Numerical Analysis of Compression Ignition Engine using Ethanol Blends

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I certify that this research work titled "*Numerical Analysis of Compression Ignition Engine using Ethanol Blends"* is my own work. The work has not been presented elsewhere for assessment. The material that has been used from other sources it has been properly acknowledged / referred.

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Abstract

The effects of ethanol (C_2H_5OH) with the diesel fuel in the proportions of 05%, 10%, 15% and 20% (by vol.) are evaluated numerically to assess the performance and the combustion behavior of a four stroke, six-cylinder, direct injection (DI), 'Mercedes-Benz', diesel engine. Simulations are performed to validate the experimental study as well as combustion model. Combustion chamber cylinder pressure, temperature and emissions plots are obtained using ANSYS FORTE. These combustion chamber pressure, temperature and heat release plots highlight about interesting aspects, that illustrates the combustion mechanism using these auspicious biofuels which can be obtained from biomass (Bioethanol). The significant results have been observed using these bio-fuels blends, reduction of SOOT, CO and NOx emissions are examined with increasing percentage of biofuels like D100E0, D95E05, D90E10, D85E15 & D80E20 respectively. Reduction in cylinder pressure has been perceived to some extent while cylinder temperatures are decreased during second part of the combustion. Emissions are reduced to greater degree compromising the engine power to a little extent. Further parametric studies are performed and effects of start of injection (SOI), duration of injection (DOI) and initial inflow droplet and air intake temperature on pressure, temperature, chemical heat release and emissions are studied. These studies show that emissions level can be reduced by slightly varying the differing chemical and physical parameters of the ethanol in contrast to the parameters existing for the diesel fuel, and results assist the precise explanation of the observed engine behavior on emissions as well as performance.

Key Words: *Biofuels, Ethanol Blends, Combustion, Emission*

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Symbols

C_2H_5OH	Ethanol
$C_{12}H_{26}$	Diesel
$C_6H_{12}O_6$	Glucose
$C_{12}H_{22}O_{11}$	Sucrose
O_2	Oxygen
N_2	Nitrogen
NO	Nitric Oxide
NOx	Nitrogen Oxides
NO_2	Nitrogen Dioxide
CO	Carbon Monoxide
CO_2	Carbon Dioxide
Ar	Argon
H_2O	Water
m_f	Mass of Fuel
LHV_f	Lower Heating Value of Fuel
V_t	Total Volume
V_s	Swept Volume
V_c	Clearance Volume
r	Compression Ratio
$\bar{\rho}$	Density
∇	Differential operator
$\tilde{u}$	Flow Velocity Vector
$\dot{\bar{\rho}}^s$	Source Terms due to Spray Evaporation
$\frac{\partial}{\partial t}$	Derivative with respect to Time
$\bar{p}$	Pressure Force
$\bar{\sigma}$	Viscous Shear Stress
$\bar{F}^s$	Rate of Momentum gain per unit Volume
$\bar{g}$	Specific Body Force
υ	Laminar Kinematic Viscosity
I	Identity Tensor
T	Transpose of a Tensor
$\boldsymbol{\tau}$	Reynolds Stress
$\tilde{I}$	Specific Internal Energy
$\bar{J}$	Heat Flux Vector
λ	Thermal Conductivity
α	Thermal Diffusivity
c_p	Heat Capacity
$\bar{T}$	Fluid Temperature
$\tilde{h}_k$	Specific Enthalpy of Species k
$\tilde{\varepsilon}$	Dissipation rate of the Turbulent Kinetic Energy

$\dot{\bar{Q}}^c$	Source term due to Chemical Heat Release
$\dot{\bar{Q}}^s$	Source term due to Spray Interactions
H	Effects of Ensemble-averaging of the Convection Term
R_u	Universal Gas Constant
W_k	Molecular Weight for Species k
n	A Constant
M_s	SOOT Mass
M_{sf}	SOOT Formation Mass
M_{so}	SOOT Oxidation Mass
M_{pre}	Mass of the SOOT Precursor
K_f	SOOT Formation Rate
A_{sf}	Pre-exponential Factor for the Global SOOT-formation Reaction
E_f	Activation Energy for SOOT Formation
MW_c	Molecular Weight of Carbon
ρ_s	SOOT Density
D_s	SOOT Particle Diameter
R_{Total}	Nagle and Strickland-Constable Oxidation Rate

Abbreviations

DI	Direct Injection
CI	Compression Ignition
PM	Particulate Matter
AFR	Air to Fuel Ratio
LCV	Lower Calorific Value
RANS	Reynolds Averaged Navier Stokes
LES	Large Eddy Simulation
ACHR	Accumulated Chemical Heat Release
SOI	Start of Injection
DOI	Duration of Injection
IAT	Initial Intake Air Temperature
IDT	Inflow Droplet Temperature
D100E0	Pure Diesel (100% Diesel)
D95E05	Diesel 95% & Ethanol 05%
D90E10	Diesel 90% & Ethanol 10%
D85E15	Diesel 85% & Ethanol 15%
D80E20	Diesel 80% & Ethanol 20%
TDC	Top Dead Center
BDC	Bottom Dead Center
BTDC	Before Top Dead Center
ATDC	After Top Dead Center
CAD	Crank Angle Degree

Units

s	Second
K	Kelvin
mm	Millimeter
nm	Nanometer
μ	Microns
g	Gram
mg	Milligram
Kg	Kilogram
J	Joule
MJ/Kg	Mega Joules per Kilogram
Kg/m^3	Kilograms per Cubic Meter
cm^3	Cubic Centimeter
cm^3/mol-s	Cubic Centimeter per Mole Second
Cal/mol	Calories/Mole
g/Kg.f	Grams per Kilogram of Fuel
rpm	Revolution per Minute
x°	Crank Angle Degree

CHAPTER 1: INTRODUCTION

The research work in this dissertation has been presented in following two parts. First part is associated with the formulation of a numerical model to simulate the processes of combustion using Diesel-Ethanol blends. The major objective of first part is to validate the combustion model of Ansys Forte for compression ignition engines using biofuel. The second half includes the parametric study related to combustion processes where the effect of start of injection (SOI), duration of injection (DOI), initial fuel and air temperatures on exhaust emissions (NOx, CO & SOOT) are studied.

1.1 Background, Scope and Motivation

European emission standards and regulations have enforced the engine researchers to concentrate on the alternative fuel related techniques [1,2]. Significant consideration has been given on the evolution of alternative fuels in several countries of the World with the foremost attention on bio-fuels which possess the additional benefit of being renewable nature [3,4]. Internal combustion engines mainly compression ignition (CI) engines are widespread and largely utilized in the automobile industry due to higher engine performance, durability and reliability [5]. Although diesel engine has higher thermal as well as combustion efficiencies and lower fuel consumption, but they are discouraged because of their exhaust emissions [6,7]. Carbon Monoxide, Nitrogen Oxides, and Particulate Matter are the major byproducts of the exhaust emissions and considered as air pollutants, which cause severe effects on the environment and are human health hazards as well [8]. Exposure to air pollutants give rise to cough, shortness of breath, wheezing, asthma, respiratory disease and high rates of hospitalization [9]. Various techniques have been developed to make sure complete combustion process like dual fuel spray methods [10], water injection [11,12] and exhaust gas recirculation [13] in compression ignition engines. Experimental investigations using biofuels as an alternating fuel have been carried out since couple of decades to accomplish the emission standards [14,15]. Nevertheless, these experimentations require a complete setup as well as real time data collection using sensors installed in the engine along with the integration to the software [16,17]. Apart from all, it is strenuous to perform parametric study on the engine test bed as it involves considerable variations in the equipment. The operating parameters such as injection timings [18] i.e. start of injection (SOI) and duration of injection (DOI), and other parameters like inflow droplet temperature (IDT) and initial air intake (IAT) temperature have notable influence on the emission quantities.

Amid all the cited solutions, this research investigates the application of alternating fuel as the use of biofuels is more practical and it doesn't require technical modifications on the diesel engine side. Beside emission reduction advantages, they are cost-effective and ecologically amicable. Also, considering the factors stated above, numerical approaches for internal combustion engine are used in this research which provides precise results and gives valuable intuition about the combustion processes take place in the engine. Along other biofuels, ethanol (C_2H_5OH), is a vital renewable fuel because it has 35% oxygen in it, compared to diesel and gasoline fuel, it needs a lesser amount of oxygen for combustion which consequences in less pollution [19,20]. Effect of ethanol fuel on the performance of a diesel engine by the use of engine simulation tool virtually are studied in the recent research by Praptijanto et al. [21]. The results exhibited that when diesel and ethanol fuels are directly blended, exhaust emission quantities such as CO, NOx, and SOOT are reduced to greater extent.

1.2 Ethanol- A Biofuel

Ethanol C_2H_5OH is a renewable fuel and it is obtained by alcoholic fermentation of sugar such as glucose and sucrose etc. from different vegetable resources, like sugar cane, corn, molasses, barley and farmed residues, such as leftover woods, hay and feedstock. Chemical reaction of ethanol fermentation using glucose and sucrose are given below:

$$C_6H_{12}O_6 \rightarrow 2\ C_2H_5OH + 2\ CO_2 \qquad (1.01)$$

$$C_{12}H_{22}O_{11} + H_2O \rightarrow 4\ C_2H_5OH + 4\ CO_2 \qquad (1.02)$$

Ethanol has advantage over other alcohols because of its renewable nature and higher miscibility with the diesel fuel.

1.2.1 Ethanol in Diesel Engine

At the present time, alcohols like methanol and ethanol are used as alternative fuels for diesel engine. Methanol can be produced economically using petrol or coal-based fuels, but methanol is used to a much smaller extent because solubility of ethanol in the diesel fuel is restrictive [18,29]. Alternatively, ethanol is a virtuous spark ignition engine fuel. Because of its higher-octane number, renewable nature and higher miscibility with the diesel fuel, it has the advantage over methanol. Researchers have been using ethanol with the diesel as an alternating fuel in the diesel engine since the twentieth century [22-24]. Komninos, et al. numerically investigated the formation of carbon monoxide and hydrocarbons emissions using isooctane and ethanol fueled HCCI engine [3]. Experimental studies on a constant speed stationary diesel engine and performance parameters using diesel-ethanol blends are performed by Ajav E. A., et al. [5]. A review study is done by Hansen, A. C., et al. on ethanol-diesel fuel blends [6]. Effects on performance, vibration and combustion behavior and knocking in a compression ignition engine by adding ethanol to the diesel fuel is studied by Taghizadeh-Alisaraei, et al. [7]. Different studies on the emissions and performance of a high-speed direct injection diesel engine operating on the diesel-ethanol blends are performed by Rakopoulos C.D., et al. [8]. Combustion heat release analysis of diesel-ethanol and n-butanol-diesel fuel blends in a diesel engine are analyzed by D.C. Rakopoulos, et al. [14]. Another experimental research using ethanol-diesel blends by Huang J., et al. examine the emission and performance of a diesel engine [15]. Physio-chemical properties of diesel-ethanol fuel blend by Li D., et al. illustrate the effects on the performance as well as emissions of the diesel engine [16]. The impact of ethanol additions on the performance and combustion characteristics of a diesel engine is discussed by Xingcai L., et al. [17].

Several experimental researches have been conducted on the combustion behavior of diesel-ethanol blends, but it has been concluded that numerical investigations are not performed yet using simulation software “ANSYS FORTE” with the innovative representations for precisely predicting engine performance and exhaust emissions.

1.2.2 Ethanol in Present Work

Numerous methods have been developed to make sure that ethanol can be fueled with the diesel in compression ignition engines. Generally, they can be classified into following: (I) Ethanol fumigation using manifold injection or carburetion to the intake air charge [24], quantity of ethanol is the constraint that can be utilized in this method, (II) Multi injection system i.e. considered impractical, as necessitate a major design alteration of the engine cylinder head [22], (III) Blending of ethanol with the diesel fuel [23-28], which is considered here as it doesn’t entail any amendment on the engine side. Ethanol is blended with the diesel fuel in the proportion of

5%, 10%, 15% and 20% (by vol.) and numerical studies are performed on the combustion behavior of a fully instrumented, six-cylinder, four stroke, direct injection (DI), ‘Mercedes-Benz’ diesel engine. Engine specifications and properties of fuel are shown in table 1-1 and 1-2 respectively. Using these biofuel blends, reduction of CO, NOx and SOOT emissions are observed with the increasing percentage of biofuels like D100E0, D95E05, D90E10, D85E15 & D80E20 respectively. It is concluded from the literature that the ethanol blends up to 20% by volume in diesel fuel are considered quite safe from the engine durability viewpoint.

Engine	**Mercedes Benz, OM-366 LA**
Bore	9.75 cm
Stroke	13.3 cm
Connecting Rod Length	23 cm
Number of Holes per Injector	5
Compression Ratio	18
Injector Hole Diameter	150 microns
RPM	1200
Total Displacement Volume	5958 cm^3
Fuel Quantity	25 mg

Table 1-1: Engine Specifications

Properties of Fuel	**Diesel $C_{12}H_{26}$**	**Ethanol C_2H_5OH**
Stoichiometric AFR	15	9
Molecular Weigh	170	46
Density at 293K (Kg/m^3)	837	788
LCV (MJ/Kg)	43	26.8
O_2 (% Weight)	0	34.8

Table 1-2: Properties of Fuel

CHAPTER 2: RESEARCH AND NUMERICAL METHODOLOGY

Compression ignition engines are the basis of exhaust emissions like CO, NOx and SOOT etc. Numerical study is carried out to analyze the combustion behavior as well as emissions produced by the diesel engine. First, engine model is designed using the ANSYS FORTE, secondly, simulations are performed to analyze the behavior of the combustion model. Parametric studies are also conducted where the effects of different parameters like start of injection (SOI), duration of injection (DOI), inflow droplet temperature (IDT) and initial air intake (IAT) temperature on exhaust emissions are considered.

2.1 Simulation Setup

The ANSYS Forte is designed for IC engine design applications. The computing resources which are practical for general design activities are utilized for the modeling approach to provide the utmost precise solutions possible for these applications. ANSYS Forte portrays the theoretical illustrations of 3-D geometry, fluid flow, spray dynamics and combustion behavior in the diesel engine a way better than other available tools.

The governing equations in ANSYS Forte are expressed to explain the ensemble-averaged stream field in the Reynolds Averaged Navier Stokes (RANS) approach, which solves the ensemble average of the stream field from many apprehensions of flows under homogeneously set circumstances and to solve the filtered stream field in the Large Eddy Simulation (LES) approach, which simulates individual flow apprehensions instead of the ensemble average of the flows. The basic form of the equations for the flow field are mentioned in a unified way as follows.

Continuity equation for the total gas phase fluid is given below:

$$\frac{\partial\bar{\rho}}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\mathbf{u}}) = \dot{\bar{\rho}}^{s} \tag{2.01}$$

The momentum equation for the fluid is given below which considers the effects of pressure, convection, viscous shear stress, and turbulent transport, as well as the influence of liquid sprays and body force.

$$\frac{\partial(\bar{\rho}\tilde{\mathbf{u}})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\mathbf{u}}\tilde{\mathbf{u}}) = -\nabla\bar{p} + \nabla\bar{\boldsymbol{\sigma}} - \nabla\cdot\boldsymbol{\tau} + \bar{\mathbf{F}}^{s} + \bar{\rho}\bar{\mathbf{g}} \tag{2.02}$$

Where $\bar{p}$ is pressure, $\bar{\mathrm{g}}$ is the specific body force, $\bar{\mathrm{F}}^{s}$ is the momentum gain rate due to the spray per unit volume, $\overline{\sigma}$ is a viscous shear stress given by following:

$$\overline{\boldsymbol{\sigma}} = \bar{\rho}\upsilon\left(\nabla\tilde{\mathbf{u}} + (\nabla\tilde{\mathbf{u}})^T - \frac{2}{3}(\nabla\cdot\tilde{\mathbf{u}})\mathbf{I}\right) \tag{2.03}$$

In equation 2.03, υ is the laminar kinematic viscosity, superscript T means transpose of a tensor. I is an identity tensor and τ is called Reynolds stress.

$$\boldsymbol{\tau} = \bar{\rho}\ (\widetilde{\mathbf{u}\mathbf{u}} - \tilde{\mathbf{u}}\tilde{\mathbf{u}}) \tag{2.04}$$

On the basis of first law of thermodynamics, the sum of pressure work and heat transfer must be equivalent to the change in internal energy. The effects of convection, turbulent transport and dissipation, sprays and chemical reactions should be considered in internal combustion engines flow problems. Equation for the internal energy transport is as follows:

$$\frac{\partial(\bar{\rho}\tilde{I})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\mathbf{u}}\tilde{I}) = -\bar{\rho}\nabla\cdot\tilde{\mathbf{u}} + \bar{\rho}\tilde{\varepsilon} - \nabla\cdot\bar{\mathbf{J}} - \nabla\cdot\mathbf{H} + \dot{\bar{Q}}^c + \dot{\bar{Q}}^s \tag{2.05}$$

where $\tilde{I}$ is the specific internal energy, $\tilde{\varepsilon}$ is the dissipation rate of the turbulent kinetic energy. $\bar{J}$ is the heat flux vector accounting for heat conduction as well as enthalpy diffusion.

$$\bar{\mathbf{J}} = -\lambda\nabla\bar{T} - \bar{\rho}D\ \sum_k \tilde{\boldsymbol{h}}_k\ \nabla\tilde{y}_k\tilde{I} \tag{2.06}$$

λ is a thermal conductivity, expressed by $\lambda = \bar{\rho}c_p\ \alpha$, where c_p is a heat capacity and α is a thermal diffusivity. $\bar{T}$ is a temperature of fluid and $\tilde{h}_k$ is a specific enthalpy of species k. $\dot{\bar{Q}}^c$ is a source term due to chemical heat release and $\dot{\bar{Q}}^s$ due to spray interactions. The H term is the effects of ensemble-averaging or filtering of the convection term, that is,

$$\mathbf{H} = \bar{\rho}(\widetilde{\mathbf{u}\imath} - \tilde{\mathbf{u}}\tilde{I}\ ) \tag{2.07}$$

An ideal gas law is supposed to follow by the gas-phase mixture for the thermodynamics relations. Whereas the mixing of the gas components follows the Dalton model, which states every component must acts like ideal gas whether it is individual or in the mixture at different temperature and the volume range.

$$\bar{\mathrm{p}} = \mathrm{R_u}\tilde{\mathrm{T}}\sum_{\mathbf{k}}\left(\frac{\bar{\rho}_k}{W_k}\right) \tag{2.08}$$

R_u is called universal gas constant, where W_k is a molecular weight defined for species k.

SOOT model used in ANSYS Forte is the two-step SOOT model comprising of oxidation steps and competing formation. The Hiroyasu Model [30] is used for SOOT formation whereas for oxidation, Nagle and Strickland-Constable Models [31] are used. The governing equations for the SOOT model are as follows:

$$\frac{dM_s}{dt} = \frac{dM_{sf}}{dt} - \frac{dM_{so}}{dt} \tag{2.09}$$

$$\frac{dM_{sf}}{dt} = K_f M_{pre} \tag{2.10}$$

$$K_f = A_{sf} p^n \exp\left(-\frac{E_f}{RT}\right) \tag{2.11}$$

$$\frac{dM_{so}}{dt} = \frac{6MW_c}{\rho_s D_s} M_s R_{Total} \tag{2.12}$$

Where p is pressure, n is a constant, M_s is a mass of soot, M_{sf} is a soot formation mass, and M_{so} is a soot oxidation mass. M_{pre} is the mass of the soot precursor, K_f is the rate of soot formation, A_{sf} is the pre-exponential factor for the global soot-formation reaction, E_f is the soot formation activation energy, MW_c is a molecular weight of carbon, ρ_s is soot density, D_s is the supposed soot particle diameter, and R_{Total} is the Nagle and Strickland-Constable oxidation rate. Further details about the SOOT model are specified by Vishwanathan and Reitz [32]. Default values of model constants used in ANSYS FORTE are given as following.

Model Constants	Value
n	0.5
A_{sf}	40 cm^3/mol-s
E_f	12,500 Cal/mol
ρ_s	2 g/cm^3
D_s	25 nm

Table 2-1: Default Values of Model Constants

2.2 Simulation Model

For modeling case, following are the sections taken care off. Geometry for diesel engine is designed using ANSYS sector mesh generator where engine parameters as well as mesh parameters are the required input data. The configurations of simulation model are completed using “Forte Simulate” and results/output are scrutinized using “Forte Monitor”.

2.2.1 Geometry/Mesh

Following parameters are defined in this section:

- Bore

  The nominal inner diameter of the working cylinder is called bore. It is show below in figure 2-1. It is usually expressed in mm.

- Stroke

  The total linear distance moved by the piston when it travels from an end of the piston cylinder to the other end as shown in figure 2-1.

- Connecting Rod Length

  Total distance between the centers of the crankshaft bore and the piston pin bore is called as connecting rod length.

- Squish

  Distance from top of a piston to head at TDC is called squish.

- Bowl Profile

  Pair of data that defines the shape of piston bowl where the first point must have z=0 and the last point of the center of the bowl must have x=0

- Compression Ratio

  The ratio of total cylinder volume V_t to the clearance volume V_c.

$$r = \frac{V_t}{V_c} \tag{2.13}$$

$$V_t = V_s + V_c \tag{2.14}$$

$$r = 1 + \frac{V_s}{V_c} \tag{2.15}$$

  Where V_s is swept volume i.e. the total volume enclosed by the piston when it moves between TDC and BDC. When piston is at TDC there is a volume in a cylinder above the top of the piston, it is called clearance volume.

- Sector

  Specification of sector angle directly or through cyclic symmetry.

- Sector Angle

  Angle of the arc used to create a sector is called sector angle

- Periodicity

  Periodic nature using sector angle.

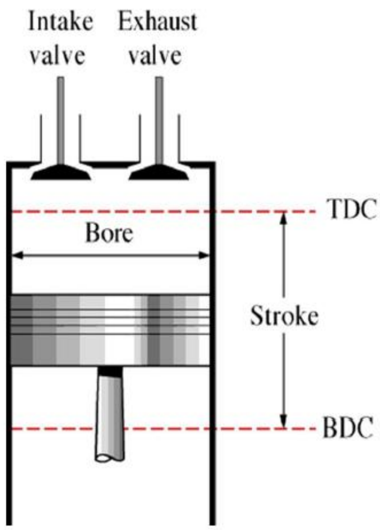

Fig 2-1: Piston Profile

Geometry and mesh profile of a piston in an engine cylinder is shown in figure 2-2.

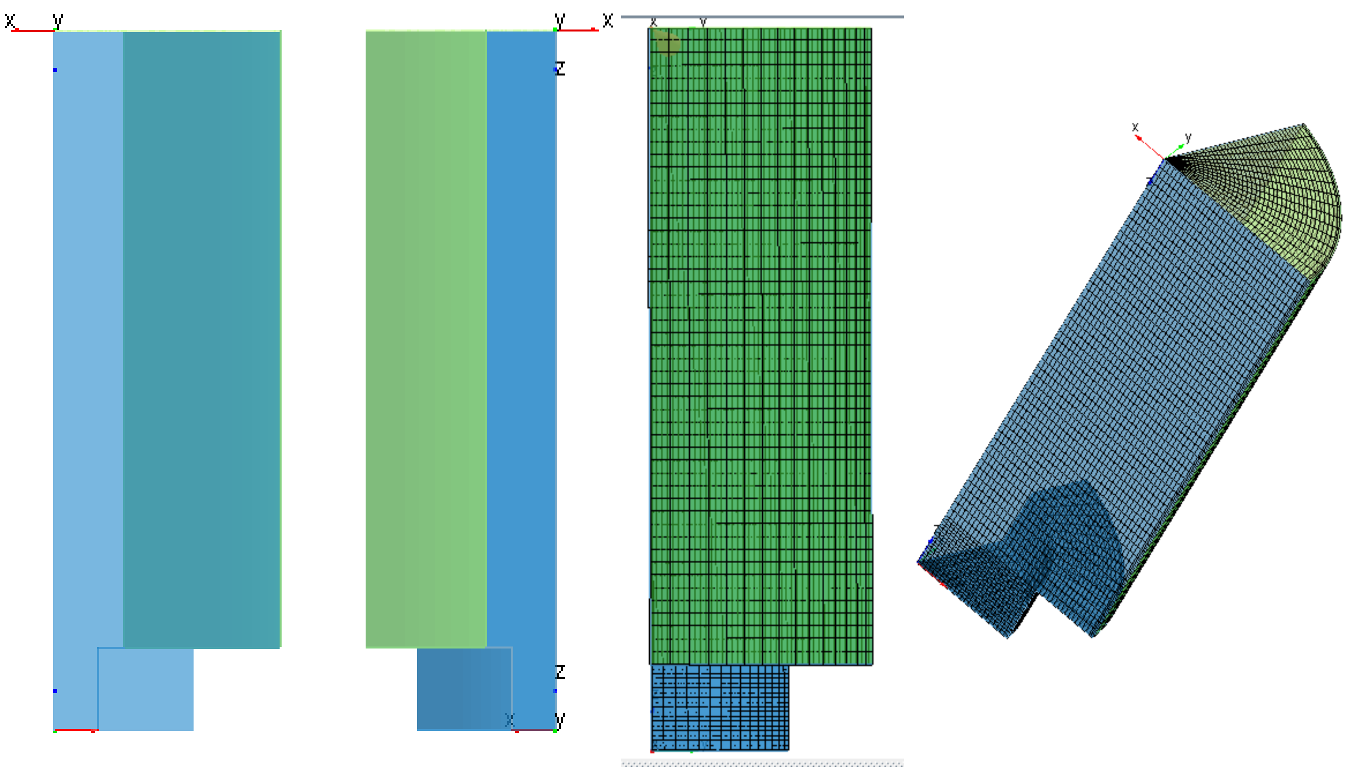

Fig 2-2: Geometry & Mesh of a Piston in a Cylinder

2.2.2 Chemistry File (Fuel and Species)

Chemistry files and fuel species are available at "Ansys Model Fuel Library". Flame speed model is used in chemistry file. RANS RNG k-epsilon model is used for turbulence.

- Diesel – SOOT Particle Tracking
- Species Definition

  Fuel species are defined in this section.

  - Ethanol (C_2H_5OH)
  - Diesel ($C_{12}H_{26}$)
- Thermodynamic Data
- Surface Chemistry
- Surface Kinematics

2.2.3 Spray Model

Different spray models for spray atomization and droplet breakup of solid cone sprays are used in ANSYS FORTE which are as following:

- KH Droplet Break Up Model

The Kelvin-Helmholtz (KH) model [33] is based on linear stability analysis of a liquid jet which is used to model the jet's primary breakup region.

- RT Droplet Break Up Model

Beyond the breakup length from the nozzle exit, the Rayleigh-Taylor (RT) model [33] is applied together with the KH model to predict the secondary breakup of spray droplets.

- Gas-jet Vaporization Model

In ANSYS Forte, the unsteady gas jet model [34] is useful to remove the mesh-size dependency for the liquid droplet-ambient gas coupling. It is based on unsteady gas-jet theory, in which the axial droplet-gas relative velocity is modeled without use of discretization on the CFD mesh.

- Radius of Influence Droplet Collision Model

ROI collision model [35] is used in ANSYS Forte to remove both time-step dependency and mesh-size dependency for the collision method of the droplet. In the ROI method, one particle can collide with another only if this particle exists in within the radius of influence of the other particle.

- **Solid Injector**
  - Injection Type
  - Parcel Specification
  - Inflow Droplet Temperature
  - Spray Initialization
  - Droplet Size Distribution
- **Nozzle**
  - Nozzle Location
  - Spray Direction
  - Nozzle Diameter

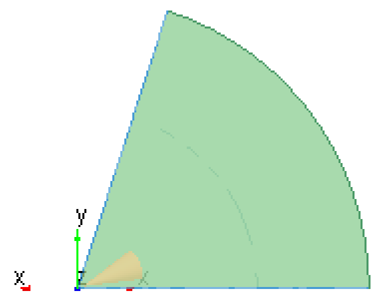

Fig 2-3: Spray Nozzle

- **Injection**
  - Injection Type
    - Pulsed
    - Continuous
  - Timing (Crank Angle)
- **Fuel Properties**
  - Composition of fuel is shown in following figure 2-4.

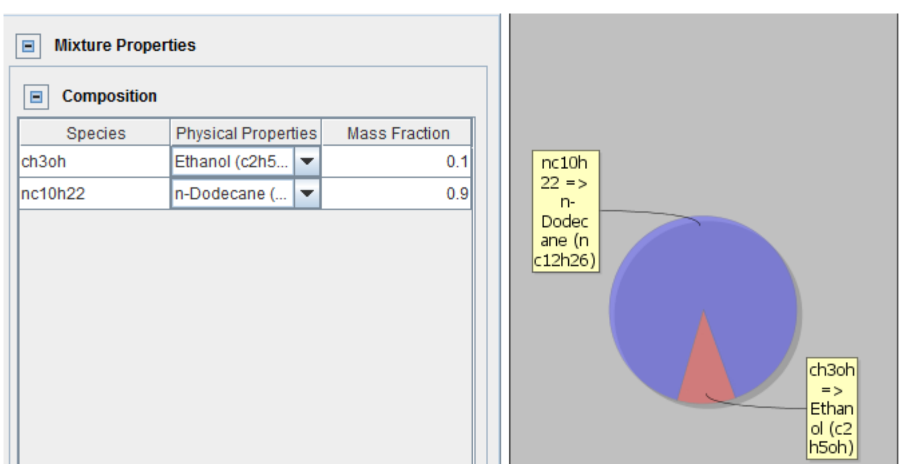

Fig 2-4: Composition of Fuel

2.2.4 Boundary Conditions

Following are the boundary conditions used in this model:

- Piston Temperature
- Head and Liner Temperature
- Sector Angle

2.2.5 Initial Conditions

Initial conditions for simulation model are given below:

- Composition of Gas Mixture

Species	**Fraction %**
N_2	78.09
O_2	20.95
H_2O	0.9
CO_2	0.04
Ar	0.02

Table 2-2: Composition of Gas Mixture

- Temperature of Gas Mixture
- Pressure of Gas Mixture

2.2.6 Simulation Controls

Different simulation controls are defined and used in this model.

- Initial Crank Angle
- Final Crank Angle
- Engine Speed (rpm)
- Cycle Type

2.2.7 Output Controls

Output controls like output units and species are defined.

- Output Species
- Output Units

- Time (Sec)
- Crank Angle Degrees (CAD)

2.3 Validation of Dual Fuel Model

The benchmarking technique which is used nowadays to validate the combustion model is accumulated chemical heat release (ACHR). It is a primary indicator that can be used to evaluate the status of combustion and fuel burning in the engine. Accumulated chemical heat release is the product of quantity of fuel and the lower heating value of fuel used.

2.3.1 Theoretical ACHR (formula) vs Numerical ACHR

Theoretical and numerical value of accumulated chemical heat release are compared for the pure diesel as well as ethanol diesel blend i.e. D90E10 (Diesel 90% and Ethanol 10%).

2.3.1.1 Pure Diesel

Mass of Fuel= m_f = 25 (mg)

Lower Heating Value of Diesel Fuel= LHV_f = 44.38 (MJ/Kg)

Theoretical ACHR = 25 (mg) x 44.38 (MJ/kg)

Theoretical ACHR = 1109.50 (J)

Numerically calculated value of ACHR = 1109.64 (J)

Percentage Error = 0.012%

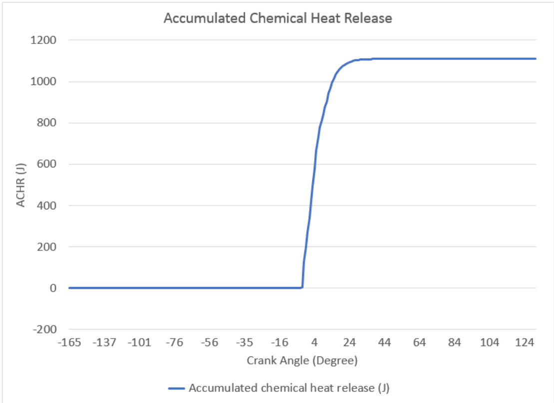

Fig 2-5: Numerical ACHR for Pure Diesel

2.3.1.2 D90E10

Mass of Fuel= m_f = 25 (mg)

Lower Heating Value of Diesel Fuel= LHV_f = 42.69 (MJ/Kg)

Theoretical ACHR= 25 (mg) x 42.69 (MJ/kg)

Theoretical ACHR= 1067.25 (J)

Numerically calculated value of ACHR= 1056.74 (J)

Percentage Error= 0.99%

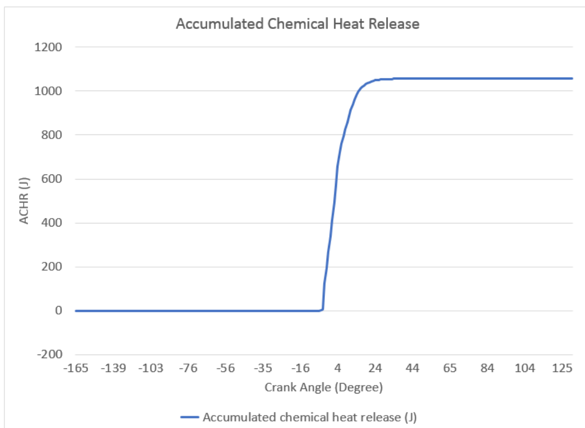

Fig 2-6: Numerical ACHR for D90E10

2.3.2 Numerical ACHR vs Heat Transfer & Work Done

Another technique which is used to validate the combustion model is the summation of accumulated wall heat transfer and work done which is equivalent to the accumulated chemical heat release.

2.3.2.1 Pure Diesel

ACHR = 1109.64 (J)

Work Done = 655.51 (J)

Wall Heat Transfer = 329.39 (J)

ACHR = Work Done + Wall Heat Transfer

ACHR = 984.90 (J)

Percentage Error = 11.2%

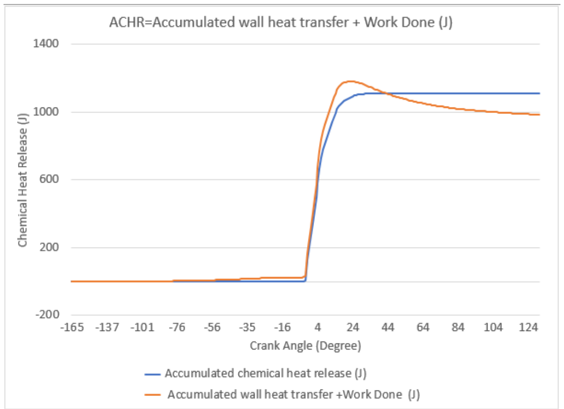

Fig 2-7: ACHR Comparison for Pure Diesel

2.3.2.2 D90E10

ACHR =1056.73 (J)

Work Done =595.27 (J)

Wall Heat Transfer =322.97 (J)

ACHR =Work Done + Wall Heat Transfer

ACHR =918.25 (J)

Percentage Error =13.1%

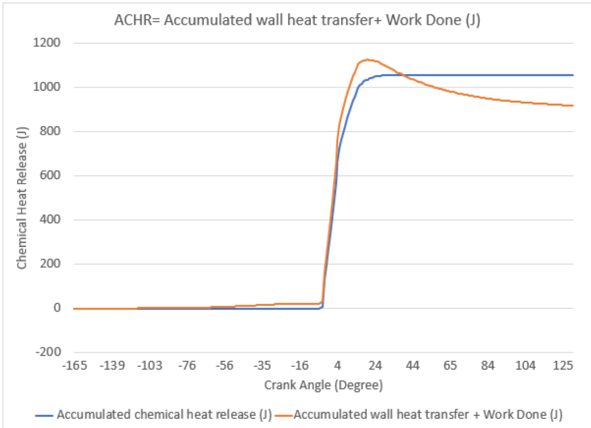

Fig 2-8: ACHR Comparison for D90E10

CHAPTER 3: FUEL BLENDS

3.1 Diesel-Ethanol Blends

Nomenclature for diesel ethanol blends is as following.

Blend	Diesel %	Ethanol %
D100E0	100	0
D95E05	95	05
D90E10	90	10
D85E15	85	15
D80E20	80	20

Table 3-1: Nomenclature for Ethanol Diesel Blends

3.2 Effect of Blends

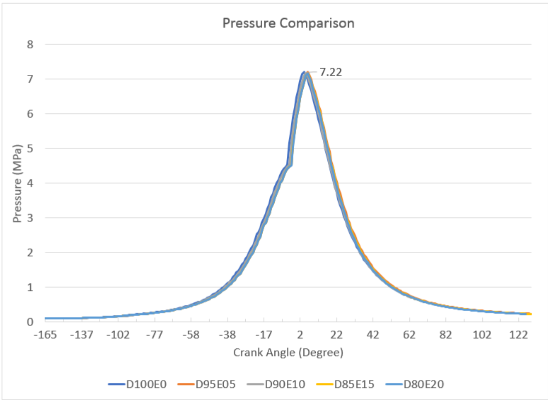

Fig 3-1: Effect of Blends on Pressure

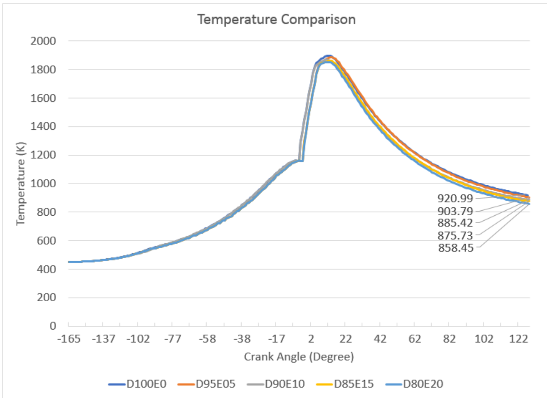

Fig 3-2: Effect of Blends on Temperature

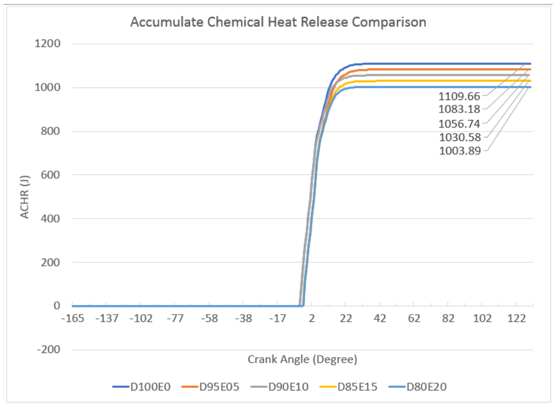

Fig 3-3: Effect of Blends on ACHR

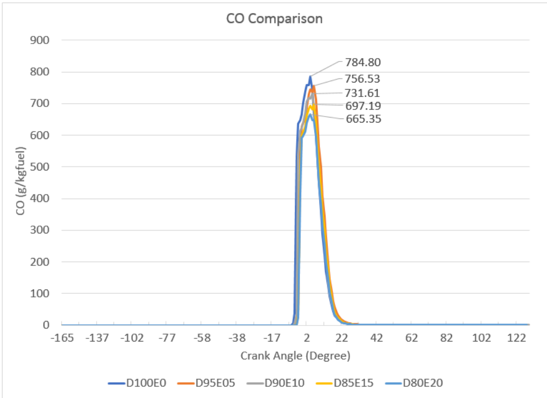

Fig 3-4: Effect of Blends on CO

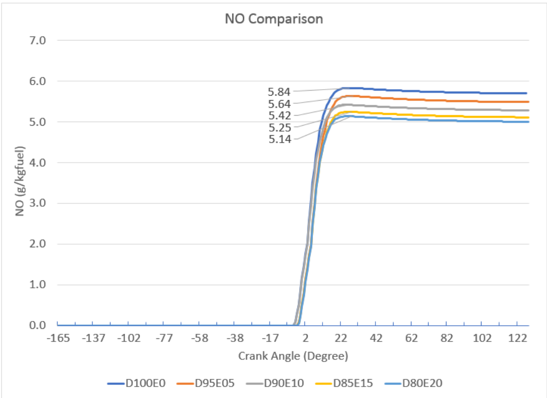

Fig 3-5: Effect of Blends on NO

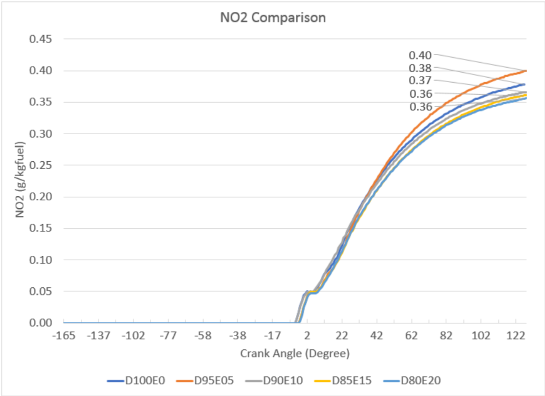

Fig 3-6: Effect of Blends on NO_2

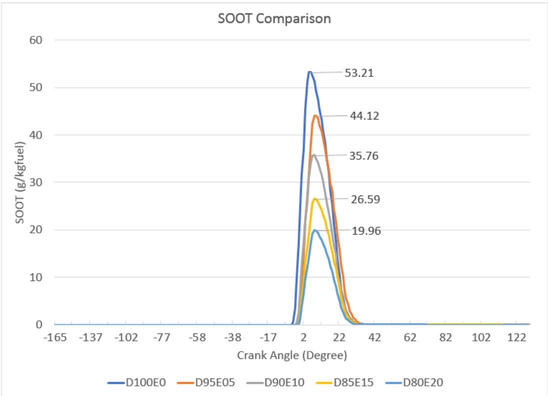

Fig 3-7: Effect of Blends on SOOT

3.2.1 Blends Analysis

Emissions are reduced to greater extent whenever the percentage of biofuels in the blends is increased. Reduction of carbon monoxides in D80E20 is almost 15% whereas decrease in nitrogen oxides like nitric oxide and nitrogen dioxide is almost 11.93% and 5.8% respectively when compared to pure diesel. A huge amount of SOOT reduction has been seen in D80E20 which is 62.92% approximately which is mainly because of the presence of oxygen molecules in the ethanol.

BLEND	**CO**		**NO**		**NO_2**		**SOOT**	
Ratio	**g/Kg.f**	**%**	**g/Kg.f**	**%**	**g/Kg.f**	**%**	**g/Kg.f**	**%**
D100E0	784.80	-	5.84	-	0.379	-	53.83	-
D95E05	756.53	3.60↓	5.64	3.41↓	0.400	5.54↑	44.12	18.04↓
D90E10	731.60	6.78↓	5.42	7.13↓	0.366	3.43↓	35.77	33.55↓
D85E15	697.19	11.16↓	5.25	10.06↓	0.363	4.22↓	26.59	50.60↓
D80E20	665.36	15.22↓	5.14	11.93↓	0.357	5.8↓	19.96	62.92↓
↑ %Increase ↓ %Decrease								

Table 3-2: Blends Analysis

CHAPTER 4: PARAMETRIC STUDY

4.1 Parameters

Following parameters are considered under the parametric study.

- Start of Injection (SOI)
- Duration of Injection (DOI)
- Inflow Droplet Temperature (IDT)
- Initial Intake Air Temperature (IAT)

4.2 Start of Injection

Usually fuel injection takes place near, at or after top dead center. Effects on cylinder pressure, temperature and exhaust emissions like CO2, NO, NO_2 and SOOT are considered. Different cases are studied under start of injection which are as following:

1. SOI -15° BTDC
2. SOI -10° BTDC
3. SOI -5° BTDC
4. SOI 0° TDC
5. SOI 5° ATDC

4.2.1 Effect of Start of Injection

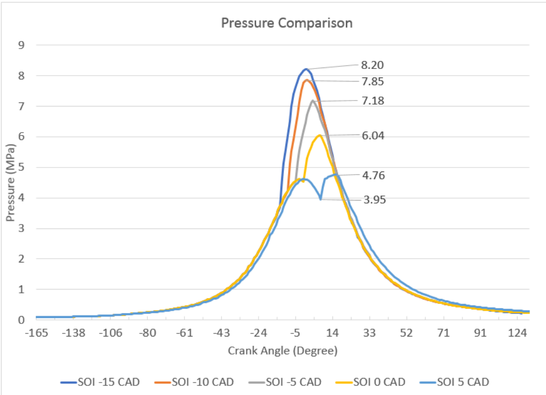

Fig 4-1: SOI Pressure Comparison

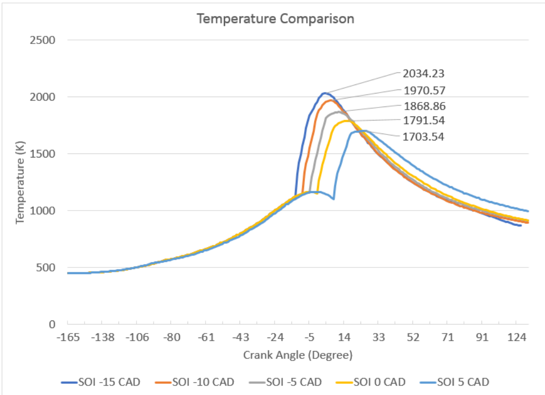

Fig 4-2: SOI Temperature Comparison

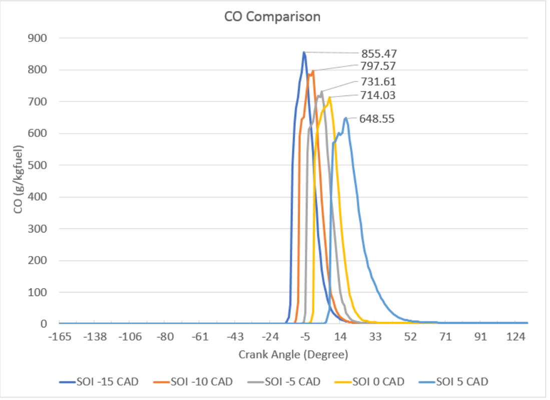

Fig 4-3: SOI CO Comparison

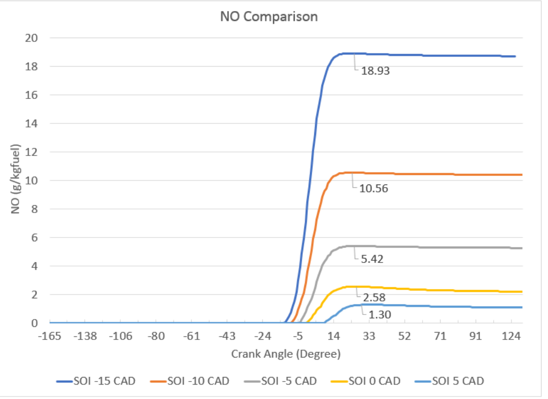

Fig 4-4: SOI NO Comparison

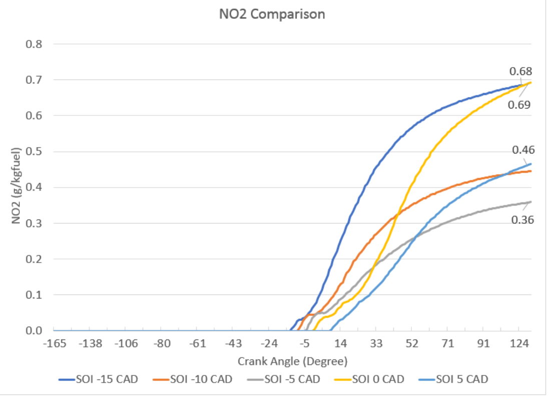

Fig 4-5: SOI NO_2 Comparison

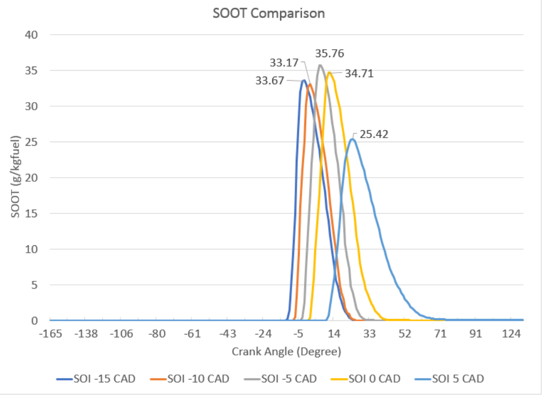

Fig 4-6: SOI SOOT Comparison

4.2.2 Start of Injection Analysis

Early injection results in more carbon monoxide i.e. 9.02% for -10 CAD BTDC and 16.93% for -15 CAD BTDC. Quantity of carbon monoxide is reduced by 2.40% for 0 CAD TDC and 11.35% for 5 CAD ATDC. Start of injection effects on nitric oxide in such a way that it is increased by 94.94% for -10 CAD BTDC and 249.38% for -15 CAD BTDC whereas it is decreased by 52.41% & 75.81% for 0 & 5 CAD ATDC respectively. Nitrogen dioxide is increased whether fuel is injected earlier or late so -5 CAD BTDC is an optimum injection point where NO_2 emissions are 0.366 gram per Kg of fuel. Effects of start of injection on SOOT emissions are minimal. This is because of premixing ratios of biofuel as well as homogenous mixtures BTDC due to the presence of ethyl alcohol in the diesel engine.

SOI	**CO**		**NO**		**NO_2**		**SOOT**	
CAD	**g/Kg.f**	**%**	**g/Kg.f**	**%**	**g/Kg.f**	**%**	**g/Kg.f**	**%**
-15	855.47	16.93↑	18.93	249.38↑	0.685	87.16↑	33.67	5.85↓
-10	797.57	9.02↑	10.56	94.94↑	0.451	23.22↑	33.17	7.25↓
-5	731.61	-	5.42	-	0.366	-	35.77	-
0	714.03	2.40↓	2.58	52.41↓	0.693	89.34↑	34.73	2.90↓
5	648.55	11.35↓	1.31	75.81↓	0.485	32.51↑	25.42	28.92↓
↑ %Increase ↓ %Decrease								

Table 4-1: Start of Injection Analysis

4.3 Duration of Injection

Different cases for duration of fuel injection are considered here for which parametric studies are performed. Plots are given below in which cylinder pressure, cylinder temperature, mass flow rate and exhaust emissions are compared. Injection duration has been increased and cases scrutinized are as following:

1. DOI 10 CAD
2. DOI 12 CAD
3. DOI 15 CAD
4. DOI 17 CAD

4.3.1 Effect of Duration of Injection

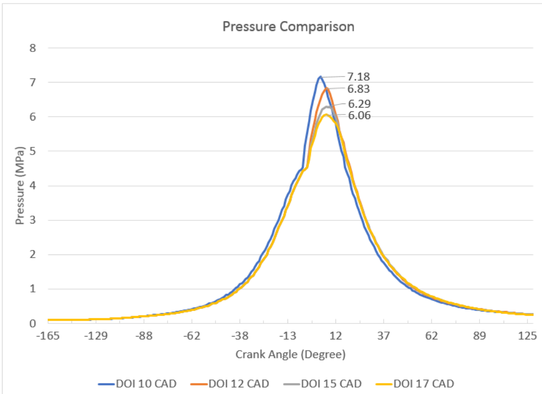

Fig 4-7: DOI Pressure Comparison

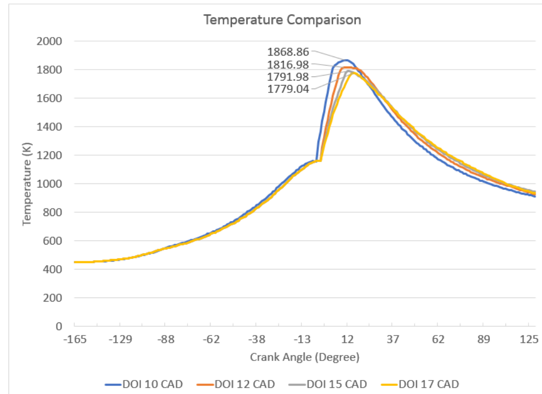

Fig 4-8: DOI Temperature Comparison

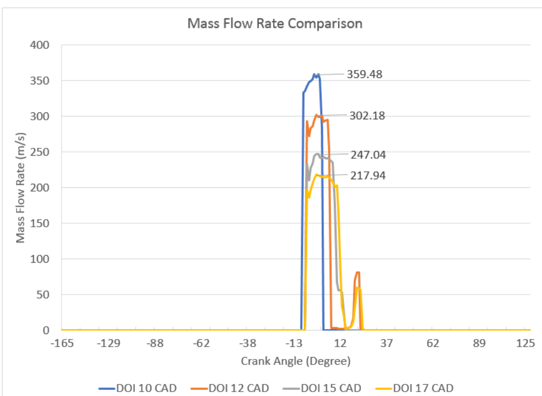

Fig 4-9: DOI Mass Flow Rate Comparison

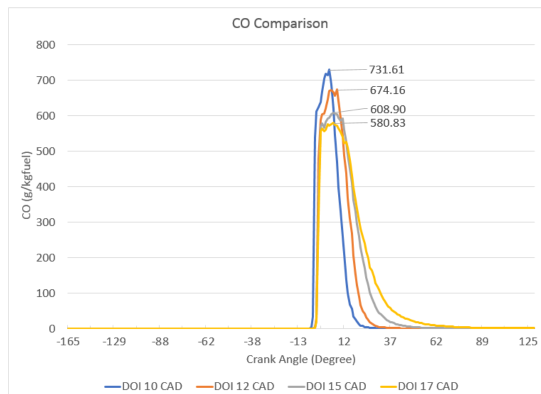

Fig 4-10: DOI CO Comparison

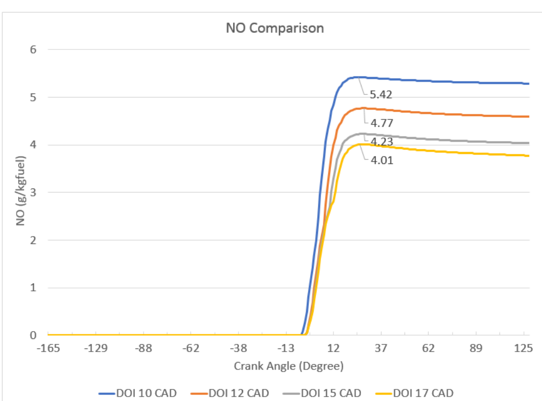

Fig 4-11: DOI NO Comparison

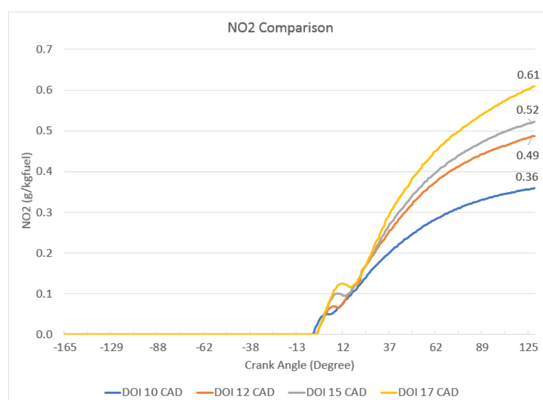

Fig 4-12: DOI NO_2 Comparison

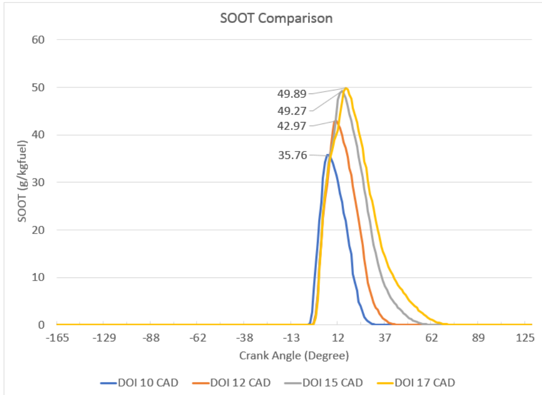

Fig 4-13: DOI SOOT Comparison

4.3.2 Duration of Injection Analysis

The increase in duration of injection results in lesser carbon monoxide i.e. 7.85%, 16.77%, and 20.6% for 12, 15 and 17 CAD respectively. Nitric oxides emissions are also decreased by increasing the duration of injection. Percentage decrease for 12, 15 and 17 CAD is 11.99% 21.91% and 20.61% respectively. When duration of injection is increased, flow rate is increased which causes rise in fuel pressure. More nitrogen dioxide is produced which is 36.07% for 12 CAD, 45.08% for 15 CAD and 66.39% for 17 CAD. Similarly, SOOT production is also increased by the increase in duration of injection which is 20.13%, 38.75% and 39.51% for 12,15 and 17 CAD respectively.

DOI	**CO**		**NO**		**NO_2**		**SOOT**	
CAD	**g/Kg.f**	**%**	**g/Kg.f**	**%**	**g/Kg.f**	**%**	**g/Kg.f**	**%**
10	731.61	-	5.42	-	0.366	-	35.77	-
12	674.16	7.85↓	4.77	11.99↓	0.498	36.07↑	42.97	20.13↑
15	608.90	16.77↓	4.23	21.92↓	0.531	45.08↑	49.63	38.75↑
17	580.83	20.61↓	4.02	25.91↓	0.609	66.39↑	49.89	39.51↑
↑ %Increase				↓ %Decrease				

Table 4-2: Duration of Injection Analysis

4.4 Inflow Droplet Temperature

Inflow droplet temperature is decreased from 320K to 300K to perform parametric study to analyze the effects on pressure, temperature as well as exhaust emissions like carbon monoxide, nitrogen oxides and SOOT etc. Following cases are considered here.

1. $T_1 = 320K$
2. $T_2 = 315K$
3. $T_3 = 310K$
4. $T_4 = 305K$
5. $T_5 = 300K$

4.4.1 Effect of Inflow Droplet Temperature

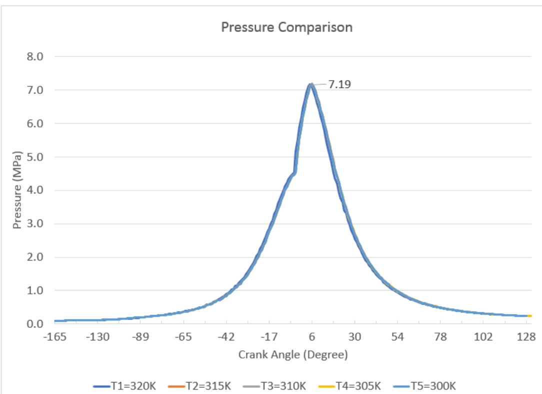

Fig 4-14: IDT Pressure Comparison

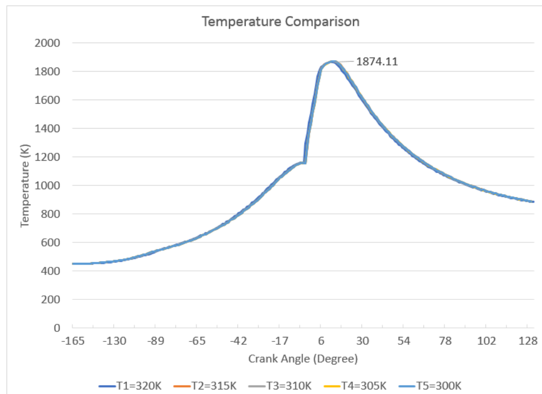

Fig 4-15: IDT Temperature Comparison

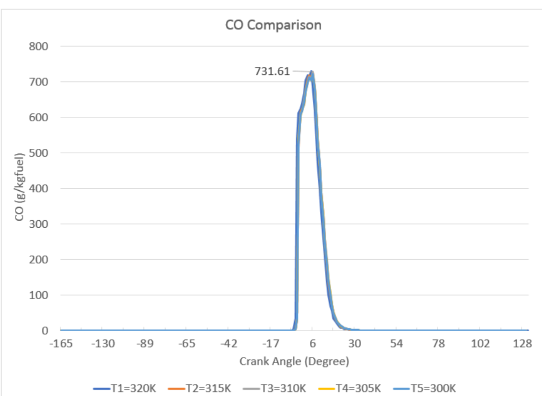

Fig 4-16: IDT CO Comparison

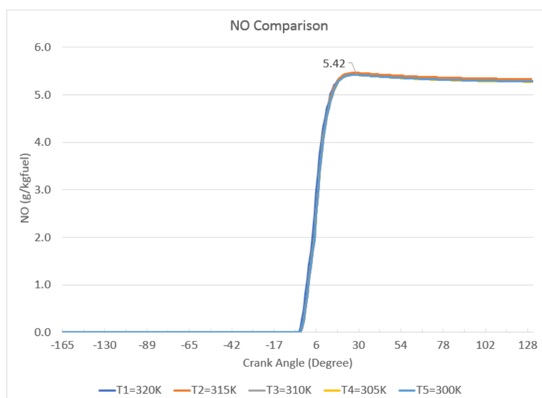

Fig 4-17: IDT NO Comparison

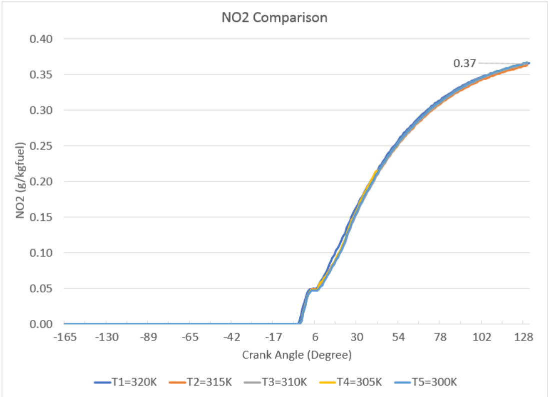

Fig 4-18: IDT NO_2 Comparison

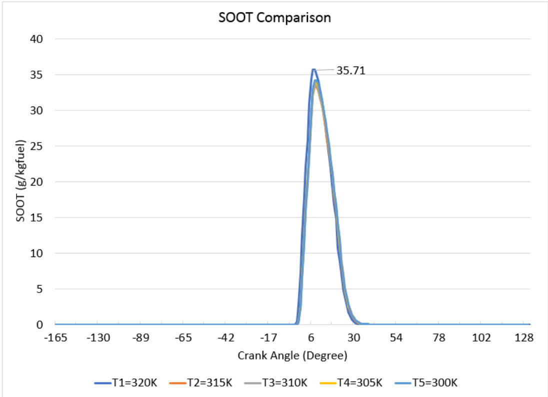

Fig 4-19: IDT SOOT Comparison

4.4.2 Inflow Droplet Temperature Analysis

A decrease in inflow fuel droplet temperature has negligible effects on carbon monoxide CO, nitric oxide NO and nitrogen dioxide NO_2 and SOOT emissions because sensible heat i.e. no phase change is considered here. Carbon monoxide is reduced by 1.47% if fuel droplet temperature is decreased by 15K. Nitric oxide is increased by 0.78% only for 315K. Quantity of nitrogen dioxide emissions are 0.366 and 0.371 gram per Kg of fuel for 320K and 305K respectively. Amount of SOOT emissions are 35.77 gram per Kg of fuel for 320K.

Fuel Temp	**CO**		**NO**		**NO_2**		**SOOT**	
K	**g/Kg.f**	**%**	**g/Kg.f**	**%**	**g/Kg.f**	**%**	**g/Kg.f**	**%**
300	723.25	1.14↓	5.419	0.00	0.368	0.55↑	34.28	4.15↓
305	720.87	1.47↓	5.418	0.02↓	0.371	1.71↑	34.01	4.91↓
310	728.24	0.46↓	5.416	0.06↓	0.367	0.27↑	33.61	6.02↓
315	725.86	0.79↓	5.461	0.78↑	0.364	0.55↓	33.42	6.55↓
320	731.61	-	5.419	-	0.366	-	35.77	-

↑ %Increase	↓ %Decrease

Table 4-3: Inflow Droplet Temperature Analysis

4.5 Initial Intake Air Temperature

Initial intake air temperature of 450K is usually used in ANSYS FORTE but it is increased from 400K to 500K to perform parametric study to analyze the effects on pressure, temperature as well as exhaust emissions like carbon monoxide CO, nitrogen oxides NO and NO_2 and SOOT etc. Following cases are considered here.

1. T_1 = 400K
2. T_2 = 420K
3. T_3 = 450K
4. T_4 = 470K
5. T_5 = 480K
6. T_6 = 500K

4.5.1 Effect of Initial Intake Air Temperature

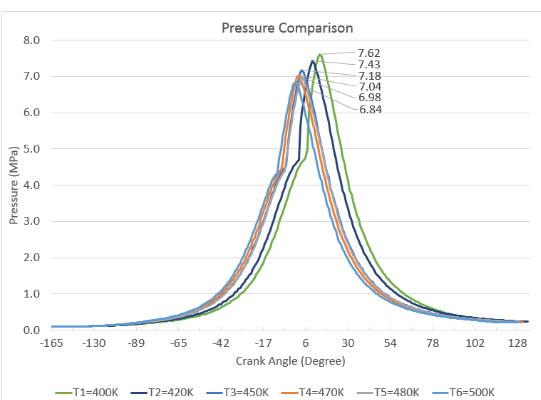

Fig 4-20: IAT Pressure Comparison

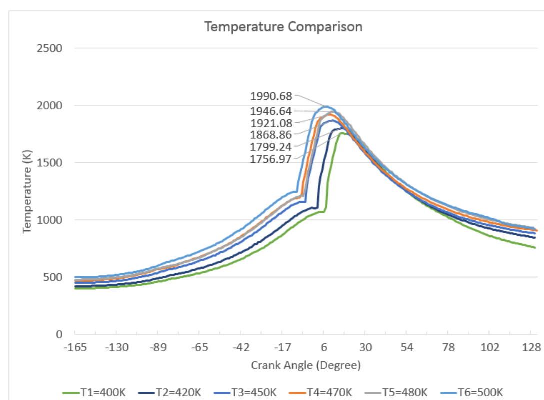

Fig 4-21: IAT Temperature Comparison

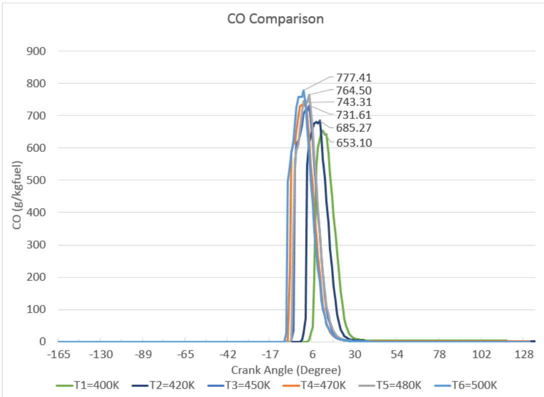

Fig 4-22: IAT CO Comparison

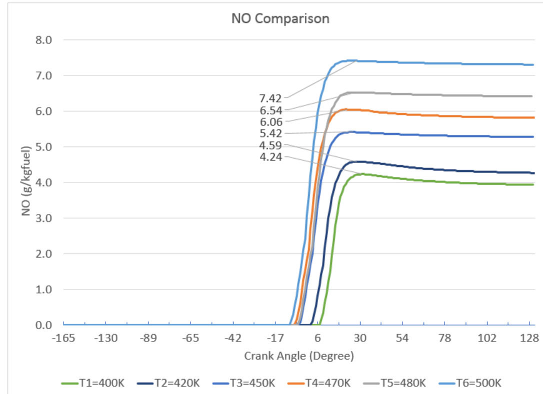

Fig 4-23: IAT NO Comparison

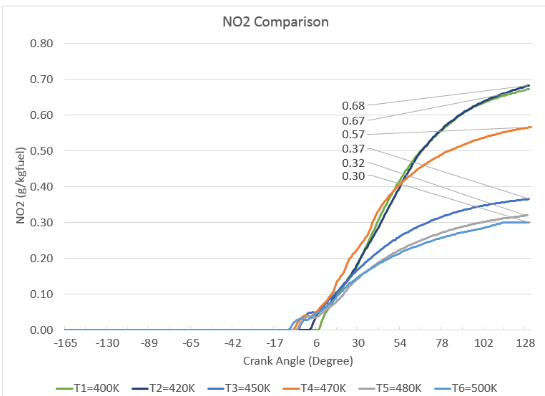

Fig 4-24: IAT NO_2 Comparison

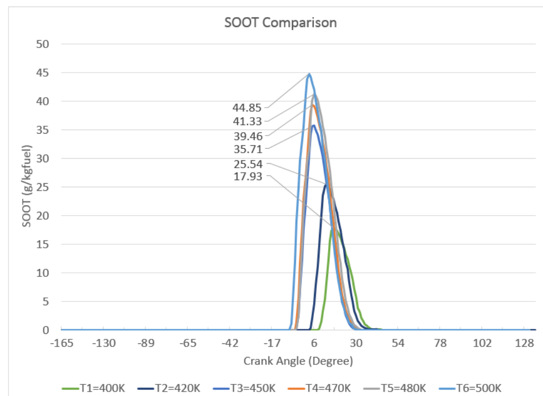

Fig 4-25: IAT SOOT Comparison

4.5.2 Initial Intake Air Temperature Analysis

The increase in intake gas mixture i.e. air temperature results in more nitric oxide, carbon monoxide and SOOT production because cold air is less dense and contains higher concentration. Increased oxygen in combustion chamber leads to complete combustion and oxidation of carbon monoxide and hydrocarbon emissions. Whereas hot air reduces oxygen quantity which causes incomplete combustion resulting more emissions.

Gas Temp	CO		NO		NO_2		SOOT	
K	**g/Kg.f**	**%**	**g/Kg.f**	**%**	**g/Kg.f**	**%**	**g/Kg.f**	**%**
400	653.10	10.73↓	4.239	21.78↓	0.658	79.78↑	17.93	49.87↓
420	685.27	6.33↓	4.589	15.32↓	0.689	88.20↑	25.54	28.58↓
450	731.61	-	5.419	-	0.366	-	35.77	-
470	743.31	1.60↑	6.057	11.77↑	0.564	54.10↑	39.46	10.33↑
480	764.50	4.50↑	6.536	20.61↑	0.600	63.93↑	41.33	15.57↑
500	777.41	6.26↑	7.420	36.93↑	0.300	18.03↓	44.85	25.39↑
↑ %Increase ↓ %Decrease								

Table 4-4: Initial Intake Air Temperature Analysis

CHAPTER 5: CONCLUSION AND FUTURE WORK

5.1 Conclusion

Emissions are reduced to greater extent whenever the percentage of biofuels in the blends is increased. Reduction of carbon monoxides in D80E20 is almost 15% whereas decrease in nitrogen oxides like nitric oxide and nitrogen dioxide is almost 11.93% and 5.8% respectively when compared to pure diesel. A huge amount of SOOT reduction has been seen in D80E20 which is 62.92% approximately which is mainly because of the presence of oxygen molecules in the ethanol.

Early injection results in more carbon monoxide and more nitric oxide and vice versa, whereas its effect on SOOT emissions is minimal. This is because of premixing ratios as well as homogenous mixtures BTDC. The increase in duration of injection results in lesser carbon monoxide and nitric oxide where more nitrogen dioxide as well as SOOT production. This is due to change of flow rate as well as fuel pressure. An increase in inflow droplet temperature has negligible effect on CO, NOx and SOOT emissions because sensible heat (no phase change) is considered here. The increase in intake gas mixture i.e. air temperature results in more nitric oxide, carbon monoxide and SOOT production because cold air is less dense and contains higher concentration. Increased oxygen in combustion chamber leads to complete combustion and oxidation of carbon monoxide and hydrocarbon emissions. Whereas hot air reduces oxygen quantity which causes incomplete combustion resulting more emissions.

5.2 Future Work

- To study the effect of Alcohols (Propanol, Butanol etc.) and other biofuels such as vegetable oils etc.
- Ignition delay using numerical methods.
- To simultaneously incorporate the Tertiary Fuel Blends and evaluate the chemical heat release and nature of emissions.

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