the main interest in this study. The discussions are then supported by the result of mass fraction burned, turbulent flame speed, laminar flame speed and thermal conductivity. This approach is needed because these parameters are the parameter that controlling the cylinder pressure.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.1 Conclusion

Computational fluid dynamic modeling approach has been used to simulate the spark ignition engine for fluid flow problems. Based on the simulation result, the constant mixture properties has the perfect fit with the experimental data. The analysis of the peak pressure and the peak pressure timing for constant mixture properties give only 2.19% and 25% deviation from the experimental data. However, it did not follow the cylinder profile of the experimental. Different with varying mixture properties analysis, it has similar profile of cylinder pressure with the experimental data which slowly increase at the start of the combustion process then highly increase before reaching the peak. But, the closest peak pressure and peak pressure timing for varying properties give as much as 22.34% and 162.5% deviation from the experimental data. The L-J parameters seem not to be accurate enough to fit the peak pressure and peak pressure timing of experimental cylinder pressure.

The results of the cylinder pressure occur due to inaccurate mass fraction burned prediction. The inaccurate prediction of mass fraction burned is highly controlled by turbulent flame speed prediction. Turbulent flame speed is an important parameter in order to produce heat and also the pressure. The increasing of temperature will cause the pressure increase. Furthermore, turbulent flame speed is depends on laminar flame speed, laminar thermal diffusivity, laminar thermal conductivity and specific heats. As conclusion, factors that affect the model prediction are recognized and critically need refinement in future works.

5.2 Recommendation

Since in this study, all of the varying mixture properties have the same trend which lacking of peak pressure and peak pressure timing deviation, L-J parameter is highly affect the trend of the pressure profile. Thus, further study in these parameter is extremely needed to ensure the perfect profile of engine combustion pressure. In order to validate the L-J parameter value, variable engine speed is suggested. As the technology is improved in lifetime, the pressure and temperature contour can be attached further to improve the understanding of combustion changes in the combustion chamber.

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