COMBUSTION MODEL DEVELOPMENT AND VALIDATION



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MASTER THESIS WORK

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DEDICATION

This research is dedicated to my parents whose prayers and support made me able to accomplish this and to my supervisor who never failed to teach and guide me.

I am highly obligated to the School of Mechanical and Manufacturing Engineering (SMME), NUST for funding this study which successfully enabled me to complete this study.

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ABSTRACT

In today's world emissions from diesel engines imparts severe damage to the environment and health of human being. The study of emission control starts with the design and development of engines and ends with the implementation and installation of exhaust control devices and equipments. While designing engine the combustion modeling plays a crucial role on emission characteristics. For this purpose various types of combustion models are available which includes the simple fast and easily operated to complicated time consuming and detailed physical and chemical models. Phenomenological combustion modeling is one which lies in the category of simple, agile and thorough modeling. This study based on one of the phenomenological modeling where the purpose is to find the rate of heat release by providing the injection profile of fuel. It enables the distinguished study of the pilot and main combustion heat release by defining the pre-combustion and mixing controlled combustion. It facilitates the survey of evaporation perspectives and modeling that involves in the fuel injection and afterwards in the combustion characterization. It also compares the credibility of model by comparing results with the experimentally pressure curve generated model. The software MATLAB/SIMULINK is exercised to build this model.

Cover Page		1					
Form TH4		2					
Dedication	Dedication						
Declaration		4					
Acknowledgment	S	5					
Abstract		6					
Table of contents		7					
List of Figures		10					
Abbreviations		12					
1. CHAPTE	R 1: Bibliographic Survey	13					
1.1 Diesel	Fuel Qualities	13					
1.1.1	Grades of Diesel Fuel.	13					
1.1.2	Cetane Number	15					
1.1.3	Knocking & Detonation	15					
1.2 IC Eng	gine Basics	15					
1.2.1	Diesel Engine	15					
1.2.2	Operating Parameters	17					
1.3 Diesel	Cycle	19					
1.4 Comb	ustion in Diesel Engine	21					
1.4.1	Geometry of the Combustion Chamber.	21					
1.4.2	Fuel Flow Ratio	22					
1.4.3	Swirl Ratio	23					
1.5 Types	of Combustion System	23					
1.5.1	Direct Injection System	23					
1.5.2	Indirect Injection System	24					
2. CHAPTE	R 2: Literature Review of Combustion Modeling	25					
2.1 Types	of Combustion Model	25					
2.1.1	Thermodynamic Modeling	25					
2.1.2	CFD Modeling	25					
2.1.3	Phenomenological Modeling	26					
2.2 Comb	ustion Models	26					
2.2.1	de Neef and Hohlbaum HRR Model	26					
2.2.2	Chmela et al. HRR Model	27					
2.2.3	Hiroyasu et al. HRR Model	27					
2.2.4	Gunner Stiesch HRR Model	28					
2.3 Fuel Spray Dynamics							
2.3.1	Spray Formation and Droplet Behavior	28					
2.3.2	Droplet Size Distribution	31					

TABLE OF CONTENTS

	2.3.3 Fuel Inject	or
	2.3.3.1 Steady	Flow Injector
	2.3.3.2 Interm	ittent Injector
	2.4 Mass flow Rate	-
	2.5 Penetration of Spr	ay
	2.6 Angle of Spray	·
	2.7 Vaporization of D	roplets
	2.8 Ignition Delay	-
	2.9 Quality of Injected	d Fuel
	2.10 Factors of Phy	vsical Process on Delay
	2.10.1 Injection T	liming
	2.10.2 Engine Lo	ad and Injection Quality
	2.10.3 Rate, Size	and Velocity of Injection
	2.10.4 Temperatu	re and Pressure
	2.10.5 Speed of E	Ingine
	2.10.6 Chamber V	Wall Effects
	2.10.7 Rate of Sw	virl
	2.10.8 Concentrat	tion of Oxygen
	2.10.9 Property o	f the Fuel
	2.10.10 Cetane Nu	umber
	2.10.11 Volatility	and Viscosity
3.	CHAPTER 3: Diesel	Fuel Spray and Emissions
	3.1 Dec et al. Spray N	10del
3.2 Structure of Diesel Flame3.3 Injection Profile3.4 Maiboom, A. Model		l Flame
		lel
	3.5 Diesel Engine Em	issions
	3.5.1 NOx Form	iation
	3.5.2 Carbon Di	oxide
	3.5.3 Black Smo	oke
	3.5.4 Noise	
	3.5.5 Diesel Par	ticulate Matter
	3.6 Variation in Exha	ust with different Engine Conditions
	3.7 CI Emission Redu	iction
	3.7.1 Changing	Ignition Delay
	3.7.2 Turbo-cha	rging and Intercooler
	3.7.3 EGR Syste	۶m
	3.7.4 Diesel Par	ticulate Filter
	3.7.5 Catalytic F	Reduction and NOx Trapping

3.7.6 Humid Air Motor System	61
3.8 Effects of Diesel Emissions on Human Health	62
4. CHAPTER 4: Phenomenological Single Zone Combustion Model	64
4.1 Introduction	64
4.2 Input parameters	65
4.3 Development of Pressure Curve ROHR Model	66
4.3.1 Cylinder Pressure	68
4.3.2 Cylinder Volume	69
4.3.3 Cylinder Temperature	70
4.3.4 Heat Capacity	70
4.3.5 Law of Thermodynamics	71
4.4 Development of Fuel Injection ROHR Model	71
4.4.1 Evaporation Model	72
4.4.2 Premixed Combustion	75
4.4.3 Mixing Controlled Combustion	77
4.4.4 Ignition Delay	79
5 CHAPTER 5: Results, Discussions & Validations	80
5.1 In-Cylinder Pressure	80
5.2 In Cylinder Temperature	81
5.3 Rate of Heat Release	82
5.4 Cumulative Heat Release	85
5.5 Recommendations and Discussions	86
References	87

LIST OF FIGURES

- Figure 1.1: Reciprocating Internal combustion engine basic geometry
- Figure 1.2: Theoretical and actual measured Diesel cycle pressure-volume diagram
- Figure 1.3: Projection of a cylinder volume
- Figure 1.4: DI Compression engine (a) multi-hole nozzle with quiescent chamber
- (b) bowl in piston chamber (c) bowl-in piston chamber with swirl
- Figure 1.5: IDI Compression engine (a) Swirl pre-chamber (b) turbulent pre-chamber
- Figure 2.1: Quasi-stationary gas jet Model in solid body flow field rotation
- Figure 2.2: Fuel injection Packet Model
- Figure 2.3: Droplet Size Distribution
- Figure 2.4: Pressure swirl atomizer
- Figure 2.5: Measured drop size distribution for a pressure –swirl atomizer
- Figure 2.6: Air blast atomizer with pilot fuel for low rundown
- Figure 2.7: Multi-hole nozzle (a) Nozzle with sac volume (b) Sacless volume
- Figure 2.8: Pintle nozzle (a) standard (b) throttling
- Figure 2.9: Vaporization rate curve for kerosene and jet fuel
- Figure 2.10: Ignition delay as a function of load
- Figure 2.11: Ignition delay as a function of reciprocal air temperature
- Figure 2.12: Effect of spray impingement on wall 100 mm from nozzle on ignition delay
- Figure 2.13: Effect of oxygen density in gas on ignition delay
- Figure 2.14: Effect of fuel cetane number on ignition delay over the load and speed range
- Figure 3.1: Test engine used for investigation of Fuel Jet
- Figure 3.2: Evolution of combustion of Fuel Jet
- Figure 3.3: Evolution of temperature and chemical composition in a Flame Plume
- Figure 3.4: Combustion vessel cross section schematic
- Figure 3.5: Lift off length versus ambient gas temperature for four gas oxygen concentrations
- Figure 3.6: Spray Jet Model
- Figure 3.7: Injection rate for a direct injection diesel engine without pre-injection
- Figure 3.8: ROHR for direct injection diesel engine
- Figure 3.9: Description of Zones
- Figure 3.10: Production of NOx and PM with respect to temperature

- Figure 3.11: Production of emissions with respect to ignition delay
- Figure 3.12: Effect of after-cooling and turbo-charging on NOx and PM
- Figure 3.13: EGR system
- Figure 3.14: A continuously regenerating diesel particulate filter, CR-DPF
- Figure 3.15: Principal sketch of the HAM system
- Figure 3.16: Relationship of Nitrogen Oxides (NOx) emissions with the formation of NO₂
- Figure 4.1: Cylinder Pressure
- Figure 4.2: Geometry of Piston Cylinder
- Figure 4.3: Change in Cylinder Volume with respect to Crank Angle
- Figure 4.4: Cylinder Temperature
- Figure 4.5: Instantaneous Injection rate with respect to crank angle
- Figure 4.6: Evaporation constant with respect to crank angle using temperature curve
- Figure 4.7: Laminar Flame Speed s_l versus Air/Fuel equivalence Ratio λ_{zn}
- Figure 4.8: Calculated ROHR of Pilot Fuel
- Figure 5.1: Measured Pressure Trace
- Figure 5.2: Selected Pressure Trace
- Figure 5.3: In-Cylinder Temperature
- Figure 5.4: In-Cylinder Temperature (2)
- Figure 5.5: ROHR Calculated from Pressure Curve
- Figure 5.6: Pre-Mixed Combustion
- Figure 5.7: Calculated Pre-Combustion
- Figure 5.8: Calculated ROHR
- Figure 5.9: Measured V/S Calculated ROHR
- Figure 5.10: Cumulative Heat Release

			GREE	<u>EK</u>	
Nor	<u>nenclature</u>		ρ De	ensity	$\frac{kg}{3}$
A	Area	m^2	λ _{an} Ai	r/Fuel equivalence ratio	m ³
С	Constant	-	-2 <i>n</i>	nometic Viscosity	m^2
C _M	Mean Piston Speed	$m_{/s}$	υ	nematic viscosity	S N
c _P	Specific heat of the gas	$\frac{KJ}{kaK}$	σ Su	rface Tension	$\frac{n}{m}$
d_N	Diameter of Nozzle	m	β Ev	vaporation Constant	$\frac{m^2}{s}$
D	Diameter	m	$\Lambda \frac{Ai}{2}$	r +Residual gas	-
D _{fu}	Diffusion constant	_	φ <u>F</u> ι	^{Fuel} Equivalence Ratio	_
f _m	Mixing frequency	<u>1</u>	$\begin{array}{c} \boldsymbol{\varphi} & A \\ \boldsymbol{\theta} & C_1 \end{array}$	<i>ir</i> Equivalence Radio	deg
f	Eraction volume of residual gas	<i>s</i>	SUBS	<u>CRIPTS</u>	
Jre	Traction volume of residual gas	- KI	0	Initial	
h _{fg}	Latent heat of vaporization	$\frac{f}{kg}$	а	Air	
k	Turbulent kinetic energy density	m^2	boil	Boiling point	
n	Turbulent kinetie energy density	s^2	ch .	Chemical	
k_g	Thermal conductivity of gas	$\frac{W}{m.K}$	cyl	Cylinder	
L	Characteristic Mixing Length	m	u diss	Disgination	
m	Mass	kg	uiss eff	Effective	
Ne	Engine Speed	rpm	evan	Evaporation	
n_N	Number of nozzle holes	-	f	Fuel	
P	Pressure	Ра	fl	Flame	
Pr.	Prandtl's number	-	Ι	Injection	
r	Radius	m	init	Initial	
Ro	Reynold's Number		inj	Injection	
ΛC		m	n	Nozzle	
s _l	Laminar Flame speed	s	pny nrod	Physical Production	
s _t	Turbulent Flame speed	$\frac{m}{s}$	re re	Residual Gas	
T	Temperature	ĸ	ref	Reference	
T _m	Temperature surrounding the droplet	t K	ub	Un burnt	
t	Time	S	Z	Zone	
11.	Turbulent Intensity	m	ABRE	EVIATIONS	
ut	Turbulent intensity	s m	SOC	Start of Combustion	
u	Velocity	s	SOI	Start of Injection	
V	Volume	m^3		Direct Injection	
We	Weber Number	_		SAUTER Mean Diameter	
			HRR	Heat Release Rate	
				Hou Roloubo Ruio	

1. CHAPTER 01: Bibliographical survey

Diesel combustion is characterized by multitude of physical and chemical processes which includes liquid fuel injection, atomization, development of spray, air fuel mixture formation, combustion, and emission formation. After the evaporation of spray it incorporates with the hot compressed air and burns itself. The basic premise of diesel fuel is its ability of releasing the chemical energy that is stored in the fuel.

The aim of this study is to develop a combustion model to describe all the physical phenomena and built a model that can predict the heat release rate in a short time by using injection rate profile.

Taking into account the stated aim of this thesis, the following bibliographic study is divided into four parts:

- ✓ The first part describes the different types of fuel used on the basis of their quality and grades
- ✓ The second part review the basics of engine parameters with their main governing equations
- ✓ The third part introduce the combustion phenomena and its basic characteristics
- ✓ *The fourth part describes the combustion types on the basis of injection.*

1.1 Diesel Fuel Qualities

Diesel fuel is a kind of liquid type fuel that is used in diesel engines. The typical type of fuel is petroleum fuel oil that is derived from the fractional distillation of crude oil at atmospheric pressure in between 200 and 350 C° . This results in a mixture of carbon chain with the 8 to 21 carbon atoms per molecule. The other type of fuel like biodiesel, gas to liquid (GTL) and biomass to liquid (BTL) are not extracted from petroleum fuel oil. The type of fuel that is derived from petroleum is commonly known as petro-diesel fuel.

1.1.1 Grades of Diesel Fuel

There are commonly three types of grades used in various types of engines depending upon their quality and engine capacity

a) 1-D

They are light middle distillate special purpose fuel. They have three categorize which include S15, S500, and S5000. They are used in the application where 15, 500 and 5000 ppm (parts per million) sulfur is required respectively.

b) 2-D

They are used in the conditions where the load and speed is changing with time. They are general purpose distillate fuel. They also lie in the category of S15, S500, S5000 depending upon the ppm of sulfur with respect to the application in which they are used.

c) **4-D**

This is a type of heavy distillate fuel that is derived from the blend of residual oil and distillate. They are used in low and high speed engines but with the constant speed and load engines.

S-500 grade represents the previous sulfur grade of low type. S-15 grade is known as ULSD (Ultra low sulfur grade). This grade is common in use now-a-days. Grade 1-D and 2-D is used in general vehicles while 4-D is used in the stationary and marine engines that are operating on constant speed and load. The difference in the fuel grades is due to their viscosity and the temperature at which the fluid flow.

The smoke in the diesel engine exhaust is due to the in-complete combustion. The white smoke type is due to the unburned fuel drops resulting from the engine ignition at low temperature. This type of smoke ends when the engine temperature rises. The type of black smoke is due to the insufficient air supply, sufficient fuel supply and high load on engine. The burning of lubricating oil results blue-grey smoke.

The design of engine is crucial in deciding the power and economy of the fuel. The fuels with higher density as ULSD type 2 gives improved mechanical efficiency and fuel economy when 1-D fuel mixes with them. The energy content of 1-D diesel type is 95% and they provide lower fuel efficiency than 2-D. They are also lower in viscosity which results in the lower lubrication in the fuel distributor and fuel pump. The varying load and speed requirement is common now-a-days. The fuel that is best for this type of condition is high volatile fuel.

1.1.2 Cetane Number

The quality of diesel fuel is determined by the centane number. The fuel volatility is also measure by cetane number. The higher rating helps in smooth engine running due to proper combustion. The 1-D and 2-D type diesel fuel cetane rating ranges from 40 to 45. Cetane number is totally different from the octane number of gasoline fuel. In octane rating, the higher the number of fuel on the scale of octane, the higher it has the capability to resist the self ignition. As the improper ignition in the gasoline engines cause knocking. While in cetane rating, the higher the rating the finer the fuel will burn. If the cetane number of the fuel is too low then it becomes very difficult to start to ignite.

1.1.3 Knocking & Detonation

Knocking also known as detonation pinging and spark knock is due to the premature combustion of the air/fuel mixture. The premature mixture auto ignites or pre-ignites in the combustion chamber. This initiates a shock wave which strike with the cylinder piston that is travelling towards the top dead centre which results in the sound of ping/knock blasting adjacent to the wall of cylinder. This causes severe damage to the engine piston and result in the complete destruction of the engine.

1.2 IC Engine Basics

Internal combustion (IC) engines produce mechanical work from chemical energy that is possessed by the fuel. Inside the engine Energy is released by oxidization of the fuel. The air fuel mixture and the burned products of combustion all include in the working fluid. For ignition and combustion a flammable air fuel mixture and an energy source is a basic requirement. In spark ignition engines the energy source comes from the spark of spark plug while in compression ignition engine this source comes from the compressed air. The higher the compression ratio the more it is useful as it takes out more mechanical energy from the given amount of air fuel mixture due to its higher thermal efficiency.

1.2.1 Diesel Engine

Diesel engines are commonly known as compression ignition (CI) engines. Light fuel oil is used in most applications. While in power generation and marine engines residual fuel in heated form is utilized. Air is injected at the time right before the combustion startup. In each cycle by varying the amount of fuel during injection the load on the engine is controlled. The flow of air inside the cylinder is consistent. Depending upon the application used the variety of engines are used as in locomotive, automotives marine and power generations. Naturally atmospheric air aspirated and forced turbocharged in which the air is forced to compress by the turbine running by the exhaust gases are also in common. On the other hand the supercharged engines in which the inlet air is compressed by the mechanically driven shaft are common in the usage of high load applications. To increase the engine output, turbocharged and supercharged are commonly used by increasing the air in the displaced combustion chamber cylinder volume with the increase in the flow of fuel. To reduce engine weight and size these methods are in common practice. The compression ratio of diesel engines is much higher than the spark ignition (SI) engines depending upon the type of engine used. It ranges from 12 to 24 [1]. The turbocharged and supercharged engines work on the higher values of compression ratio. Both SI and CI have same valve timings. During the intake stroke the air is induced and then compressed to 4 MPa pressure and a temperature of 800 K approximately at the time of compression. Before the top dead centre of the cylinder at the angle of 20 degrees the fuel is injected in the cylinder. The liquid fuel atomizes and the already compressed air entrains. In the combustible proportions the evaporated liquid fuel blends with the air. The pressure and temperature of air are higher than the ignition point of fuel. Consequently after some time delay auto-ignition of uneven fuel air mixture starts the combustion process instantly. The cylinder pressure rises. In the region of injected fuel the flame advances immediately. Following the combustion in the expansion phase the mixing of air fuel and gases pursue. The exhaust stroke is identical to the SI engines. The whole cycle start again after the completion of exhaust stroke.

While in the 2 stroke CI engines all the processes are same except the intake and exhaust strokes which are not alike. Inlet and exhaust ports are on the same side of the cylinder and are unveiled at the time of approach of Bottom dead centre of the cylinder. The pressure of cylinder drops instantly after when the exhaust ports are open. The ports of inlet air open when the pressure of cylinder drops below the inlet pressure. The fresh charge of air removes the already burned gases. As the piston starts in the compression stroke after the shutting of the ports, all the processes proceeds in the same way as in the four-stroke cycle of compression ignition.

1.2.2 Operating Parameters

Several geometric and thermodynamic parameters characterize the performance of an engine. For a single cylinder, piston, connecting rod, crankshaft and head assembly is represented as



Figure 1.1: Reciprocating Internal combustion engine basic geometry

For calculation of different operational parameters following geometrical particulars are considered: crank radius a, bore b, connecting rod length l, stroke s, crank angle θ . The one half of the stoke length is crank radius. The crankshaft position at $\theta = 0^{\circ}$ is referred as top dead centre (TDC) or top centre (TC) of engine. The volume at this time is at its minimum position. This volume is commonly known as clearance volume V_c . The crankshaft position at $\theta = 180^{\circ}$. The volume V_t is at its maximum position and it is referred as bottom dead centre (BDC) or bottom centre (BC). The ratio of maximum to minimum volume is known as compression ratio

$$r = \frac{V_{BDC}}{V_{TDC}} = \frac{V_t}{V_c}$$

For a single cylinder the displacement volume is calculated as

$$V_d = V_t - V_c = \frac{\pi}{4}b^2s$$

Rate at which the work is done is known as brake power BP. Work done per unit rotation of crank is known as torque τ . The dynamometer is used to measure the brake power of the engine. Brake power is the output power of and engine.

$$BP = 2\pi N\tau$$

The ratio of work done to unit displacement volume is known as mean effective pressure. Two types of mean effective pressures are used i.e. brake mean effective and indicated mean effective pressure. During compression and expansion the net work done to unit displacement volume is termed as indicated mean effective pressure. The ratio of external shaft work done by engine to volume is known as brake mean effective pressure.

For 4-stroke engine type

$$bmep = \frac{4\pi\tau}{V_d}$$

For 2-stroke engine type

$$bmep = \frac{2\pi\tau}{V_d}$$

To calculate the fuel consumption with respect to brake power, the brake specific fuel consumption is used as

$$bsfc = \frac{\dot{m}_f}{BP}$$

It is the measure of efficiency of engine. By using the heat of combustion q_c from the engine the brake thermal efficiency η_b is calculated as

$$\eta_b = \frac{BP}{\dot{m}_f q_c}$$

Another parameter used to optimize engine is volumetric efficiency η_{ν} . It is the mass of air and fuel induced in the cylinder to the mass it would displaced at the intake manifold at the density ρ_i . Intake manifold configuration, timing of lifting of valve, valve size and lift changes the volumetric efficiency.

$$\eta_{v} = \frac{2(\dot{m}_{a} + \dot{m}_{f})}{\rho_{i} V_{d} N}$$

1.3 Diesel Cycle

In diesel cycle is also known as constant pressure cycle. In this cycle heat is supplied to the system at constant pressure. Neither constant volume nor constant pressure cycles are used in modern compression engines. An intermediate cycle in which some part of heat is added at constant volume and other at constant pressure is termed as Dual cycle. It is used to model the combustion processes which are rapid than constant pressure and slower than constant volume. It provides the algebraic equation to model performance parameters like thermal efficiency. The amount of heat addition is decided by the designer that is specified by the type of fuel used, the engine geometry and the fuel injection system. It is used to limit the peak pressure of the cycle. It is also known as limited pressure cycle. The processes are given as

- 1-2: Reversible Adiabatic Compression Process
- 2-3: Heat Addition at constant Volume
- 3-4: Heat Addition at constant Pressure
- 4-5: Reversible Adiabatic Expansion Process
- 5-1: Heat rejection at constant Volume



Figure 1.2: Theoretical and actual measured Diesel cycle pressure-volume diagram

Heat Supplied = $mC_V(T_3 - T_2) + mC_P(T_4 - T_3)$ Heat Rejected = $mC_V(T_5 - T_1)$

Net Work done = Heat supplied - Heat rejected

Thermal efficiency η_{th} in terms of temperatures is given as

$$\eta_{th} = \frac{Net Work \ done}{Heat \ Supplied} = 1 - \frac{T_5 - T_1}{(T_3 - T_2) + \gamma(T_4 - T_3)}$$

Where γ is specific heat ratio and given as

$$\gamma = \frac{C_P}{C_V}$$

1.4 Combustion in Diesel Engine

For off road and on road heavy duty transportation diesel engine is very preeminent. It is also dominant in the industrial power generation and marine engines. Some of the light duty diesel engines have gone through problems like noise weight and pollutant emissions. If the issue of emission is settled then they offer an advantage of improved fuel economy. Diesel engines follow the 4-stroke engine cycle but the only difference lies in the compression cycle.

In the Otto cycle combustion occurs at the constant volume while in this type at the constant it occurs at the constant pressure. While in actual both the volume and pressure changes at the time of combustion. For the same spark ignition (SI) and diesel engines the later have the same higher thermal efficiency and compression ratio. SI engine have intake port for the mixing of air and fuel experience knocking while combustion. While in these type the direct injection of diesel does not cause knocking and thus have higher value of compression ratio. The time delay between the injection of fuel and start of ignition is known as ignition delay. The timing for the start of combustion is controlled by the injection timing. The delay between the injection and combustion start should be short.

By changing the fuel injection during each cycle the torque of engine is controlled. The requirements related to the pumping work are very low which results in the improved mechanical efficiency in comparison to the SI engines. The formation of soot results from the increased amount of fuel injected. The excessive amount of fuel encounters problems while air utilization during combustion. For a given ratio of expansion the diesel fuel has higher conversion efficiency than the SI engines because the diesel fuel always operates with the lean air to fuel ratios.

During the designing the combustion chamber the important thing that should be focused is the complete rapid air fuel mixing and to finish the process of combustion in the convenient crank angle duration adjacent to top dead centre. The burning rate of fuel is controlled by the mixing rate. More persuasive air movement is mandatory while low penetration of fuel is decisive.

1.4.1 Geometry of the Combustion Chamber

Cylinder and piston are included in the combustion chamber. Air enters in the combustion chamber through the port and intake valve and the fuel is introduced from the

injector. The combustion products leave the combustion chamber from the exhaust valve. Fuel injector is placed in the center of the cylinder head. The pressurized fuel is injected through the injector holes which are generally four to eight in numbers. To suspend the infraction of the spray on the head of piston the head is designed in the form of symmetrical recesses bowl.



Figure 1.3: Projection of a cylinder volume

1.4.2 Fuel Flow Pattern

The characteristics of fuel flow inside the cylinder depend upon the factors like configuration of valve and port and the piston head shape. The piston moves away from the top dead centre and sucking air inside the cylinder through the intake valve. Due to the curve shape of the intake ports the swirl motion around the cylinder axis produces. The intake valves then shut off and piston travels towards the upside direction forcing the air of the cylinder to move in the bowl of the piston generating a radial type squish flow. According to momentum conservation theory the swirl increases in the bowl when the radius of the swirling gas decreases. The velocity of the piston and the air above the piston should be same when the piston moves upward. The squash velocity of the air is imparted by the movement of piston. The swirl and squash velocity are equal in intensity.

1.4.3 Swirl Ratio

Ratio of swirl to engine revolution per minute is defined as the swirl ratio. If the ratio of swirl is one then it is taken as very low and the chamber design of such types are known as quiescent even though the flows inside the cylinder is turbulent. For the small bowl to bore ratios, Induction swirl ratio from 3 to 4 results in the 10 to 15 swirl ratio of the bowl. Larger engines have low swirl ratio while smaller engines have high ratio of swirl. There is moderate fuel injection pressure (13 - 340 atm) with low number of injector holes in high swirl engines. The numbers of injector holes are typically eight and the injection pressure is comparatively high from 500 - 1400 atm in the low swirl engine [2]. Low swirl engines have a deep while high swirl engine have shallow bowl in the head of the piston. The mixing between the air and fuel is affected by the swirl. Low swirl causes the generation of tumbling vortices that shifts from one cycle to another. High swirl can cause increased heat transfer and light hot products to push to the centre which lowers the mixing rate and penetration of spray. This produces partially burn lean mixture which in the end releases hydrocarbons and CO emissions.

1.5 Types of Combustion System

According to the design of combustion chamber design the engines are classified into two categories.

Direct Injection (DI) Combustion

Indirect injection (IDI) Combustion

1.5.1 Direct Injection Combustion

In this type of system the fuel is injected directly in the single open combustion chamber and It is used in the engine where the need of mixing rate is least demanding. The energy and momentum of the injected fuel is used for the mixing. The design of combustion chamber comprises of the shallow bowl with central multi-hole injector. The swirl in the air is produced by carefully designing the inlet port and its direction. When the piston is moving upward by pressurizing the air towards the axis of cylinder a great amount of swirl is generated.



Figure 1.4: DI Compression engine (a) multi-hole nozzle with quiescent chamber (b) bowl in piston chamber (c) bowl-in piston chamber with swirl

1.5.2 Indirect Injection Combustion

The modifications in the piston have not contributed sufficient in achieving high value of mixing rate in small engines. The divided chamber injection or indirect injection is used for this purpose. IDI is further classified in the in swirl chamber system and pre-chamber system. The auxiliary chamber is used which is located above the main chamber. First the air is forced in the auxiliary chamber which results in the persuasive flow. At lower injection pressure the fuel is injected in the auxiliary chamber which develops the combustion in the auxiliary chamber. The fluid is forces towards the main chamber due to the pressure rise where the jet mixes with the main air of the main chamber.



Figure 1.5: IDI Compression engine (a) Swirl pre-chamber (b) turbulent pre-chamber

2. CHAPTER 02: Literature Review of Combustion Modeling

The purpose for the modeling is to design and develop an engine which meets the emission legislation and is parameterized on the basis of new changes. Today the evolution in the technology of computer has enabled us to study various extensive processes in just a second. Such model can be utilized to understand complex phenomena of the combustion characteristics and their effects on the emissions. The subject of engine modeling is used in the various applications like gas exchange processes, design of a component and solely for the development of combustion.

2.1 Types of Combustion Models

On the basis of approach to calculate and model all the processes in combustion, the combustion modeling falls in the following type of categories.

2.1.1 Thermodynamic Modeling

The modeling of combustion in any device begins with the basic laws of thermodynamics. These laws include mass and energy balance equations. Spatial changes in the cylinder and conservation of momentum are not considered in this type of modeling. The area of combustion chamber is treated as complete homogeneous region. Spray evolution, injection timings changes and other sub-processes cannot be analyzed in these types of models. On the other hand the ease of calculation and efficient computation time are the main convenience of these models. They are used in the time when the interest is to acquire the average information related to combustion process.

The parameterization of different characteristics is not predicted without measurement. The assumptions of ideally mixed combustion chamber and the empirical relations while calculating the main sub-processes are the main reason of deficiency in thermodynamic models. The rates of pollutant formation that is distressed by the mixture formation and the inside temperatures are not modeled by using this model.

2.1.2 CFD Modeling

Computational fluid dynamics (CFD) models comprises of flow equations of multidimensional type that are resolved through numerical simulation. The detailed studies of chemical and physical processes are investigated. The nature of flow of fluid like turbulence and steadiness is governed by the principles of energy, mass and momentum conservation. The partial differential equations that are based in the time and space are integrated numerically. All the diverse and complicated processes and phenomena of the engines are intensively studied in the CFD models.

These models are used when there is no compulsion of time and cost. Actually the calculation time for a single cycle lies in the region of hours. At first the meshes are generated over the entire flow of the fluid in the combustion chamber. The computation time depends on the type of meshing as the amount of data increased while refining the mesh. Initial and boundary conditions are then defined over the flow. The equations of fluid mechanics are investigated in this type of modeling.

2.1.3 Phenomenological Modeling

In phenomenological modeling there is a division of combustion area in the different zones of varying composition and temperature is performed. They are also known as quasi-dimensional models. They are different from thermodynamic (zero-dimensional) models in which combustion chamber is considered as ideally mix. These models give solution without taking account three dimensional turbulent flow to minimize the time for calculation.

The main objective is to explore the heat release rate (HRR) of chemical and physical processes in the combustion chamber without utilizing the pressure curve. The division of chamber in the different zones depending upon composition and temperature helps to calculate emission characteristics.

2.2 Combustion Models

Various combustion models have been studies using different approaches to calculate combustion characteristics. Few of them are as given below

2.2.1 de Neef and Hohlbaum HRR Model

In order to find HRR, stationary gas jet theory by Abramovich was utilized by de Neef and Hohlbaum [3] [4]. Evaporation advances rapidly relative to the formation of mixture of air and fuel. In the rotational flow of idealized body, fuel injection is depicted as gas jet of quasistationary state. Through the formation of air fuel mixture rate combustion rate is evaluated.





2.2.2 Chmela et al. HRR Model

A zero dimensional HRR model has been studied by Chmela et al. [5]. This model lies in the category of phenomenological and zero-dimensional (thermodynamic) models as it is not giving the subdivision of combustion area in the zones of various temperature and composition and on the other side not giving the HRR as an empirical function like in the VIBE function of thermodynamic models. It works on the difference between the injected fuel mass and burnt. As it calculate available fuel mass at every time and also considering the turbulent kinetic energy. The turbulent kinetic energy \mathbf{k} is served as a model for the mixing speed of fuel and air in the cylinder.

$$\frac{dQ}{d\phi} = \left(m_f - \frac{Q_f}{lh\nu}\right) \exp\frac{\sqrt{k}}{\sqrt[3]{V_{cyl}}}$$

Simple description of the phenomena and short calculation time are the key advantages of this model. The effects of injection parameters like injection pressure, nozzle orifice shape and numbers are also discussed in this model. On the other hand this model fails in describing the ignition delay and the premixed fuel combustion. These processes really influence the combustion characteristics.

2.2.3 Hiroyasu et al. HRR Model

For diesel engine combustion a relatively simple model was described by Hiroyasu et al. [6]. This model is commonly known as packet model. The entire injection spray was subdivided into many small zones called packets. These packets are considered as separate control volumes. Various energy and mass balances equations are solved for these control volumes. The pollutant formation, droplet evaporation and other sub processes are calculated within these c volumes. A distinctive history of temperature and composition is achieved. Total HRR is achieved after addition of burning rates in each packet.



Figure 2.2: Fuel injection Packet Model

2.2.4 Gunner Stiesch HRR Model

The approach used by Stiesch [3] was derived from packets model of Hiroyasu. It assumes that after compression there is only one zone in the combustion chamber which is ideally mixed. The affects of products of combustion and fresh air is also taken into account. Spray packets are generated continuously in the zone during injection. Despite more than one nozzle orifice only one zone of fuel spray is considered. Different nozzle holes spray Interaction is not considered. During injection at each time step a new axial packets disc is generated. At first only the liquid type of fuel is considered in the packet. After some time the small atomized drop and the entrainment begins. Hot gases heat up the fuel droplets which then evaporate. After the ignition delay, the air fuel mixture burn which result in the temperature rise of the packet and formation of pollutant.

In the boundary of packet evaporation, atomization and combustion carried out. All the calculation must be separately calculated for these packets. The change in rate of temperature composition and volume is calculated using mass and energy balance equations for each packet. Pressure is taken as a function of time.

2.3 Fuel Spray Dynamics

2.3.1 Spray Formation and Droplet Behavior

The difference between combustion of liquid and gaseous fuel is that liquid has to first evaporate and then burn. In case of gaseous fuel we study heat release rate, flame temperature, flame speed and energy density. In liquid fuel we also consider heat release rate, flame speed, flame temperature and energy density of liquid but all these are dependent on the rate of evaporation of the liquid fuel as liquid has to evaporate first. In case of gasoline in SI engines the vaporization and combustion processes are uncoupled while in case of CI engines they are interlinked. In first phase the gasoline is vaporized and mixes with the air and then in 2nd phase it is introduced to the cylinder.

Liquid fuel shattered into liquid droplet spray then it is introduced to the combustion chamber in all most all the cases. Boilers, gas turbines, oil fired furnaces, and diesel engines used liquid fuel droplet sprays to increase the combustion and vaporization rate as fuel surface area increases in droplet sprays. Breaking a drop of 3 mm into 30 μ m droplets results in the increase of a million droplets which increase the area of surface of the fuel by 100 times [2]. Burning rate of droplet is inversely proportional to the squared diameter so the rate of burning increases up to ten thousand times. Whereas favorable atomization which is the generation of uniform and fine droplet sprays is fundamental to smooth combustion and low emission rate.

Liquid is broken into large number of various sizes and velocities drops upon the injection of liquid fuel. On the basis of ambient conditions and the density of liquid fuel in the chamber some of the droplet continues to break up in further small drops and some collide and combine again. In this procedure the fuel starts to shatter and evaporate as well. Either because of surrounding temperature or because of flame front the fuel vapor start mixing with the air in the chamber and starts burning. The combusted and non combusted products mix and gives a delay time to combust completely. In the end fuel completely converts to combusted products.

There are number of ways in which sprays is generated. Pressurized atomization and air blast atomization is commonly used. By pressurizing a liquid through an orifice with relatively high velocity as compared to the surrounding gas or air, spray is generated in pressurized jet atomization. In case of air blast, spray is generated by intruding a high velocity air flow with a jet of low velocity moving liquid. The process of breakup may be seen in a sequence that starts with the narrowing and stretching followed by the ligaments, protuberances and ripples which results in the swift disruption of liquid into small droplets. Due to the shear and vibration further breakup occurs with the accumulation of some of the droplets if the spray is not dilute. Three dimensionless numbers are used to characterize the spray formation.

a) Reynolds Number

It is the ratio of inertia to viscous force.

$$Re = \frac{\rho_l \ v \ d_{jet}}{\mu_l}$$

b) Weber Number

It is the ratio inertial force to force of surface tension.

$$We = \frac{\rho_g \, v^2 d_{jet}}{\sigma}$$

c) Ohnesorge Number

$$Oh = \frac{\mu_l}{\sqrt{\rho_l \sigma \, d_{jet}}} = \frac{\left[(\rho_l / \rho_g) We \right]^{1/2}}{Re}$$

1,

The subscripts in the above mention equations are l and g which define the properties of liquid jet that is being atomized, the gas in which it is going to atomized. d_{jet} refers to the liquid jet diameter and σ shows the surface tension of the liquid jet [2].

When a liquid flows into an orifice a swirl is generated in the liquid. As in the case of plain jet the liquid jet forms a wider sheet of conical shape and then shatter in the wave like manner. Before coming in the inactive state of air, spray of swirl type travels to a certain distance. In the case of breakup due to the aerodynamic shattering these dimensionless numbers are viewed as droplet rather than liquid jet. The numbers are then

$$Re_{dr} = \frac{\rho_l \, v \, d_{drop}}{\mu_g}$$

$$We_{dr} = \frac{\rho_g \, v^2 d_{drop}}{\sigma}$$

In the case of $We_{drop} > 12$ the breakup of droplet happens. The liquid droplet stripped from the main parent liquid droplet in case of large valves of We_{drop} .

2.3.2 Droplet Size Distribution

With the help of optical techniques measurement of droplet size of spray is possible. A short laser pulse is utilized to inject in the spray and light up a camera screen of high resolution. These images are then transferred to computer to analyze size distribution. By counting the liquid droplets for a specific volume a spatial distribution at a given time is obtained [2]. By calculating droplets passing through a specified surface area the temporal distribution is obtained. These distribution is plotted as a histogram as shown below





 ΔN_i is the liquid droplet fraction which is calculated in the interval of size Δd_i . The histogram takes the shape of differential number distribution as the size interval become short. The other way to examine size distribution is through cumulative number fraction.

$$CNF = \frac{\sum_{i=1}^{k} (d_i \Delta N_i)}{\sum_{i=1}^{\infty} (d_i \Delta N_i)}$$

Also the cumulative volume fraction is given as

$$CVF = \frac{\sum_{i=1}^{k} (d_i^{3} \Delta N_i)}{\sum_{i=1}^{\infty} (d_i^{3} \Delta N_i)}$$

The shape of histogram is changed in smooth curve with the sign of summation converted in the sign of integration as

$$CVF = \int_{0}^{d} \left[d^{3} \frac{dN}{d(d)} \right] d(d)$$

To describe the distribution size of liquid droplet there are different types of measurements involved. These include area mean diameter, volume mean diameter, most probable diameter, mean diameter and Sauter mean diameter (SMD). The diameter of droplet with largest fraction of drops in it is known as most probable diameter. Average diameter of groups of droplets of liquid is known as mean diameter.

$$d_{avg} = \sum_{i=1}^{\infty} (d_i \Delta N_i)$$

Area mean diameter of droplet is based on the fraction with the surface area of average diameter.

$$AMD = \left[\sum_{i=1}^{\infty} (d_i^2 \Delta N_i)\right]^{1/2}$$

Volume mean diameter is based on the fraction of droplet with the given volume of average diameter.

$$VMD = \left[\sum_{i=1}^{\infty} (d_i^{3} \Delta N_i)\right]^{1/3}$$

Whereas the Sauter mean diameter is the ratio of VMD and AMD.

$$SMD = \frac{VMD}{AMD}$$

2.3.3 Fuel Injector

The sole purpose of a fuel injector is to provide good mixing of fuel with the air. It is done when it enables to help the fuel in good penetration and dispersion of fuel into small droplets. The time that is taken by the atomization rely on the time taken by the liquid to vaporize, mix and then combust. On the basis of flow there are two types of fuel injectors i.e. steady and intermittent injectors.

2.3.3.1 Steady Flow Injector

It is the simplest injector with the plain orifice of hole length L and diameter of nozzle d_n injecting into quiescent air. Cone angle of spray ranges from 5° to 15°. They rely on the surface tension and viscosity of the fluid. The relation for the plain orifice for SMD is given by Tanasawa and Toyoda (1955)

$$SMD = 47 \frac{d_n}{v} \left(\frac{\sigma}{\rho_g}\right)^{0.25} \left(1 + 331 \frac{\mu_l}{(\sigma \rho_l d_n)^{0.5}}\right)$$

This equation depends on the parameters of particular sets of units not depending on the dimensionless numbers. The swirl or simplex atomizer is shown in





These injectors have a good dispersion rate. The angular momentum in the fluid is created with the tangential slots of the atomizer. This enables the fluid to eject in the form of hollow cone which forms the core vertex of air inside the cone. The angle of spray is up to 90 degrees. The SMD of an atomizer of a pressure swirl type rely on the surface tension and viscosity of the liquid. It also depends on the rate of mass flow and the change in pressure of liquid across the atomizer. The relation for SMD is given by Radcliffe as

$$SMD = 7.3 \ \sigma^{0.6} \ \vartheta_l^{0.2} \ \dot{m}_l^{0.25} \Delta p^{-0.4}$$

The size distribution of the droplets for density number and mass is derived from nozzle of pressure swirl. The SMD for this type of atomizer is $45 \,\mu m$ in average. The rate of flow in case of pressure swirl atomizer is directly proportional to the injection pressure differential square root. The flow rate ratio of 20:1 is required in the turbine of aircraft. A pressure of about 400 *atm* is required for higher flow rate. This pressure shows the lower end of the injection

pressure in diesel engines. They are very much for the steady flow of turbines and furnaces. Other forms of air blast atomizers are used in oil fired furnaces and turbines.

An atomizer as shown in figure **2.5** utilizes low injection pressure and gives very fine droplets. This type of atomizer is known as pre-filming air blast. The option of additional air in this type of atomizer increase mixing and minimize the formation of soot. The SMD for pre-filming air blast atomizer is given by



Figure 2.5: Measured drop size distribution for a pressure –swirl atomizer [7]



Figure 2.6: Air blast atomizer with pilot fuel for low rundown

The dp is the diameter of pintle in this case. The momentum of air is presented by the first expression while droplet surface tension is denoted by the second expression of the equation above. To create the small droplets of the liquid higher densities and higher velocities work.

Higher density and more surface tension with larger droplets are effective in bearing breakup. For the balance of surface tension and viscosity the second expression is used. High viscous fluid bears the distortion. There is minor effect on increasing the ratio of air to liquid more than five.

2.3.3.2 Intermittent Injector

They operate once short pulse in a single cycle of combustion. It is also used in the SI engines. The injection in diesel works on the high pressure of about 300 - 1400 atm to get fine atomization during injection [10]. There is inward opening of the needle with the plain orifice type injector.



Figure 2.7: Multi-hole nozzle (a) Nozzle with sac volume (b) Sacless volume

Figure shows a multiple injection system nozzle. In figure (a) there is sac volume below the needle of the injector which helps in the dribbling of the liquid at the end time of injection. In figure (b) there is no sac volume. The 2^{nd} type eliminates the exhaust smoke.



Figure 2.8: Pintle nozzle (a) standard (b) throttling

This type of injector is standard and throttling type pintle nozzle. They are of single hole type. Throttling type prevents the slow injection at the time of start of injection and close faster to eliminate dribbling effect at the end time of injection.

Different equations for SMD of diesel fuel

Elkotb [9]

$$SMD = 3.08 \times 10^6 v_f^{0.385} \sigma^{0.737} \rho_f^{0.737} \rho_a^{0.06} \Delta p^{-0.54}$$

Knight [10]

$$SMD = 1.605 \times 10^{6} \Delta p^{-0.458} \dot{m}_{f}^{0.209} v_{f}^{0.215} \left(\frac{A_{orf}}{A(t)_{ef}} \right)^{0.916}$$

Hiroyasu and Kadota [8]

$$SMD = 2.33 \times 10^{6} \Delta p^{-0.135} \rho_{a}^{0.121} v_{f}^{0.131}$$

These equations depict the different types of SMD used in the case of lower injection pressure. They are used in early 1990s in the heavy diesel engines. They help in the understanding of the trends of sprays. These formulas give the similar trend while calculating the SMD but there are some differences as the viscosity effect is minimize by the Hiroyasu and Kadota's equations and on the other hand effect of air density is neglected by Knight's equation. Due to droplet clustering there is increase in the SMD due to the increase in the density with the increase in the density of air.

2.4 Mass flow Rate

The mass flow rate of the injected fuel depends on the pressure difference across the nozzle with the liquid density and shape of nozzle hole. The combustion characteristics and dynamics of spray rely on the timing and the rate at which the fuel is injected in the combustion chamber. Assuming the flow nature as quasi-steady, one–dimensional and incompressible then flow rate is calculated using [1]

$$\dot{m}_f = C_D A_n \sqrt{2\rho_l \Delta p}$$
C_D , A_n are the discharge co-efficient and area of the nozzle hole respectively. Whereas at the tip of nozzle hole the velocity is calculated as

$$u_i = C_D \sqrt{2\Delta p / \rho_l}$$

2.5 **Penetration of Spray**

Depending upon the conditions there are several equations to find the distance of penetration of spray in the quiescent air. The tip of the liquid spray moves in a liner relation with time. After the injection the spray length is directly proportional to the square root of time of injection.

Correlation for spray penetration before and after the breakup of spray is given as [11] Before breakup of spray $0 < t < t_b$

$$S = C_D \left(\frac{\Delta p}{\rho_l}\right)^{0.5} t$$

The value of discharge co-efficient C_D is taken as 0.6 to 0.8 in today's modern diesel engines.

After breakup of spray $t_b \leq t$

$$S = 2.95 \left(\frac{\Delta p}{\rho_a}\right)^{0.25} (d_n t)^{0.5}$$

And the time of breakup t_b is given as

$$t_b = 4.351 \frac{\rho_l \, d_n}{C_D^{\ 2} (\rho_a \Delta p)^{0.5}}$$

2.6 Angle of Spray

The angle of spray is given by the relation [11]

$$\theta = 0.025 \left(\frac{\rho_a \Delta p \, d_n^2}{\mu_a^2}\right)^{0.25}$$

The correlation by Reitz and Bracco [15]

$$\tan(\theta) = \frac{1}{A} 4\pi \left(\frac{\rho_a}{\rho_l}\right)^{0.5} \frac{\sqrt{3}}{6}$$

In which A is

$$A = 3.0 + 0.28 \left(\frac{l_n}{d_n}\right)$$

Where l_n is the length of nozzle hole and μ_a is the viscosity of the gas.

2.7 Vaporization of Droplets

In the designing of combustion the important parameters that should keep in mind are the rate at which the evaporation occurs and the time that it takes to evaporate completely. The vaporization relies on the factors like gas pressure and temperature, size of droplet and relative velocity between gas and droplet. It also depends on the latent heat of vaporization and boiling point. The relative velocity between the gas and the droplet is very low that is neglected in many cases. The boiling point of pure fuels are well defined while the mixtures like jet fuel and diesel fuels have a range of boiling points depending upon the quality of the fuel. The latent heat is considered as zero. The vaporization rate is measured by appending the droplet on the thermocouple wire and examining the change in diameter with time. It is examined that the diameter changes in a square relation with time.

$$d^2 = d_0^2 - \beta t$$

The β is the constant of vaporization. The vaporization comprises of two process evaporation and boiling. The boiling process is a phase transformation phenomena from liquid to gas that happen at or above the boiling temperature. While evaporation is also phase transformation from liquid to gas phase but it occurs below the temperature of boiling at the given temperature.



Figure 2.9: Vaporization rate curve for kerosene and jet fuel [14]

2.8 Ignition Delay

In diesel engine ignition delay is defined as the time or delay in terms of crank angle between the time at which the injection of fuel is start and the time when first vapor of fuel start to combust. The injection is taken from the needle lift of the injector as seen from the nozzle needle lift indicator. The time of start of combustion is very difficult to find. It is sort out from the lifting of the heat release curve that is derived from the pressure curve. Also it is observed from the pressure curve lifting as it changes suddenly due to the start of combustion. In the direct injection the right point of combustion start is easy to find while in case of indirect injection it is very difficult to find. For the first sign of flame propagation flame luminosity sensors are used. There is minor difference between the indication. This creates uncertainty while designing the engine combustion characteristics.

Actually at the time of combustion both physical and chemical processes start. The physical processes include atomization, vaporization and mixing while chemical processes include combustion reactions of air fuel and the residual gases which results in the auto-ignition. All of these processes are affected by the design of engine and its operating parameters.

For the fine atomization of liquid fuel, high pressure of during injection, suitable viscosity, small orifice diameter of nozzle hole and the high compressed pressure of air is necessary. The vaporization relies on the size, distribution and the velocity of droplets of fuel. It also depends on the temperature and pressure of the combustion chamber as it helps in the vaporization of droplets. For the rapid air fuel mixing in the combustion chamber piston is designed to increase the rate of swirl to create turbulence. The number of nozzle holes and the placement of their location in the injector decide the pattern of the spray. These details change the cone angle of spray. The penetration distance depends on the air density, pressure of injection, characteristics of air fuel flow and the size of droplet.

The spontaneous ignition process of diesel engine is heterogeneous in nature. Ignition mainly occurs in the phase of vapor but the process of oxidation proceeds in the phase of liquid with the cracking of large hydrocarbons to smaller is happening. These processes are dependent on the pressure, temperature and physical processes described above.

The characteristics of operating engine parameters like noise, emissions, smooth running are affected by the ignition delay. Cetane number is the measure ignition quality. It is sort out by differentiating the ignition delay of the fuel with the reference fuel that is used in the standard engine testing. If the cetane rating is low then rapid burning occur at the time of start of combustion which results in the high temperature and pressure peaks. This leads to the diesel knock. If the cetane rate is very much low then incomplete combustion with the low power output and low conversion efficiency of fuel occur. For the high centane rating fuel burn before the injection of total fuel happens. The heat release rate and rise of pressure is maintained in this case which results in the smoother engine running.

2.9 Quality of Injected Fuel

The quality of fuel is prescribed by its cetane rating. The process to find the quality of gasoline knocking and diesel knocking is totally different. The scale to find the quality of diesel fuel depends on the n-hexdecane $C_{16}H_{34}$ and heptamethyalnonane (HMN). n-hexadecane is a hydrocarbon with very high ignition quality of cetane rating 100. On the other hand hetamethaylnonane represents the low ignition quality with cetane rating of 15. The formula for cetane rating is as

$$CN = percent n - cetane + 0.15 \times percent HMN$$

The standard engine used to find cetane rating operates on special loading conditions with special instruments to acquire the data. The test procedure and the operating conditions are denoted by ASTM D613 method [16]. The requirements are intake air temperature $65.6 C^{\circ}$, injection timing before 13° top dead centre of cylinder, 900 *rpm*, and injection pressure of 10.3 *MPa*. The compression ratio of engine is then changes to starts combustion exactly at top dead centre with the ignition delay time of 13°. When a fuel that is used for reference is used, compression ratio is fixed to get 13° delay. Compression ratio of actual fuel is sorted out by the readings acquired by the two blends of reference fuel changing in a difference of cetane number five. It is then evaluated by interpolation between the values of compression ratio utilized by the two blends of reference fuel.

2.10 Factors of Physical Process on Delay

The physical factors like velocity, temperature and pressure during mixing take part in deciding the delay time. They depend on the design combustion chamber, injection system and other operating parameters. The variables of injection system like spray type and form, size, quantity and velocity. The values of delay are different for the different time of engine operating conditions. The design parameters for delay during the startup time and warm up time are different then the completely warmed up engine. All these precautions are kept in mind while deciding the ignition delay.

2.10.1 Injection Timing

The minimum ignition delay occurs at the time of start of fuel injection for a warmed up engine operating at low to medium speed. The value of delay at this time is 10 to 15 degrees from bottom dead centre [17]. After the earlier or later injection timing the increase in ignition delay occurs. This is due to the temperature of air pressure changes near to top dead centre. Delay increases if injection starts earlier as the initial pressure and temperature of air is are lower. The pressure and temperature are at higher value, if the injection starts later, they decrease as the delay continues. The suitable condition for the injection lies in between them.

2.10.2 Engine Load and Injection Quality

With the increasing load the delay, the ignition delay decreases. The wall and residual gas temperature increases with increasing load. The result of which is higher charge temperature and slight high charge pressure with short ignition delay time. Under normal operating conditions the increase in the quantity of fuel has no powerful effect on delay. The delay increases at the time of start of engine as the temperature of mixture is low.



Figure 2.10: Ignition delay as a function of load [18]

2.10.3 Rate, Size and Velocity of Injection

The value of the parameters like size rate and velocity are defined by injector nozzle size and shape and injection pressure. These parameters have negligible effect on the delay of the ignition. At constant injection pressure and increasing the size of hole diameter by two times results in the increase of drop size. This results in no change in the delay. Also the size, shape and length of nozzle hole have an insignificant effect on delay.

2.10.4 Temperature and Pressure

The intake pressure and temperature affect the charge conditions which then affect the delay of ignition. At the time of injection below 1000 K the ignition delay is strongly affected by the intake charge temperature. Ignition delay is not affected by the charge temperature above 1000 K. At this temperature range there is significant effect of pressure on delay time. The delay is shorter if the pressure is high. The charge inlet air temperature and pressure also affect the other parameters that changes the delay time. Ignition delay is also decreased by increasing the compression ratio.



Figure 2.11: Ignition delay as a function of reciprocal air temperature [22]

2.10.5 Speed of Engine

There is a minor decrease in the delay at constant load and increased speed. The temperature and pressure time relationships changes at change in engine speed. The Pressure of injection increases at the increase in engine speed. During the stroke of compression the peak value of compression temperature rises with the increase in the speed of engine. This is due to the smaller heat loss during compression.

2.10.6 Chamber Wall Effects

The mixing and fuel evaporation processes are affected by the impingement of fuel spray on the chamber walls. In all the engine types the impingement happens weather it is small or high speed or load engine. The impingement in the M system of combustion chamber achieves a smooth pressure increase.



Figure 2.12: Effect of spray impingement on wall 100 mm from nozzle on ignition delay [21]

Figure shows the effect of various experimental results carried to study the effect of wall impingement on delay. In this a constant volume bomb combustion bomb is used with the various ranges of temperature and pressure to calculate ignition delay. The wall is placed 100 mm from the tip of nozzle and set perpendicular to the spray direction. At the lower pressure and temperature the presence of wall decreases the delay. At high pressure and temperature there is negligible effect on the delay. In this study the impingement angle of jet changed from the zero to perpendicular to wall. They delay increases as the angle decreased.

2.10.7 Rate of Swirl

Evaporation of fuel and mixing is affected by the rate of swirl. Swirl also changes the heat wall transfer and the temperature at the injection of fuel. At normal conditions of load and speed the change in delay is very small due to change in swirl. At the time of start of engine in which the engine speed is low this change in delay is prominent.

2.10.8 Concentration of Oxygen

The concentration of oxygen in which is fuel is injected influence the delay. The delay is also affected by the exhaust gas recirculation in the cylinder as it decreases the concentration of oxygen in the cylinder. The results due to change in the concentration is shown in figure



Relative Oxygen density

Figure 2.13: Effect of oxygen density in gas on ignition delay [20]

These studies are carried out at 1800 *rpm* and air to fuel ratio 30:1. In this experiment the concentration of oxygen is changed by introducing the cooled exhaust gas in the single cylinder of diesel engine. Ignition delay increases as the oxygen concentration decreases.

2.10.9 Property of the Fuel

Ignition delay is defiantly affected by the cetane rating. It also changed by the quality of fuel used. The normal alkanes like paraffinic compounds of straight chain molecule have the highest ignition quality. With the increase in length of chain the ignition quality increases. Aromatic compounds with the branched chain molecules have the lowest quality of ignition. Alcohols are also low quality for ignition. There are difficulties in using the alternative fuels like ethanol and methanol as they are of low quality for ignition. Ignition quality is improved by the addition of normal alkanes except alkanes with low carbon number and n-pentane.

2.10.10 Cetane Number

The cetane number imporves with increase in chain length of paraffin. If the branching is concentrated at the one side of isoalkanes then thay also help in the ignition quality. Cetane number is reduced in the case of cycloalkanes and aromatics. The cetane number changes in an inverse relation with the octane number. The cetane number for normal fuel diesel engines ranges between 40 to 55. Ignition delay with respect to the different operating conditions in diesel fuel is shown in figure below



Figure 2.14: Effect of fuel cetane number on ignition delay over the load and speed range [19]

There is linear trend in the variation at the normal operating conditions however ignition delay rapidly decreases with the decrease in cetane number from 38 to below. With the help of additives, refining processes and accelerators that helps in ignition the cetane number is monitored. As in the case of spark ignition engine the knocking is reduced by adding anti-knock agents in the fuel. Various sulfur compounds nitrates, nitrites and organic peroxide are include in the additives of ignition accelerating. These include isopropyl nitrate, primary hexyl nitrate, octyl nitrate and primary amyl nitrates. There is an increase in the 10 cetane number when these additives are added in 0.5 percent by volume in the distillate fuel. The main effectiveness is dependent on the base fuel composition. Cetane number decreases if the additives are add in incremental way. The addition of additives helps in the use of alcohols in the compression ignition engines.

2.10.11 Volitlity and Viscocity

With the cetane rating of about 38 to 53 experiments with the front end volatility of fuels does not show any significant change in the ignition delay. Variations in the viscosity of about 2.5 shows a minor change that is very insignificant for the change in ignition delay. In case of warm up engine the changes in the penetration of spray, vaporization rate and fuel atomization does not affect the delay of ignition.

3. CHAPTER 03: Diesel Fuel Spray and Emissions

For the design modeling and optimization of combustion, understanding of diesel fuel jet is very crucial. Jet of diesel fuel attributes directly correlates with the emissions characteristics. In this chapter a detailed study of previous fuel spray model is carried out. These models form the basis for the new models.

3.1 Dec et al. Spray Model

Dec et al. [23, 24] have presented a structure for the combustion process based on the chemical kinetics model. This model gives a new view about ignition and process about formation of particulate. This model was tested with the laser diagnostics. This leads to the improvements in the computational efficiencies. It is used to find the temporal sequence and structure of flames of diesel fuel. This forms the basis for the description of burning spray plume. Images of the structure of flame give details for the understanding of combustion phenomena. This proves the importance of kinetic process valuable for the study of air fuel mixtures. The temporal and spatial description has been linked with the calculations of chemical kinetics. The calculations of NOx and particulate are qualitatively speculated by this model. The analysis of chemical kinetics has been practiced on wide area of pressure, temperature and air/fuel ratio.

Laser imaging process has been utilized. It focuses on the methods and chemical analysis used to evaluate the value of reaction, generation of chemicals and heat release. A complete picture of the phenomena like injection of fuel, initial reactions of oxidation and ignition of fuel has been portrayed in this model. Planner imaging of laser based is utilized in this method. An optically accessible engine for research is applied.

A 4-stroke single cylinder engine based on Cummins N series DI diesel engine is utilized. The engine parameters are 152 mm bore and 140 mm stroke. The original cylinder head is used to see the flow characteristics. The piston used is of extended piston design with the window in crown piston. For the orthogonal optical access which is used for 2-D imaging additional windows are added around the cylinder wall top. The laser sheet enters in the combustion chamber horizontally through these windows in the direction of axis of jet of fuel. The installation details are as shown in the figure below



Figure 3.1: Test engine used for investigation of Fuel Jet [23, 24]

The operating conditions include 1200 *rpm* with a top dead centre temperature of 992K and pressure of 50 bars. The engine was heater to 368K with the $\emptyset = 0.26$. Needle lift of injection nozzle and rate of heat release are given as



Figure 3.2: Evolution of combustion of Fuel Jet [23]

Figure shows the propagation of jet of fuel when its temperature increases and stabilize. The first image shows the increase in temperature of jet of fuel and the air entrainment in the cylinder. The second shows the 3 D axis image of the fuel jet. The first axis shows the correlation of fuel jet with the angles of crank. The second axis shows the time traveling with the fuel evolution. The third axis shows the relation of equivalence ratio with the jet. These are evaluated using Siebers [13] correlations. In quiescent conditions, the fuel jet temperature increases from 350 to 650 K. Due to the direct transfer of heat from the air to fuel there is an increase in temperature. Exothermic reactions start at the higher temperatures and the temperature reaches to 825K. The rapid oxidation of components of fuel starts and further temperature rises. Low temperature oxidation energy is enough to raise the temperature of air fuel mixture in the fuel jet more than 1150 K. At this temperature all the oxygen in the mixture is consumed. The temperature continues to increase due to these reactions and reaches to 1600 K.



Figure 3.3: Evolution of temperature and chemical composition in a Flame Plume [23, 24]

Above mentioned image provides the comprehensive image of the chemical and thermal processes of the fuel jet. A diffusion flame in the form of envelope surrounds the fuel jet at the place where there is oxidation. Fuel fragments and particulate matter are converted to water vapor and CO_2 in this envelop. NO_x generates at this high temperature region. A rich premixed zone of combustion is inside this hot envelop. At the surface of diffusion flame rich combustion products are oxidized.

For the concentration of oxygen in intake air and flame lift-off length a correlation was performed by Siebers et al. [25]. Lift-off length is the distance between the injector nozzle hole

surface and the position where the combustion starts at the jet. A constant volume combustion chamber of length 108 mm on each side is used in the experiment. On one of the wall of chamber fuel injector nozzle is fixed while for visualization other walls have sapphire port of 105 mm diameter.



Figure 3.4: Combustion vessel cross section schematic [25]

The setup is provided with the option of different composition, temperature and density in injection. The variation range for temperature is between 600 to 1400 K while the variation in density ranges from 3.6 to $60 kg/m^3$. The apparatus test results are as fellows



Figure 3.5: Lift off length versus ambient gas temperature for four gas oxygen concentrations [25]

There is inverse relation between oxygen concentration and lift-off length. With the decrease in oxygen concentration, lift-off length increases but due to the two parallel effects ambient oxygen concentration does not change with the amount entrained oxygen upstream of the lift off length. The two parallel effects that cancel each other are increase in lift-off length that accepts the total ambient gas and rate of reduced oxygen entrainment due to smaller fraction of oxygen in the entrained gas. This results in the dilution of jet due to the increase amount of diluents in the ambient gas [25]. The trend of oxygen concentration and lift-off length shows reduction of reaction between fuel evaporation process and combustion.

With the increase in quantity of ambient gas and fuel the formation of soot decreases. It is minor when entrainment of oxygen is more than enough to decrease the average equivalence ratio in the fuel air jet less than two at the point of lift-off length. The areas of soot formation and combustion is pushed further and stretched in the cylinder as the concentration of oxygen in the ambient gas lowers. This is due to the lift-off length increase and per length decrease in the oxygen entrainment with decreasing ambient oxygen concentration. This decrease the rate of combustion, increase in lift-off length and the time required to end the combustion.

3.2 Structure of Diesel Flame

To show the nature of combustion, various structures have been studied. One of the studies has been carried out by Chiu [27]. This model supposed that the spray is made of rich fuel core of high density enveloped by increasing leaner fuel/air mixture.



Figure 3.6: Spray Jet Model [27]

The hot compressed air that is enclosed in the chamber is entrained by the jet of fuel as the fuel injection start. The temperature of fuel jet rises due to the entrainment of air and helps in the vaporization of fuel. The fuel jet is surrounded by the vaporized fuel in the form of envelop with the temperature rise of 750 K. The chemical reaction starts after this process. From these reaction and further entrainment, the temperature of jet of fuel rises to the 825 K. Basic oxidation reaction takes place at this instant. The chemical products include C₃H₃, C₂H₂, CO and H₂O. The production of soot is due to the short chained fuel components that are the main structure of polycyclic aromatic hydrocarbons (PAH). The jet temperature rises up to 1600K during these reactions. The products of combustion are forced out by the by the jet of fuel. After this they reentrained into the jet in the cylinder. In this way the jet of fuel is stabilized.

3.3 Injection Profile

A fuel injection is shown in the figure





For the fuel injection a curve on the bottom shows the rate of burning for the each part of injected fuel. The ROHR curve is shown below. In these figures the 180 degrees of crank angle movement and TC are the same reference points.

The combustion process is divided into four stages on the basis of this injection profile.

At first stage the fuel is injected into combustion chamber. In the heated air fuel injector injects fuel. Due to the high velocity of fuel jet or jets in case of multi orifice injector causes the fuel to atomize. This helps in the mixing of fuel with the air and evaporation. After evaporation the droplets start to move away from the core of the fuel jet. An air/fuel mixture starts to generate with the help of high temperature with no significant amount of energy release. Ignition starts to take place in the outer fringes of the fuel jet vapors envelop with the pressure rise above the compression line. The first part of the combustion stops here. This part is known as the ignition delay of the combustion.





In the combustion 2nd part a large amount of energy is released as the injected fuel burns completely. This is shown in the above figure between the b and c. In this part the air fuel mixture combust instantly and then fall off. This part of combustion is known as pre-mixed combustion. The 3rd part is known as the diffusion combustion or mixing controlled combustion. This part is between c and d. The rate of combustion is controlled by injection of fuel. 4th part of combustion continues till the expansion stroke. This is mainly due to the partially unburned fuel. Some part of energy is also present in the combustion products and soot. This energy is released if the better mixing of air fuel mixture happens. The processes are very slow as the required temperature to help the reaction is very low at the end of expansion stroke. This range between the d and e is known as late combustion part of the combustion.

3.4 Maiboom, A. Model

A new detailed six zone combustion model has been studied by Alain Maiboom [28]. The chamber of combustion is categorized in six zones which are as fellows



Figure 3.9: Description of Zones

- The 1st zone is the zone of liquid fuel zone. It starts from the nozzle hole to the point of maximum distance of penetration of fuel
- The 2^{nd} zone is the region of air fuel mixture. It starts from the end of penetration length L to the lift-off length H. If the distance of liquid penetration length is higher than the distance of lift-off length then the fuel is of totally evaporated type down towards the penetration of liquid. If the penetration length is less than the distance of lift-off length then it contains liquid fuel downstream of the length of lift-off.
- 3rd zone is the zone of pre-mixed combustion zone. It comprises of the combustion of phase of air-fuel vapor that arises during the delay of ignition.
- 4th zone is the diffusion zone. It starts from lift-off length to penetration distance of vapor phase fuel mixture.
- 5th zone is also diffusion zone but it consists of diffusion flame that is enveloping the 3rd and 4th zones.
- 6th zone is the zone of gas (air and EGR) that surrounds the whole zones.

3.5 Diesel Engine Emissions

Diesel exhausts are the gases that are released by the combustion of diesel fuel locomotives. They are known as clag. The condition in the exhausts of diesel fuel is different from the SI engine as the combustion is not controlled by the amount of intake oxygen as in case of SI engines. The sufficient amount of oxygen is present when the engine is running on idle condition. Diesel fuel release very much amount of smoke when they are not provided by the sufficient supply of intake oxygen. The lean burning mixture of diesel and high temperature and pressure results in the generation of nitrogen oxides. Modern diesel engine should utilize selective catalytic converters for emissions as the process of exhaust gas recirculation is not enough for NOx reduction. Also the generation of particulate matter imposes a great concern on human health.

3.5.1 NOx Formation

NO together with the NO_2 are collectively known as NOx emissions. Nitric oxide is the main oxide that is produced inside the cylinder. The main source for the formation of NO is the reaction of oxidation of molecular atmospheric nitrogen. The gasoline engines emissions contain minor amount of nitrogen while diesel emissions contain more nitrogen. NO formation is mainly due to the atmospheric nitrogen. In combustion of stoichiometric air fuel mixture the main reaction that governs the formation is as fellows.

$NO + H_2O \rightarrow NO_2 + OH$

The critical time period for the formation of NOx is the time when burned gases temperature is very high. For NO formation the critical equivalence ratio at high temperature and pressure is close to stoichiometric.

3.5.2 Carbon Dioxide

Diesel fuel produces low carbon dioxide as compared to the petrol engines. This is one of the bases of diesel engine improved fuel economy. Due to the recent changes in the climates and the emission standards biodiesel fuels are now in practice as they emit less net some carbon dioxide as most of it is utilized by plants that are used as fuel. There are also concerns about the growth of plants that are used to form biodiesels as they are taking place the land and water that can be used for other plants that is used for both humans and animals. At the low power range there is sufficient amount of oxygen present in the cylinder that is used to combust the fuel completely. The diesel fuel generates significant quantity of carbon dioxide when it is working under a high load.

3.5.3 Black Smoke

The fuel of diesel does not burn completely unless it is not provided by the enough amount of compressed oxygen before the power stroke. If high amount of fuel is injected against the low amount of oxygen then it results in the black smoke due to incomplete combustion. Modern engines are provided with the facility of changing the injection timing with respect to the load. This helps in the controlled amount of fuel to be burnt. In this type the engine temperature, rpm, boost temperature and load is sensed by electric control and then signals the injection to adjust. Diesel fueled engines are commonly recognized by the specific type of smell. This smell is now reduced due to the removal of sulfur while refining of fuel. Diesel exhaust comprises of a list of toxic components. These components are harmful for the health of humans and environment also.

3.5.4 Noise

Diesel engines are commonly recognized by the specific distinctive noise. This noise is known as diesel knock or clattering of diesel. This is due to the sudden injection that results in the generation of pressure wave. This is controlled by the use of pre-injection, indirect injection and timing of injection. The higher cetane diesel fuel improves the combustion process and reduces the noise. Cetane number can be increased by introducing an additive or catalyzing the fuel. This is also controlled by multiple injection system. For the improvement of diesel noise the multi nozzle fuel injection with the pilot and main injection with the exhaust gas recirculation have turn down the problems in common rail diesel engines and have improved the efficiency of diesel fuel.

3.5.5 Diesel Particulate Matter

Diesel exhaust particles (DEP) or particulate matters are the particulate constituents of exhaust. It comprises of diesel aerosols and soot like ash particles, silicates, sulfates and metallic abrasion particles. They accumulated in the form of chain aggregates or individual particles within the range of 100 nanometers when released in atmosphere. They are also known as ultrafine particles.

3.6 Variation in Exhaust with different Engine Conditions

The amount and quantity of nano size particles changed with the operating temperature and pressure. They also rely on the fuel mixture type, atmosphere mixture type and the presence of an open flame in the cylinder. The type of emissions from different engine capacity and different quality fuel is not comparable. 95% percent of nano particles of volatile component is unburned lubricating oil. Diesel engines produce black smoke from diesel particulate matter. This black smoke consists of such carbon particles that cannot be combusted because of low temperature in the area where the fuel jet is not atomized. This condition occurs at the cylinder wall and at the periphery of the large droplets that are created due to the shattering of fuel jet. The mixture is rich at the areas where it is cold. Rich fuel mixture side has low amount of oxygen form combusting so some of the fuel converts into carbon deposit. To capture carbon particles diesel particulate filter is used in modern engines and then combust it completely by injecting extra fuel into the filter. This helps in the reduction of carbon particles at the expense of small fuel. Black smoke limit is the standard to recognize the full load limit. After this point the fuel is not combusted completely. It is stoichiometircly lean so it is exceeded to get more power out of it. But exploiting it causes loss in the combustion efficiency, dense smoke and high consumption of fuel.

At the time of cold start the engine combustion efficiency is very low. This is due to the fact during compression stroke cold engine block extracts heat out of the cylinder. This result in the incomplete combustion with blue and white smoke with reduced power until the engine is warmed up complete. This is more prominent in the case of indirect injection system of combustion because they are thermally insufficient. This is adjusted with the help of electronic injection system that alter the injection depending upon load, speed pressure and temperature.

Some engines have mechanical type of injection control system that alters the injection with hydraulic governor control system with the aid of multiphase glow plugs that are controlled electrically. Plugs stay on for a short period to ensure the smooth and clean combustion. Plugs are then switched off to lower power to prevent them from burning.

NOx emissions are generally of thermal source and are formed on the lean side of the diffusion flame while soot is formed on the rich side of the diffusion flame. CO and HC level are generally very low. There exists comprise on the NOx and PM (particulate matters) while modeling combustion parameters. As the higher combustion temperature favor particulates oxidation, but

increase NOx production rates. At the source reduction of NOx generally entails an increase in the particulate emissions and an increase in fuel consumption.



Figure 3.10: Production of NOx and PM with respect to temperature

3.7 CI Emission Reduction

3.7.1 Changing Ignition Delay

Retarding the timing of injection results in the reduction of peak cylinder temperature and pressure this softens the combustion process and helps in reducing the NOx production with the increase in relative increased amount of PM



Figure 3.11: Production of emissions with respect to ignition delay [1]

3.7.2 Turbo-Charging and Intercooler

Turbo-charging is the first technique that is used to reduce the emission of diesel fuel. It is now accompanied with the intercooler. Majority of heavy duty diesel engines are utilizing this facility. The power output of the diesel engine depends on the amount of fuel injected in the cylinder and combusted. If the amount of fuel is increased then power out also increased. There is a requirement that for the increased amount of fuel there should be enough amount of air to burn it completely. For this, large amount of air is gathered through two types of changing. Either the cylinder volume should be increased or the increased amount of induced air is pressurized enough to fit for the increased amount of fuel. Devices commonly used for pressurizing are compressor and turbochargers. The turbocharger is preferable because it utilize energy from the exhaust gas for driving its shaft. Compression of air is obtained with the minimum power loss and fuel loss. Infect it imparts increase in the efficiency as utilizing the waste energy. So it lowers the fuel consumption as compared to the naturally aspirated engine of the same specifications. So it promotes the power density of the engine.

Increase in the boost pressure lower ignition delay which in results reduces PM. On the other hand boosting pressure and reducing fuel to air ratio increase intake temperature and NOx emissions. The injection timing is adjusted accordingly. NOx is also reduced if with the retardation in the injection timing charge air cooling is utilized. It is the intercooler that is placed between intake manifold and compressor of the turbocharger. The peak temperature during combustion and intake air temperature are reduced by this way and the supplied air become dense. It also decreases PM at acceptable brake specific fuel consumption.



Figure 3.12: Effect of after-cooling and turbo-charging on NOx and PM [26]

3.7.3 EGR System

Exhaust gas recirculation technique was first utilized only by the spark ignition engines but now it is also adopted by the diesel engine systems. It comprises of low and high recirculation systems. In high pressure system some of the portion exhaust gas is circulated back into intake manifold while in low pressure system first the exhaust gas is circulated through after-treatment device and then rooted to the intake manifold or compressor of the turbocharger. EGR system reduces the NOx emissions [29]. The oxygen concentration is reduced because it is diluted by the combustion products. Also the peak combustion temperature is reduced due to the dilution and products of combustion. On the contrary if high amount of EGR is utilized then there is an increase in the particulate matters. If EGR is used with the DPF then both the reduction of NOx and particulate matter is possible.



Figure 3.13: EGR system

3.7.4 Diesel Particulate Filter

Diesel particulate filters (DPF) are of many types depending upon the type of engine used. They are accompanied with regeneration methods. The most common DPF in practice is continuous regenerating type developed by Johnson Mathey [29].



Figure 3.14: A continuously regenerating diesel particulate filter, CR-DPF

It is very much durable and it has been utilized for a period of time. Low sulfur fuel is used in DPF. Filter is consist of a catalyst of an oxidation type with the active particle filter. The function of catalyst is to convert nitrogen oxide to nitrogen dioxide. This nitrogen dioxide is then used for continuous regeneration of actual filter. NO₂ burns soot at low temperature while O₂ does not. The whole system regenerates NO₂ which is then burns and under heavy load trapped soot at the favorable temperature of about 200-450 C° . The reaction that takes part in the conservation of soot is as fellows

$$NO_2 + C \rightarrow NO + CO$$

 $2NO_2 + C \rightarrow 2NO + CO_2$

DPF also reduce the carbon dioxide and hydrocarbon in the exhaust gas. For hydrocarbon about 85% conservation occurs after high mileage. While CO and PM conservation rates are 90%.

3.7.5 Catalytic Reduction and NOx Trapping

NOx emissions are reduced through the selective catalytic reduction by using urea and ammonia as a reducing agent. The urea is converted to ammonia and is injected as catalytic converter for reaction with the NOx to extract nitrogen out of it. The efficiency of reaction is dependent on the supply of ammonia. If the saturation reaction exceeds the limit then there is a disadvantage of ammonia slippage. A proper infrastructure is required for this operation. The SCR technique with the particulate filter technique shows great advantage in reduction of NOx. SCR gives lower fuel consumption as compared to other techniques.

$$2NH_3 + NO_2 + NO \rightarrow 2N_2 + 3H_2O$$
$$4NH_3 + O_2 + 4NO \rightarrow 4N_2 + 6H_2O$$
$$8NH_3 + 6NO_2 \rightarrow 3N_2 + 6H_2O$$

3.7.6 Humid Air Motor System

It is an interesting that the introduction of water in the combustion process results in the decrease of generation of NOx emissions. the advantages of using water is that it is nontoxic, cheap, and it is basically inert. When vapor of water are mixed with the air in supercharged form three of the following mechanism happens that results in the decrease of NOx.

- 1. Water molecules dissociation
- 2. Water vapor is replacing air in dilution of supercharged air

3. Increase in specific heat capacity of air fuel mixture

Water is injected in many forms in the combustion chamber. It is introduced in the cylinder in the form of emulsification of water in fuel, as fume in the charge air and directly injected in the cylinder. Practically NOx is decreased upto 30-40%. For this purpose an additional tank which should be in size of fuel tank should be added with the engine. The principle of HAM developed by Munthers Europe AB, Sweden [reference] is that compressed air from the turbo is forced to pass through a tower for humidification.





In the tower, the compressed air is introduced to heated water in the mode of counter-flow mode. Some of the water vaporized and humidity of air increase near the saturation point. A heat exchanger is utilized to heat the water. The energy for heating is carried from the cooling system of engine. So no such heat source is required. A reduction of about 55 to 80% is achieved by this process. The main problem in using this type of configuration is the amount of water that is used for the road engine.

3.8 Effects of Diesel Emissions on Human Health

Effects of NOx and PM on health come from various medium of information. This information is related to the study of factors that are harmful for the health of population. It also

includes observational controlled exposure of humans to the pollutant and animal toxicology test. It is derived from outdoor study where the pollutant emission of the ambient air includes NO₂. The fine particles and soot is released from the exhaust of diesel fuel. Some toxic exhausts are in sufficient amount and some of them are in enough amounts that they impose certain health problems when accumulated in a sufficient amount. These soot and fine particles can cause the human cancer. Heart, lung and mental functioning can also be damaged due to these particles. The particulate of diesel emissions comprises of fine particles. The surface structure of these particles can be easily combines with the other toxics of the environment. They are of very small size that they can penetrate into the lungs.

Motor vehicles emission is the common source of NO_2 . NO_2 is a precursor of other secondary air pollutants which includes photo oxidants, nitrite part of aerosols and nitric acid. The situation of examining and observing NOx is complicated as photochemical reaction take place and air travels to a distance before the generation of secondary pollutants. Health risks come from the direct inhalation of NO_2 or its secondary pollutants including O_2 .



Figure 3.16: Relationship of Nitrogen Oxides (NOx) emissions with the formation of NO₂

4. CHAPTER 4: Phenomenological Single Zone Combustion Model

4.1 Introduction

For the prediction of combustion process various models have been studied. These models range from high complex time consuming models like CFD models to the simple one zone phenomenological models. In this chapter a simple phenomenological combustion model is described with the parameterization of main diesel processes.

The prediction of combustion processes in diesel engine requires user friendly parameterization and considerable short computing time. The optimization does not take place in the actual existing engine, but instead in a model, which contemplate mechanical, thermodynamic and chemical model for the description of technical processes. The combustion is characterized by injection, atomization, spray evolution, vaporization, fuel air mixing, combustion and emission formation.

Combustion models can be categorized into thermodynamic, phenomenological and CFD models. Thermodynamic (0-dimensional) models based on heat release empirical equations while neglecting pollutant formation. Phenomenological (quasi-dimensional) based on chemical and physical sub models while CFD models give the detail physical description of physical processes. Calculation time in CFD models for a cycle transformation takes hours and in phenomenological models it takes seconds. The spatial development of combustion into zones of changing temperature and formation is achievable in phenomenological models which help in predicting the aspects of emissions.

Cylinder pressure analysis cannot be overpass in the evolution of internal combustion engines. It is most important in distinguishing the knocking and understanding of the insights of combustion process which include heat release rate, inflammation duration, ignition delay and heat paths. This can be done by thermodynamic analysis. The analysis of HRR in phenomenological models can be obtained without using pressure trace.

Wiebe [32] model of exponential decay function neglects the changes in combustion chamber and injection rate. Hiroyasu et l. [6] divided injection jet into several short zones, so called packets which acted as separate control volumes. The energy and mass equations are solved on these control volumes. Droplet evaporation pollutant formation and combustion rates are calculated within these limits. Chmela et al. [5] approach on the basis of kinetic energy of injection only describes the mixing controlled combustion while neglecting premixed combustion and wall impingement. While this model takes into account both premixed and mixing controlled into consideration.

The given model allows for parameterization study of combustion phenomena. Common rail injection engines give a variety of specifications to deal with, like duration of main and pilot injection, injection timing, ignition delay, EGR rate and boost pressure. All these changes require very short computing timing to study variations and their effects. The main target of every combustion model is to calculate HRR.

4.2 Input parameters

A 2.0 liter HSDI diesel engine is used for this model with the low pressure EGR system with following specifications:

No. of Cylinder	4
Engine Type	Euro 4
Displacement	1998
Architecture of cylinder	In line
Bore × Stroke (mm)	85 × 88
Compression Ratio	18
Injection System	Common rail, Piezoelectric injectors,2 nd Generation
No. of Injector Orifices × Diameter (mm)	7 × 0.150
Injection Pressure (bar)	1.6
Combustion Chamber Type	Re-Entrant bowl piston
EGR System	High Pressure Cooled EGR
Intake Temperature	26.24°C or 298.64K
Ambient Temperature	16.5°C
Cylinder Wall Temperature	510 K
Exhaust Temperature	615.07 K

Table 4.1: Engine Specifications

Ambient Pressure	1.01 bar
Clearance Volume	$0.29374e-4 m^3$
Displacement Volume	4.9936e-4 m ³
Total Volume	$5.2873e-4 m^3$
Mean Piston Speed	5.85 m/s
Relative Humidity	83%
Connecting rod length, l/Crank Radius, a=S/2	3.295
Mass of air induced in the cylinder, m_{ai}	7.724e-4 kg/stroke

It has been installed with the charge-cooler to cool the charge of air after the compression from turbo charger. Charge-cooler requires a large quantity of air to flow similar to that installed at the front of an automobile.

4.3 Development of Pressure Curve ROHR Model

In this section the detailed numerical model is presented. The numerical model is further divided into parts to facilitate the detail insight study of the combustion process. The gases used in the internal combustion engine as working fluids are treated as ideal gases. These gases include oxygen, nitrogen, water vapor and carbon dioxide. They are usually considered as ideal gases. For this specific volume of superheated and saturated water vapors are tabulated against pressure and temperature.

- 1. Properties of superheated water vapors
 - Specific volume, m3/kg against
 - 38 Press. values range from 0.00061-60Mpa
 - 58 Temp. values ranges from 0-3000 C
- 2. All Inputs
- 3. Properties of saturated water vapors
 - Specific volume, m3/kg against
 - 55 values of temp, ranges from 273K to 647.3K

- 55 values of press, ranges from 0.0061 bar to 221.2 bar
- 4. Finding the values of pressure and specific Vol. against ambient temp(289.65K)
- 5. Finding the values of pressure and specific Vol. against exhaust temp(615.07 C)
- 6. Finding the mass of air pressure of air and vapor initially in the clearance volume
- Perform interpolation to find the value of sat. vapor pressure and specific volume at ambient temperature i.e. 289.65K

Table 4.2: Properties of Saturated Water Vapors

Properties of Saturated Water Vapors				
No.	Temp,T_vap(K)	Pvap_sat(bar)	Vvap(m ³ /kg)	
4 th	285	0.0139	99.400	
Х	T_amb=289.65	0.0188	V _w =71.7790	
5 th	290	0.0192	69.7000	

$$V_w = \frac{V_w}{H_{rel} \times 100} = \frac{71.7790}{0.83 \times 100} = 86.4807 \frac{m^3}{kg}$$

 Perform interpolation to find the value in between the 49th and 50th at exhaust temp. (615.07 C=888.22K) which gives an array of 38 values of specific volume at Pressures in between 0.00061--60MPa

Table 4.3: Properties of Superheated Water Vapors

Properties of Superheated Water Vapors				
No.	Temp, K	Sp.Volume m ³ /kg at 1Mpa		
49 th	873.15	0.4011		
49.301 th	888.22	0.4081		
50 th	923.15	0.4245		

$$V_w = 86.4807 \frac{m^3}{kg}$$

Properties of Superheated water vapor at Exhaust Temperature 615.97C=888.22K			
No.	Sp.Volume m ³ /kg	Pressure MPa	
2^{nd}	634.321	0.00061	
2.923 th	86.4807	0.00928	
3 rd	40.9906	0.01000	

Table 4.4: Properties of Superheated water vapors at Exhaust Temperature

 $P_v = Press. of vapor in the clearence Vol.$

$$P_v = 0.0098 MPa = 9.2803e3 pascals$$

 $m_{ai} = mass \ of \ air \ in \ the \ clearnace \ Vol. = 2.689e - 5 \ kg$

 $P_a = Press. of air in the clearance Vol.$

$$P_a = \frac{m_{ai} R T_{exh}}{V_c} = 1.661e5 \ pascals$$

4.3.1 Cylinder Pressure



Figure 4.1: Cylinder Pressure

Piezo-resistive pressure sensor is used to find out the pressure of cylinder [28] for compression and expansion strokes. The intake pressure is 1.6 bar and exhaust pressure is 1.7 bar, while the maximum pressure is 97.73 bar.

4.3.2 Cylinder Volume

By using compression ratio r the volume of cylinder $V(\theta)$ can be estimated with respect to crank angle movement. It also utilizes the bore, connecting rod length and stroke.



Figure 4.2: Geometry of Piston Cylinder [33]

$$V(\theta) = \frac{V_d}{r-1} + \frac{V_d}{2} \left[\frac{l}{a} + 1 - \cos\theta - \left(\left(\frac{l}{a}\right)^2 - \sin^2\theta\right)^{\frac{1}{2}}\right]$$



Figure 4.3: Change in Cylinder Volume with respect to Crank Angle



Figure 4.4: Cylinder Temperature

$$PV = (maw + mai)RT_{cyl}$$
$$T_{cyl} = \frac{PV}{(maw + mai)R}$$

4.3.4 Heat Capacity [38]

If
$$T > 600$$
 then

$$Cp = 166.3 + \frac{24.5}{\emptyset} \log (T - 70 - \frac{120}{\emptyset})$$

If $\emptyset < 8$ then

$$Cp = (975.5 + 0.28T) - (11.92 + 0.06T\log(\emptyset))$$

Else

$$Cp = 1000 + 2.85 * exp\left(\frac{T - 273.15}{100}\right) 0.88$$

 $Whereas T = T_{cyl}$
 $C_P = C_V - R$

4.3.5 Law of Thermodynamics

$$dqp = Heat \ loss \ across \ the \ cylinder \ wall = hA(T_{cyl} - T_w)$$
$$dQ = Rate \ of \ Heat \ Transfer(ROHR) = Watts = \frac{J}{s}$$
$$dU = Internal \ Energy \ (j) = (m_{aw} + m_{ai}) \ C_v \ dT$$
$$dW = Work \ Done = P \ dV$$
$$ROHR = dQ = (m_{aw} + m_{ai}) \ C_v \ dT + P \ dV - hA(T_{cyl} - T_w)$$

$$A(\theta) = \frac{\pi}{2}b^2 + \pi b \frac{s}{2} \left[\frac{l}{a} + 1 - \cos\theta + \left(\left(\frac{l}{a}\right)^2 - \sin^2\theta\right)^2\right]$$
$$h = \left(\frac{W}{m^2 K}\right) = 130 \left(V_{cyl}^{-0.06} P^{0.8} T^{-0.4} (V_p + 1.4)^{0.8}\right)$$

1

4.4 Development of Fuel Injection ROHR Model

The Fuel injected model does not require the use of cylinder pressure values. It is based on the fuel injection timing. It directly affects the pressure due to heat release. The injection profile [28] used for this modeling is shown in figure below. In which pilot injection starts at -**19.05**° before reaching the cylinder to top dead centre at crank angle of **180**°. The duration of pilot injection is **0**. **2032** *ms*. The main injection starts at -**0.42**° before reaching the cylinder to top dead centre at crank angle of **180**°. The main injection duration is **0**. **9352** *ms*. The minus sign indicates that this value is to be subtracted from the position of top dead centre of cylinder i.e. **180**°. The crank angles for the start of injections are **160.95**° and **179.58**° for pilot and main injection respectively.



Figure 4.5: Instantaneous Injection Rate with respect to Crank Angle

4.4.1 Evaporation Model

Evaporation of fuel starts just after the injection of fuel. The term evaporation, vaporization, and boiling point have nearly same meaning as all of them are phase transition processes. Vaporization of an element or compound is a generally a transition of liquid phase to gas phase. Evaporation is transition from liquid to gas phase but it occur below boiling temperature at given pressure where as boiling process is also phase transition from liquid to gas phase but it occur below boiling the phase but it occur at or above the temperature of boiling.

The evaporation starts just after the injection of fuel due to the temperature of compressed air. The evaporation is calculated according to d^2 law of droplet vaporization which relies on vaporization constant beta(β). The droplet diameter after evaporation is calculated by subtracting the evaporation from it. D_0 is the initial diameter at the time of injection. This model assumes the fuel as a single zone and considers all the further processes in focusing that spherical zone of fuel. Actually all the fuel no matter from which injector it is coming from is gathered in one spherical zone. The diameter of droplet after injection in the cylinder decreases in linearly squared relation with respect to time *t*.

$$d^2 = d_0^2 - \beta t$$

By putting d = 0 and after rearranging, for droplet size d_0 vaporization time is calculated as


Figure 4.6: Evaporation Constant with respect to Crank Angle using Temperature Curve

Heat transfer from the environment heat-up the droplet and it start vaporization. It helps to increase the vapor pressure of the droplet and the rate of evaporation rises. Evaporation helps to release the heat from inside of droplet. The mass of a liquid droplet in a sphere shape is given as

$$m_l = \frac{\rho_l \pi d^3}{6}$$

The value of vaporization constant increases with the increase of atmospheric temperature and pressure

Fuel	Air Temperature	Beta (mm^2/s)
Gasoline	971	1.06
Gasoline	1068	1.49
Kerosene	923	1.03
Kerosene	971	1.12
Kerosene	1014	1.28

Table 4.6: Vaporization Constant for selected Fuels in Air at 1 atm Pressure [35]

Kerosene	1064	1.47
Diesel Fuel	437	0.79
Diesel Fuel	971	1.09

The unit of beta is m^2 /s. The evaporation constant under convection is used as [8]

$$\beta = \frac{c \, k_g}{\rho_f \, c_p} \ln(1+B)$$

$$B = \frac{1}{h_{fg}} \{ c_p (T_{cyl} - T_{boil}) \}$$

The injection of fuel mainly depends on the pressure at which it is injected. After injection from nozzle it depends on the conditions inside the combustion chamber. The compressed air temperature and pressure causes the fuel jet to shatter into several droplets. These liquid droplets then relay on the inertial and surface tension forces that decide the time and amount of shattering of liquid droplets into further droplets. Reynolds number and Weber numbers are two dimensionless numbers that decide the turbulence and amount of droplet shattering as they rely on inertial force and surface tension respectively. The initial droplet diameter is calculated from SMD as under [9]. The value of constant c is taken as 4.

$$D_{0} = SMD = c. d_{N}. (Re. We)^{-0.28}$$
$$Re = \frac{u_{d,0}. d_{N,eff}}{\vartheta_{f}}$$
$$We = \frac{u_{d,0}^{2}. d_{N,eff}. \rho_{cyl}}{\sigma_{f}}$$
$$u_{d,0} = \frac{\frac{dm_{inj}}{dt}}{\rho_{f}. A_{n,eff}}$$

The initial droplet velocity is calculated by using injection profile. As $\frac{dm_{inj}}{dt}$ is the instantaneous injection rate. The surrounding temperature of droplet is calculated from the in cylinder temperature using ideal gas law. It is presumed that evaporated fuel after injection accumulated in a zone. The unburned gaseous fuel mass mf_{ub} is taken as input for this model.

4.4.2 Premixed Combustion

The fuel is injected in mainly two steps comprising of pilot and main injection. The pilot fuel injection is of very small quantity commonly known as pre-injection. Longer ignition delay of main combustion comes from the early pilot injection because it gives short time to burn completely and gives a higher premixed peak of the main combustion. Combustion noise is mainly due to the high pressure that generate due to the abrupt combustion. The reduction of combustion noise is the preeminent goal of pre-injection by softening the main injection pressure.

The pilot injected fuel burn as premixed combustion. Pilot injection reduces the ignition delay of main injection by increasing the temperature and pressure of the combustion chamber and also helps in the reduction noise and NOx. The premixed combustion includes mixing and combustion models. The mixing model gives the local air to fuel ratio during mixing. The injected fuel from each injector hole forms one homogeneous spherical zone [24]. The turbulent mixing takes place during the ignition delay which leads to the growing zone with leaner air to fuel ratio because air and residual gas is increasing relative to the fuel. The combustion starts due to pilot injection from a point. The exact location of the flame generation is not explicit [24]. First surging indication of heat release comes from the turbulent flame generation of that point. After that flame generation starts from other locations of the zone which provides the declining indication of the heat release curve of the premixed combustion.

It is assumed that constant initial mixing of fuel with air and residual gases take place during the pilot injection. When the mass of fuel **mf** evaporates then initial air and residual gases is added to the premixed region. The mixing is treated as turbulent mass transport mixing due to the presence of fuel in the different combinations in the region. Equation 1 describes the fuel diffusion out of that region. The value of diffusion constant $D_{fu} = 1.0e - 4 \frac{m^2}{s}$.

$$\frac{dm_f}{dt} = D_{fu} \cdot Re^{0.5} \cdot A_z \cdot \frac{\rho_f}{D_z}$$

During mixing the air and residual gases mixes with the fuel in the region and this goes on developing with the increasing amount of air and residual gases.

The velocity of flame generation due to turbulent mixing is portrayed by Damkoehler [34]. The turbulent velocity u_t changes directly proportional to the mean piston speed. Burning of air fuel mixture changes with the turbulent flame velocity s_t and flame surface area A_{fl} .

$$\frac{dm_1}{dt} = \rho_{ub} \cdot s_t \cdot A_{fl}$$

$$s_t = s_l \cdot \left(1 + c_1 \left[\frac{u_t}{s_l}\right]^{c_2}\right)$$

$$s_l = s_{lo} \cdot \left(\frac{T_{cyl}}{T_{cyl,0}}\right)^{\gamma} \cdot \left(\frac{P_{cyl}}{P_{cyl,0}}\right)^{\delta}$$

$$s_{lo} = \beta_m + \beta_2 \cdot \left(\frac{1}{\lambda_{zn}} - \frac{1}{\lambda_{sl,max}}\right)^2$$

$$\gamma = 2.18 - 0.8 \cdot \left(\frac{1}{\lambda_{zn}} - 1\right)$$

$$\delta = -0.16 + 0.22 \cdot \left(\frac{1}{\lambda_{zn}} - 1\right)$$

 $c_1 = 1.6, c_2 = -0.85, \lambda_{sl.max} = 0.91, \beta_m = 0.276, \ \beta_2 = -0.47, T_{cyl.0} = , P_{cyl.0} = 1.6 \ bar$



Figure 4.7: Laminar Flame Speed s_l versus Air/Fuel equivalence Ratio λ_{zn}

The declining indication of heat release due to the flame propagation form the other points of zone is calculated with below expression. $m_{f,ub,z}$ is the available unburnt mass of fuel that is the limiting factor for the premixed combustion. Whereas r_z is the radius of that zone and considered as length of the transmission of flame



Figure 4.8: Calculated ROHR of Pilot Fuel

4.4.3 Mixing Controlled Combustion

The main injection burns completely as mixing controlled combustion flame. Mixing controlled combustion depends on the time of mixing and turbulent kinetic energy. Mixing of air fuel is mainly due to the turbulence. The concept of frequency model for predicting mixing controlled combustion is well described by Boulouchos et al. [36] and utilized by Weisser et al. [37].

Mixing frequency f_m is calculated from characteristic mixing velocity and characteristic mixing length. The portion of combustion chamber which gives place for proper combustion is changing

with respect to crank angle. This characteristic length decides the time for mixing controlled combustion. This length is calculated as [37]

$$Ch. Length = \sqrt[3]{\frac{V_{cyl}}{\lambda. n_N}}$$

Mixing velocity is generated by the turbulence in the cylinder. The turbulence is mainly due to the high pressure of injected fuel. Due to this pressurized flow the phenomena like swirl and squish-flow of fuel happens in the cylinder. This helps in the thorough mixing of the air and injected fuel. The homogeneous turbulence model k-l is used for mixing frequency. This involves the production and dissipation of kinetic energy [1]. The production of kinetic energy is directly calculated from the injection of fuel and initial droplet velocity $u_{d,0}$. Whereas the kinetic energy of dissipation is calculated from turbulent velocity u_t as it is restricting the flow of fluid. Turbulent kinetic rate is taking part in deciding the characteristic velocity of the flow and it is calculated as

$$\frac{dk}{dt} = -c_{diss} \cdot \frac{1}{d_N} \cdot k^{\frac{3}{2}}_{diss} + c_4 \frac{dk}{dt}\Big|_{prod}$$
$$\frac{dk}{dt}\Big|_{prod} = \frac{1}{2} \frac{dm_{inj}}{dt} u_{d,0}^2 \frac{1}{m_{cyl}}$$
$$k_{diss} = \frac{3}{2} u_t^2$$
$$Ch. velocity = \sqrt{c_G \cdot c_M^2 + c_K \cdot k}$$
$$f_m(k) = \frac{Ch. velocity}{Ch. length} = \frac{\sqrt{c_G \cdot c_M^2 + c_K \cdot k}}{\sqrt[3]{\frac{\emptyset. V cyl}{n_N}}}$$
$$\frac{dm_f}{dt} = f_m(k). m_f$$
$$\frac{dm_f}{dt} = f_m(k). (m_{inj} - m_b)$$

$$\frac{dQ}{dt} = LHV.\frac{dm_f}{dt} = LHV.f_m(k).(m_{inj} - m_b)$$

$$c_{diss} = 0.04, c_4 = 0.3, \qquad c_G = 1.8 - 3, c_K = 0.1 - 0.4$$

4.4.4 Ignition Delay

The duration from start of fuel injection to start of combustion is termed as ignition delay (ID). Ignition delay depends mainly on the temperature and pressure of combustion chamber. It comprises of physical and chemical delay. In physical delay is taken from evaporation time that is the time at which mixture of gaseous fuel and air is formed. While chemical delay is calculated from Arrhenius type relation.

- Duration of Pilot Fuel=4° (161-164)° Crank Angle
- Duration of Main Fuel=14[°] (179-192)[°] Crank Angle

$$\int_{\theta^{SOC}}^{\theta^{SOC}} \frac{\mathcal{A}^{ai}(p(\theta))}{N_e} d\theta = 1$$
$$p(\theta) = (P(\theta), T(\theta), \emptyset)$$
$$\mathcal{A}^{ai}(p(\theta)) = c_5 \cdot \emptyset^{C_6} \cdot \left(\frac{P(\theta)}{P_{ref}}\right)^{C_7} \cdot \exp\left(\frac{-T_A}{T(\theta)}\right)$$
$$c_5 = 0.04, c_6 = -0.2, c_7 = -1.2, T_A = 6000$$

- SOC of Main Fuel Injection=183.6 Crank Angle
- Ignition Delay=22.6 Crank Angle

5. CHAPTER 5: Results, Discussions & Validations

This chapter includes the results, discussions and future recommendation for combustion modeling. It comprises of the rate of heat release curves that are generated by the pressure curve and fuel injection modeling. It also includes the comparison of measured pressure curve and calculated fuel injected models.

5.1 In-Cylinder Pressure

Pressure of cylinder is analyzed for 8 different points [28] Figure 5.1 shows the pressure signals after applying filter. From the Figure 4.3 (Instantaneous Injection Rate with respect to Crank Angle) it is clear that the pilot injection starts from 161 degrees of crank angle and main injection starts from 179 degrees. The variation in the pressure curve is directly related to the injection profile of the cylinder. In this study only one sample of pressure curve is analyzed for which the intake pressure of the air is at 161746 Pa and exhaust pressure is at 175334 Pa. The first rise of peak of pressure traces is due to the pilot fuel injection while after a short interval the second rise appears which is due to the main injection. The difference between the time start of pilot /main fuel injection and the time start of pressure rise is due to the ignition delay.



Figure 5.1: Measured Pressure Trace



Figure 5.2: Selected Pressure Trace

5.2 In-Cylinder Temperature

As it is difficult to measure the inside temperature of the cylinder directly, so it is measured indirectly by using the pressure trace. The ideal gas law is used for this purpose as





The measured intake temperature of air is 299.24 K and the exhaust temperature is 888.22 K. The temperature and pressure of air are higher at the exhaust side which helps to run turbocharger and ultimately sucks more air from the atmosphere at the time of intake.



Figure 5.4: In-Cylinder Temperature (2)

Figure 5.4 shows the calculated in-cylinder temperature. The first rise of the temperature is due to the pilot and second rise to temperature is due to the main fuel injection. At start the temperature first drop slightly and then start to increase. This is due to the fact that the fluid fuel injection process comes with the evaporation process and evaporation causes decrease in temperature. The temperature rise due to the pilot fuel is of very short interval as the pilot fuel burns incompletely whereas the temperature of main injection falls very smoothly due to the complete burning main injection fuel.

5.3 Rate of Heat Release

Rate of heat release (ROHR) is the main output of a combustion process. ROHR is calculated in Watts as it is the energy released in joules from one Kg of fuel burning in one second. Energy that is released is due to the complete combustion of fuel with the oxygen. The fuel in this case is diesel fuel together with the high temperature compressed air for proper combustion. Figure 5.5 shows the rate of heat release curve that is calculated using measured pressure trace. SOI-P shows the start of injection of pilot fuel while SOI-M shows the start of injection of main fuel. The difference between the start of injections and afterward peaks shows the ignition delay in the model. After the ignition delay, for the duration of few crank angles combustion of pilot fuel occurs very rapidly. The temperature of cylinder rises which helps in the smooth start of burning for mixing controlled combustion. Lots of phenomena happen during this

phase which includes evaporation, air fuel mixing and other chemical reactions. The rate of mixing is controlled by the burning process.



Figure 5.5: ROHR Calculated from Pressure Curve



Figure 5.6: Pre-Mixed Combustion

In the Figure 5.6 the initial start of burning curve is less than zero which clearly shows the effect of evaporation at the time of start of injection. One of the reasons of ignition delay is evaporation time that delays the starting time of burning.



Figure 5.7: Calculated Pre-Combustion

Figure 5.7 shows pre-combustion that is calculated using mixing model from air to fuel ratio. The measured pre-combustion and calculated pre-combustion are in good agreement. Thus precombustion model is validated as the peak values are nearly same with a little bit of difference.



Figure 5.8: Calculated ROHR



Figure 5.9: Measured V/S Calculated ROHR

Figure 5.9 shows the measured and calculated ROHR, the red line indicates the calculated ROHR while blue dotted line indicates the calculated ROHR. The difference in the curves is due to the fact that the measured ROHR is calculated using precise pressure curve values while calculated ROHR is an approximation using mixing model and frequency model approach. The purpose of this model is fulfilled i.e. combustion modeling and validation. A good approximation is achieved. As the difference between calculated and measured ROHR shows a good agreement.

5.4 Cumulative Heat Release



Figure 5.10: Cumulative Heat Release

The product of LHV and injected fuel mass is known as cumulative heat release CHR. It is given as

$$CHR = LHV \times m_f$$

$$LHV = 4.27 \times 10^7 \frac{J}{kg}$$

$$m_f = 4.0198 \times 10^{-5} kg/stroke$$

$$Actual CHR = 1.716 \times \frac{10^3 J}{stroke}$$

$$CHR of Pressure Curve Model = 1.7175 \times 10^3 \frac{J}{kg}$$

$$CHR of Injection Profile Model = 1.5456 \times 10^3 \frac{J}{kg}$$
%Error (In case of CHR of Pressure Curve Model = 0.11%)
%Error (In case of CHR of Injection Profile Model = 9.95%)

The green straight line in the Figure 5.10 shows the CHR as calculated above. Whereas, the peak value of calculated heat release curve (black dotted line) from phenomenological model is $1.5759 \times 10^3 I/stroke$. This leads to about 90% accuracy in the model.

5.5 **Recommendations and Discussion:**

From the above % error, Injection profile model proves to be in a good agreement with the ideal pressure curve model. This proves that without using experimental setup rate of heat release can be calculated with the best possible results with detailed inside investigation of involved processes. This model can be utilized to find the emissions in the exhaust gases by using the rate of heat release and temperature. Emissions can be reduced by optimizing the operating parameters and processes.

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