Numerical Analysis of Exhaust Gas Recirculation and Water Injection Process in Diesel Engine

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Declaration

I certify that this research work titled "Numerical Analysis of Exhaust Gas Recirculation and Water Injection Process in Diesel Engine*"* 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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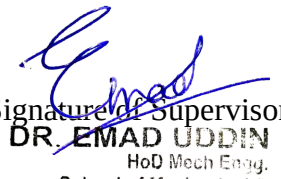

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Abstract

Combustion Process in internal combustion engine consists of various steps. Numerical solution and simulation of the internal combustion engine provide a useful insight into the details of sub-processes of the combustion. Emissions such as CO, NO, and NO2 have a harmful impact on the environment as well as human health. The processes of Exhaust Gas Recirculation and Water Injection reduce the quantity of emissions produced in internal combustion engines. In this study, the combustion process in the diesel engine has been simulated. The engine used in the simulations was Peugeot Citroën Dw-10b. The result of the experimental data was compared with the simulation data, and it was found that the numerical solution obtained is very close to the experimental data. Value of Accumulated Chemical Heat Release (ACHR) obtained from numerical solution was also compared with the analytical value, and both values were very close to each other. Ansys Forte 2019 was used for the simulation of exhaust gas recirculation and water injection processes. The validation of the numerical solution was done for both EGR and WI processes. A parametric study was also performed to evaluate the effect of operating parameters on emissions. Parameters such as intake air temperature, fuel droplet temperature, the start of injection, and duration of injection were varied and the quantities of the nitrous oxide emissions, carbon monoxide emissions, and soot production were studied. The study is useful in understanding the effects of various input and operating parameters of the diesel engine on emissions.

Key Words: *Exhaust Gas Recirculation, Water Injection, ACHR, Numerical Simulation*

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CHAPTER 1: INTRODUCTION

Diesel engines are highly efficient, durable, and have low operating cost. Diesel engines are more preferable in the category of internal combustion engine in European region due to low fuel consumption and higher values of performance parameters. These engines normally have high torque and power output. The direct injection diesel engines have mainly higher efficiencies due to better fuel conversion efficiencies. However, these types of engines are criticized due to the exhaust emissions. The exhaust emissions such as NOx (Nitrogen Oxides), CO (Carbon Monoxide), and Particulate Matter (PM). These are tough European standards and regulations related to emissions of diesel engines. These emissions have a harmful effect on the environment, and they contribute a lot towards the environmental pollution. Moreover, these emissions seriously affect the human health. The basic objective of diesel engine manufacturers and designers was to decrease the fuel consumption [1]. The goal of reducing the fuel consumption was also the aim of the transporters keeping in view the competition [1]. The fuel consumption is directly related to the emissions, particularly carbon monoxide[1]. The overall objective of reduction of fuel consumption was linked to the reduction of carbon monoxide emissions, while the general intention was to reduce the emissions and fuel consumption as well. Reduction of emissions was also necessary in order to comply with the regulations.

In order to comply with emission standards, the engine designers test various fuel spray methods, employ the techniques of water injection (WI), exhaust gas recirculation (EGR), and devise different strategies to ensure complete combustion process. The operation parameters of the engine such as, start of injection (SOI), duration of injection (DOI), and other parameters that are, intake air temperature, and fuel droplet temperature have a significant impact on the quantities of the exhaust gas emissions. Normally experimental method is employed to perform parametric study using engines can be obtained. However, the method is expensive, requires the installation of sensors, and integration of electronic hardware with the software. Moreover, by using experimental method, it is almost impossible to study the effect of variations of various operating variables in a single iteration. The parametric study in case of experimentation requires substantial changes in the hardware. Compared to experimental method, numerical method of solving internal combustion engine provides accurate solution and gives useful insight about the local phenomena.

Internal combustion engine processes are primarily fluidic in nature and also consists of different physics such as thermodynamics, chemical kinetics, and dynamics of spray as well. In order to effectively study the sub-processes in detail, an approach of subdividing the complete process into various sub parts should be adopted. This particular method is useful in defining and identifying the equations as per phenomena, and finally coupling all the equations to solve the complete problem to find a solution. There are various steps for setting internal combustion engine problems numerically. Traditionally, internal combustion engine simulation can be regarded as computational fluid dynamics (CFD) problem. In order to reduce the fuel consumption and also keeping the emissions of exhaust gases low, detailed understanding and knowledge of pre-combustion processes, such gas mixture, temperature of inlet gas mixture, and other operating parameters is required as spray, formulation of droplets, spray length, spray characteristics, composition of. Setting up the internal combustion engine problem numerically step by step is a better approach because the designer or user has got a more control over the defining variables. Similarly, visualization techniques in the current numerical simulation packages is very much elaborative. The display of the variables during pre-combustion and post engine combustion phases provides a better understanding of the process and is helpful in in heat release rate, pressure distribution within cylinder, and co-relation of these variables will provide an insight about the processes and burning of fuel, in this way designers and manufacturers can co-relate the operating variables, fuel, chemical understanding the trend in general. The soot production, emission of exhaust gases, variations mechanism, fluidic parameters, and engine performance. Engine designers require more fast methods for designing so that the design process can be accelerated overall [2]. Moreover the mathematical models of internal combustion engine gives discrete values, the main advantage of numerical methods is visualization[2]. There are two different ways of performing numerical simulations. The first method is based on writing a computer code by the user in any language and the equations are also incorporated in the computer program, the method can be applied using many software packages such as FORTRAN, MATLAB etc. The second method is based on using the commercial software packages available for simulations such as ANSYS, COMSOL Multi-physics. There are advantages and disadvantages associated with both methods. The defining of the equations in the computer program allows the user or designer to control and define the variables in a better way. Normally the designers write and use their own codes for engine design and simulations, however, the process is time taking and requires very

accurate definition of boundary conditions, moreover the user has to define the graphical conditions and GUI as well for the self-written codes. The usage of commercial software package is less time taking, and the GUI is available, moreover, the enhanced visualization features allow the user to analyze the variations in variables in the cylinder during combustion cycle, however, the limitation is the limited liberty to define the operating conditions and variables. Moreover, the tweaking of equations is not fully possible in the commercial software packages. The usage of commercial software package for simulation of internal combustion engine problems is a smart approach to accurately model the engine processes in a very short time and get the accurate results for inferring the conclusions. The approach that is normally adopted in simulating the internal combustion engine problems is that the experimental conditions are first duplicated and the results are verified, this is done for the benchmarking of method and approach, the benchmarking ensures that the approach of simulations, numerical method, and boundary conditions are correct. On the basis of benchmarking, further variations in the operating conditions and input parameters is done and the trend is studied, the trend is then related to the possible logical and scientific reasoning. The similar approach has been adopted in this case

1.1 Diesel Engine and Diesel Cycle

For effectively simulating and modeling the combustion in diesel engines, it is important to understand the principle of diesel engines, and its working in detail. Diesel engines are compression ignition engines, the mixing of air and fuel takes place in the engine cylinder and the gas mixture (air) is compressed within the chamber [3]. This results in the generation of very high temperatures that are high enough to ignite the diesel upon injection[3]. The diesel engines then utilize the heat to emit and release the chemical energy from the fuel and it is then converted into force that is mechanical in nature [3]. The diesel engine in the category of internal combustion engines produces greatest overall efficiency, even more than 50 percent in case of huge and the slow operating[3]. The pre-ignition characteristics of diesel engine combined with other characteristics such as low fuel consumption, low emissions, and less running noise have resulted in increasing the significance of diesel engine[3]. The diesel engines can be further classified as two stroke and four stroke diesel engines. Diesel engines have one or more cylinders, the combustion of air fuel mixture results in the upward and downward motion of the piston, due to the

movement of piston it is called as reciprocating one[3]. Linear motion of the piston which is reciprocating in nature is converted into rotational movement with the connecting rod on the part of a shaft called crank shaft[3]. The flywheel is connected at the end of crankshaft that ensures the smooth rotation of the shaft and continuous rotation and helps in the reduction of the uneven rotation that is caused by the periodicity in the combustion in the different cylinders[3]. The engine speed is referred to as the rotational speed of crank shaft[3]. Figure 1 shows the schematic of four cylinders with different parts labelled[3].

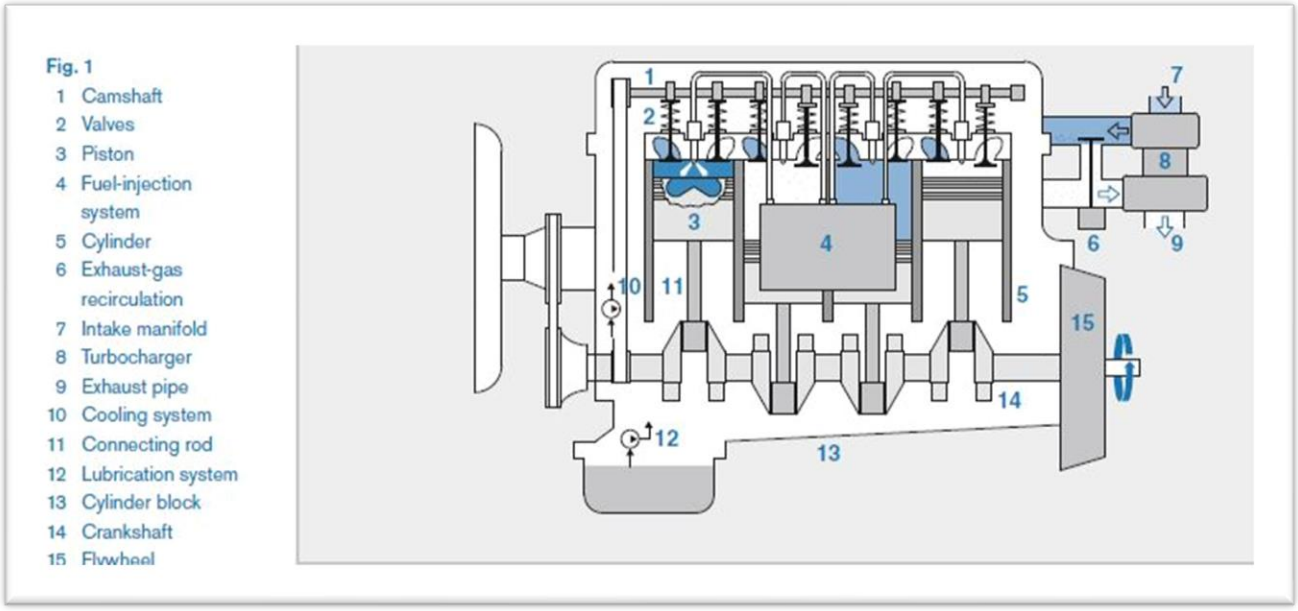

Figure 1 Schematic of the four cylinder diesel engine with different parts labelled

Current study is related to four stroke diesel engine cycle. This section will also provide the short description of four stroke diesel engine cycle. In four stroke diesel engines, the inlet and exhaust valves control the incoming intake air and expelling of exhaust gases. The intake of air and expulsion of exhaust gases are done via intake and exhaust ports respectively. The intake and exhaust ports may contain one or two valves.

1.2 4 Stroke Diesel Engine

- The first step that takes place in the four stroke diesel engine cycle is the intake or induction stroke. At the start of the intake stroke, the piston is at top dead center, the downward movement of the piston increases the volume of the center thus

making room and capacity. At this moment inlet valve is opened and air is allowed to move in the cylinder. The cylinder capacity of containing the air is maximum when piston reaches the bottom dead center.

- The second step is the compression stroke. During compression stroke, inlet as well as the exhaust valves are closed. Piston moves in upward direction and compresses the gas that is present in the cylinder. Volume is significantly reduced and the temperature of the air rises up. The rise of the temperature is dependent upon the compression ratio of engine. During compression stroke, temperature of the gas rises up to 900 degrees centigrade[3]. Just before the completion of compression stroke, fuel is injected at very high pressure. The fuel injection in the compressed hot air is the main core functionality of the diesel engines. Volume of the cylinder is minimum at the Top dead center (TDC). The air is hot enough that the diesel fuel is able to be ignited. Diesel engines are called compression ignition engines due to the ignition of fuel in the hot compressed gas.
- The third stoke is termed as ignition stroke. After the ignition delay in which the crank shaft moves a few degrees, the ignition stroke starts. The highly atomized droplets of the diesel that is easily combustible, the spontaneous burning of the diesel fuel takes place. The burning of the diesel takes place due to the high temperature of the compressed gas. Consequently the developed charge is heated more and this results in the rise of the cylinder pressure. The amount of the heat energy that is released depends upon the quantity (mass) of the fuel injected. High pressure in the cylinder provides a pushing force in downward direction. During the compression stroke, the chemical energy that is released as a result of combustion is converted into the kinetic energy, the piston's kinetic energy is converted into the torque by the drive system of crank shaft.
- Before the arrival of piston at bottom dead center, exhaust valve opens and results in expulsion of high pressure gases, upon the upward motion of piston towards the top dead center, the remaining exhaust gases are forced out of the cylinder via exhaust port.

When the exhaust stroke completes, two revolutions of the crankshaft are completed, and the four stroke cycle starts again with the intake stroke.

Figure 2 shows the complete four stroke cycle of diesel engine[3]. The parts of the cylinder have also been labelled. Position of the piston, as the cycle progresses is also shown in the figure[3]. The visual representation will help in understanding the details of cycle.

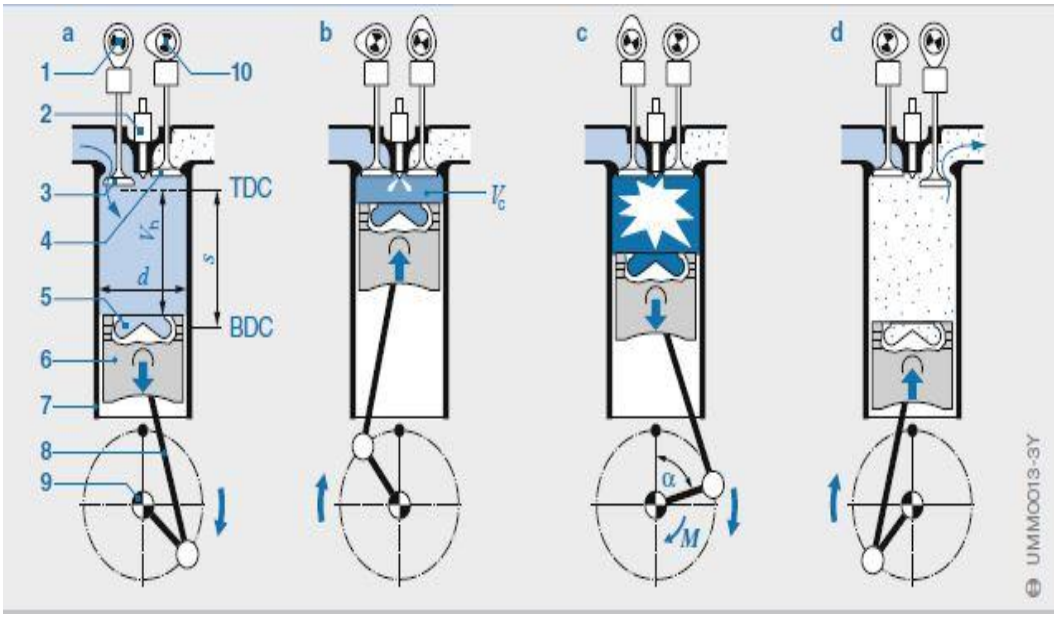

Figure 2 Operational stages of four stroke diesel engine with different parts labelled. The position of piston at various strokes have been shown

In the figure above the labels refer to following

α	Crankshaft angle of rotation
d	Bore
M	Turning force
s	*Piston* stroke
*V*c	Compression volume
*V*h	Swept volume
TDC	Top dead center
BDC	Bottom dead Center

a	Induction stroke
b	Compression stroke
c	Ignition stroke
d	Exhaust stroke
1	Inlet-valve camshaft
2	Fuel injector
3	Inlet valve
4	Exhaust valve
5	Combustion chamber

6	Piston
7	Cylinder wall
8	Connecting rod
9	Crankshaft
10	Exhaust-valve camshaft

1.3 Ideal Diesel Cycle

Rudolph Diesel invented the diesel cycle in 1893. The cycle is also called as constant pressure cycle, because heat addition is done at constant pressures. The ideal diesel cycle consists of four processes, these processes are two isentropic processes, a single constant pressure process, and a volume constant process. These four processes are as follows

- Isentropic Compression that is reversible adiabatic
- Heat addition at constant pressure
- Isentropic Expansion
- Heat rejection at constant volume

During isentropic compression, piston movement is from bottom dead center to top dead center, and isentropic compression of air takes place. During this stroke air is compressed, pressure rise is evident from P1 to P2 in figure 3, and consequently temperature increase from T1 to T2 and during this process the entropy remains same.

The second process is heat addition at constant volume process, during this process, the piston stops for a moment at top dead center, pressure during this process remains constant, and there is an increase in volume from V2 to V3, there is a rise in temperature from T2 to T3, and the entropy rises from S2 to S3

Third process is isentropic expansion, during this process, after the heat has been added in the system, expansion of the air takes place, in the isentropic manner, and the work is gained. The piston moves in downward direction and reaches at bottom dead center, there is a drop in pressure, increase in volume, and drop in temperature, however, the entropy remains constant.

The fourth process is the rejection of heat from the system at constant volume. During this process there is a slight rest of piston at bottom dead center, there is a decrease in pressure from P4 to P1, a temperature drop, and decrease in the entropy of the system, however, the volume remains constant. Figure 3 shows the Pressure volume plot and temperature entropy plot of ideal diesel cycle[4]

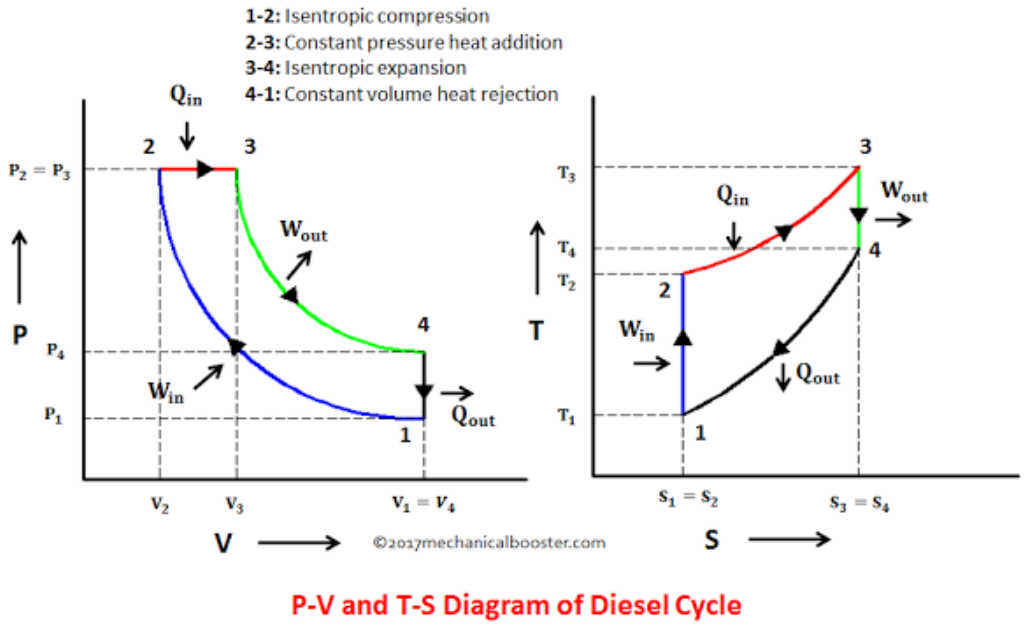

Figure 3. Pressure-Volume and Temperature Entropy plot of ideal diesel cycle (source: mechanical booster)

1.4 Exhaust Gas Recirculation

Exhaust gas recirculation is a process in which a portion of engine exhaust gases is recirculated back into the combustion chamber. This process can be done either internally by managing the timings of valves properly, or ether by the usage of piping. The exhaust gas that is recirculated in the chamber act as an inert gas, and it does not gets involve in the combustion reaction. For the naturally aspirated diesel engines the implementation of exhaust gas recirculation is comparatively simple due to reason that the exhaust pipe's back pressure is higher compared to intake air pressure, a path is thus established between intake manifold and exhaust manifolds and the flow is regulated with the help of throttling valve [5]. Figure 4 shows the simplified pictorial representation of exhaust gas recirculation[5].

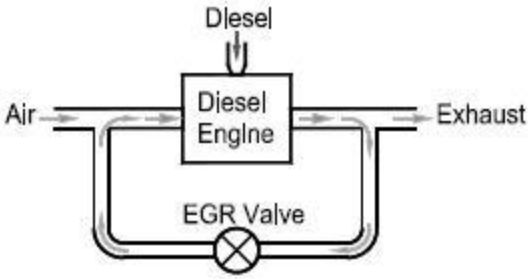

Figure 4 Exhaust gas recirculation system for diesel engines

Exhaust gas recirculation is also classified into further two types, these are hot exhaust gas recirculation and cooled exhaust gas recirculation. If the exhaust gases are directly introduced then the process is called hot EGR, and if cooling is applies with the help of a cooler for lowering the temperatures of the exhaust gas, then the process is called cooled EGR. Higher compression ratios of the diesel engines aid in achieving the high temperatures that are required for the auto-ignition of the fuel, as a result the higher values of the expansion ratios make the engines discharge less heat energy in the exhaust, consequently the temperature of the exhaust gases is not very high[5]. For the compensation of the non-homogenous aspect of the fuel scattering and distribution, an extra amount of oxygen is necessarily required for complete combustion reaction. However, in reality the condition is changed in reality due to the higher values of the flame temperature and the locally stoichiometric air fuel ratios are prevalent instead of lean fuel in the heterogeneous combustion conditions[5]. As a result the diesel engines produce large quantities of NO_x due to the higher value of flame temperatures in the conditions where oxygen and nitrogen are present in the abundant quantities[5].

Exhaust Gas recirculation is done to reduce the amount of exhaust gas emissions. Keeping in view the stoichiometric way of burning of fuel in diesel engines, the more efficient approach would be to reduce the ratio of specific heat capacity of the fluids for reduction of the flame temperatures[5]. With EGR, carbon dioxide is introduced in the intake manifold of the engine, it effectively increases the specific heat capacity[5]. EGR also helps in diluting the oxygen concentration of the working fluid. In this way the production of NO_x can be reduced significantly. The introduction of the exhaust gases is difficult in the modern diesel engines that are normally turbocharged, a positive pressure difference is usually achievable between the outlet of turbine and

inlet of the compressor. Figure 5 shows the low pressure loop EGR circuit diagram with components labelled[5].

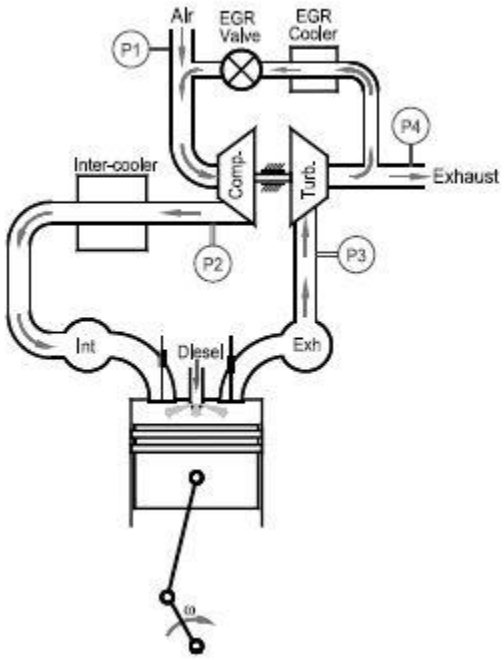

Figure 5 Low pressure loop EGR concept. The arrangement of turbine and compressor can also be seen in the image shown above

The possible reasoning for reduction of NO_x by the usage of exhaust gas recirculation process is that the EGR reduces the combustion flame temperatures in different ways. In the presence of inert molecules of exhaust gases, fuel molecules require more time to find the oxygen molecules, this results in the reduction of the peak temperatures that are achieved in the combustion due to the slowing down the overall speed of the combustion process. The same amount of heat energy released during combustion, but it takes more time to release. In the presence of EGR, the heat energy will have to heat a large amount of gas, and with the dilution of intake air with exhaust gas, the amount of the gas portion that needs the necessary quantity of oxygen is also large in case of EGR lower value of combustion temperature reduces the amount of NO_x emitted. The co-relation between NOx formation and peak combustion temperatures can be viewed and studied from figure 6[6]

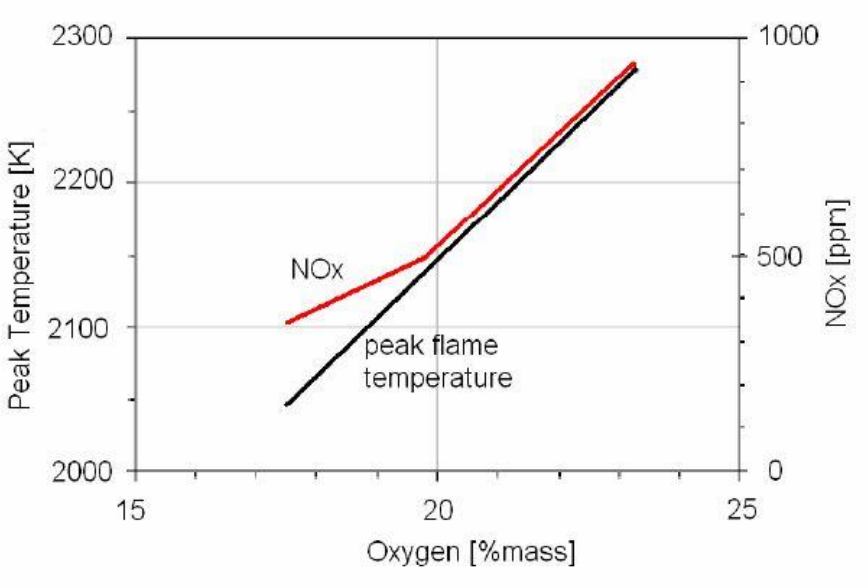

Figure 6 Peak temperature of combustion relationship with NOx formation

As it can be viewed the NO_x formation increases with the increase in the peak combustion temperatures. The goal of the EGR is to reduce the peak combustion temperatures and also slows down the combustion process.

1.5 Water Injection

Another strategy that is employed to reduce the amount of emissions in diesel engines is the injection of water. The direct and indirect injection of water of water into the combustion chamber is one of the efficient and most cost effective tool used for the reduction of emissions such as NO_x and Particulate Matter (PM)[7]. Different researchers have developed various systems for introducing water in the combustion chamber. The development of different systems of water injection are being under development from the era of the development of aircraft piston engines[7].

The key pollutants that are produced from the diesel engines are nitrogen oxides, unburnt hydrocarbons, smoke, carbon monoxide, carbon dioxide, sulphur oxides, and particulate matter. The formation of NO_x and particulate matter (PM) is a major concern for the diesel engine designers and manufacturers. It must be mentioned that the NO_x formation and particulate matter (PM) are temperature dependent phenomena[7]. The formation of both these emissions are normally contradictory in nature with one another [7]. The attempts to reduce one normally causes an increase

in the other [7]. The mechanism and process related to water injection is the reduction in the temperature of the combustion flame and products due to the vaporization of water, and ultimately the dilution of species that are in gaseous phase[7]. For the emission of particulate matter (PM), the water present in the chamber at the time of soot formation appears to reduce the rate of soot particle formation, and aid in their burning by providing hydroxyl (OH) species[7].

There are many ways of introducing water in the combustion chamber, and these methods have been used by the engine designers as well as the researchers. These methods are water diesel emulsion, fumigation, and the direct injection of water[7]. These methods have their own advantages and disadvantages. These types will be shortly described in this section, and the advantages and disadvantages of these methods will also be explained.

Generally emulsion is a mix of two liquids that are not generally miscible with each other, one liquid is generally present in the droplet form, while the other exists in dispersed phase[7]. The emulsion of diesel and water that is used in the engines should be stable, and that stability is achieved with the help of surfactants[7]. There is another requirement for the usage of surfactants in case of diesel water emulsion, that is, the burning of surfactant should be easy and it should not produce soot, moreover, it should not contain sulphur and nitrogen[7]. In literature, experimentally, the emission reduction as per regulations have been reported with the usage of water diesel emulsion. However, there are mixed observation about the increase or decrease in the power output of the engine if the emulsion is used, and the variation in the trend of power output is related to the percentage of water present in the emulsion. There is a need of exploration and detailed studying about the effects of usage of emulsion, percentage of water, and the outcomes of the usage on the emissions as well as performance parameters.

Fumigation is another method that is employed to introduce water in the combustion chamber. In fumigation, the water is injected in the intake manifold during the intake stroke of the diesel engine. Fumigation is comparatively simpler method of introducing water, and the integration of system is easy with the present technologies of the engine[7]. Further variation in the fumigation is the multipoint and single point of water injection. If comparison is made between fumigation and emulsion, it is reported that the amount of water required for reduction of NO_x using fumigation is large compared to the emulsion[7]. The fumigation has a positive impact on reducing the emissions in the diesel engines. The mixing of the water with the incoming air and characteristics of the spray, exact timing of water injection are the main factors that play a critical

role in this regard. Moreover, the vaporization of water, and the timing of vaporization are also the important variables that play an important role. The location of water injector, injection pressure, and temperature of the water injected also have an impact on the role of water in reducing the temperature of combustion chamber and ultimately reducing the emissions. Simulations can help a lot in studying the effects of different factors related to fumigation method of water injection, and it would be easier to change and adjust the above mentioned factors in the simulation. The effects of these variables can also be studied experimentally, however, many major and minor changes are required in the hardware and components.

The direct water injection system consists of a dual feed nozzle with a water supply system. It is almost impossible to change the percentage of water during the transient engine running conditions, however, there are also many liberties related to injection of water during the compression stroke when direct injection method of water is used. Moreover, the degree of freedom for water injection is more in the direct water injection systems compared to the fumigation and emulsion.

All three methods of injecting water seems effective in reducing the emissions of NOx as well as particulate matter. The water diesel emulsion method is yet to be explored further particularly with reference to the volume of water used in the formation of emulsion. The cost of conversion of the normal engine into the system with which water can be injected should also be kept in mind when selecting a system. Fumigation as well as direct water injection systems also include the aspects of spray dynamics that play a significant role in the current situations.

It must be mentioned that EGR and water injection both reduce the emissions by reducing the combustion peak temperatures. The EGR also alters the availability of oxygen atom present in the combustion chamber, and plays it role in the controlling the rate of combustion, in many cases the heat released during the combustion when EGR is introduced released at the later stages when compared to the cases in which EGR was not used.

CHAPTER 2: RESEARCH METHODOLOGY

The study is based on the numerical simulation of EGR and Water Injection in the diesel engine. A comprehensive research methodology was adopted to develop an understanding of the processes, and to provide the useful insight about the numerical simulation processes of EGR and WI and the extent up to which these processes help in reducing the exhaust gas emissions such as CO, NO_x, and soot. A parametric study was also performed to study the effect of operating parameters such as start of injection (SOI), duration of injection (DOI), and initial temperatures on the emissions.

2.1 Research Aim and Objective

- The aim of the research was to formulate a numerical and simulation model for studying the processes of exhaust gas recirculation and water injection using Ansys Forte.
- To validate the combustion model of Ansys forte for diesel engines, especially for the cases of EGR and WI
- To study the combustion Process in Diesel Engines and the effect of SOI, DOI, and initial temperatures on exhaust emissions (NOx, CO, Soot).

Figure 7 shows the step by step approach that was used in carrying out this study.

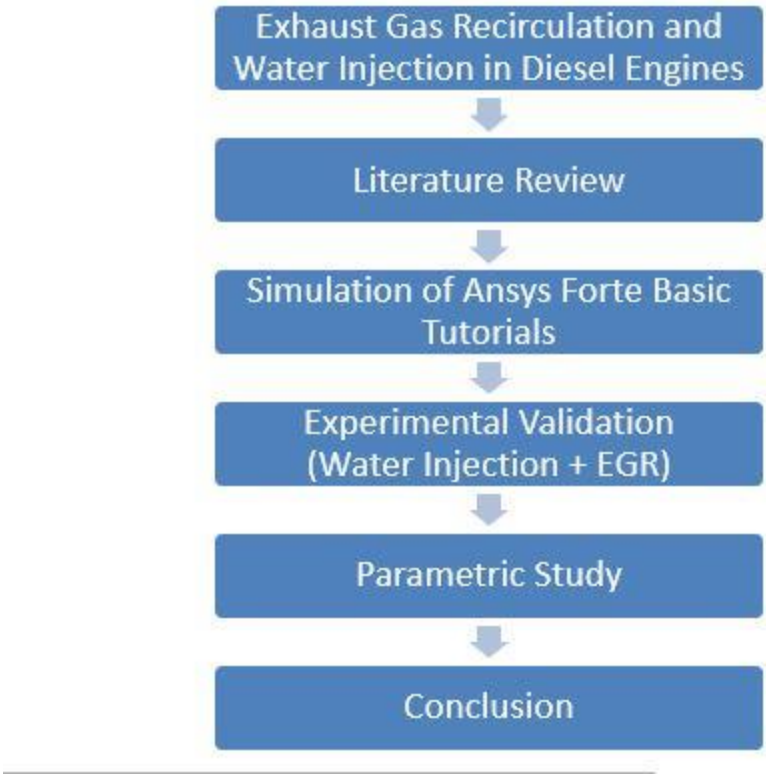

Figure 7 Steps used in carrying out the current study.

- The first step in carrying out the study was the detailed study of Exhaust Gas Recirculation (EGR) and Water Injection (WI) processes. During this study, a detailed understanding of working of compression ignition engines was developed
- Second step was the review of literature about the numerical techniques, CFD codes, algorithms, and steps of diesel combustion processes. In this steps various commercial software packages were also considered and ease of setting up problem, visualization, accuracy, and the objectives were kept in mind while selection. ANSYS FORTE was selected for the numerical simulation.
- In order to develop understanding about the procedure, setting up the simulation, and mathematical models, the tutorials that were provided by the ANSYS about combustion, sector mesh formation, and spray were replicated.
- The fourth step was the replication and validation of an experimental study of EGR and WI for benchmarking.

- Once the validation was done, a parametric study was performed to study the effect of input and operating parameters on the emissions.
- The last step was drawing of the various conclusions based on the results obtained and general understanding of the processes

CHAPTER 3: NUMERICAL SIMULATION OF INTERNAL COMBUSTION ENGINE AND THEORATICAL FRAMEWORK

This section will provide a basic theoretical and mathematical framework of numerical simulations. Different models that are normally employed in modeling different stages of combustion. The current section also presents the simulation of the EGR and Water Injection for a diesel engine. The experimental conditions were replicated in the commercial software ANSYS, and then cases of EGR and Water injection were studied. A parametric study was also performed in which various parameters were changed and the effect of variations of these parameters on emissions was studied.

With the time there is a strong sense of realization and acknowledgment among the researchers and designers that experimentation alone is not enough to give a complete insight about the local phenomena, CFD simulations are necessary to perform parametric study, and CFD simulations are able to capture the details of local phenomena and processes [8]. The number of publications presenting computational fluid dynamic codes applied to internal combustion engine problems is increasing day by day. Normally the researchers present the results primary in the form of pressure curve attained from the experiment and the numerical simulations, and finally a comparison is made. The results that have been presented normally are in very close agreement with the experimental results. The verification is necessary for validation of the computational fluid dynamic (CFD) code.

As mentioned previously, various researchers have performed simulations regarding the internal combustion engines and verified the experimental results. Soni and Gupta simulated the methanol powered diesel engine using CFD approach[9], and the difference in the experimental and numerical values was merely 3-4 bars[8]. Guo et al studied the fuel injection effects on the performance parameters of free piston diesel engine generator using CFD approach, and also verified the experimental and numerical results[10]. Verma et al performed CFD modeling of EGR and injection timing, the combustion was studied with different EGR percentages injection timings, and the effect of these parameters on the emissions and combustion in diesel engine was reported[11]. Abay et al performed CFD simulations of diesel engine by constructing the 45 degree sector, and the simulations were reactive in nature, the researchers used commercial CFD code called as FORTE (reaction design) and the chemical solver CHEMKIN [12]. The effects of EGR on

NOx emissions and soot formation was also reported by the researchers. The research provided detailed parameters and equations that are used in the Forte reaction design code[12]. The research that was performed by Abey et al. is similar to the work that is being presented here, however, there are many aspect that have been reported in the current study which will provide useful insight about the EGR, WI, other operating parameters and emissions.

3.1 Numerical Modelling of IC Engines

In the internal combustion engine problems, the air and fuel mixture and the products after the combustion reaction are considered normally as working fluids. The current study includes the simulation of diesel engine using the commercial CFD code Forte Reaction Design by ANSYS. The turbulent reaction flow mechanisms are modelled by the Navier-Stokes equations. The transport equations of mass, energy, and momentum are modified for the compressible flows, gaseous phase, and turbulent flows. The interaction between liquid spray and gaseous droplets when the fuel or water is injected in liquid form are accounted for by the usage of exchange reactions. For the derivation of main equations, many assumptions were used. Following are the assumptions that were used for deriving the equations that are related to the flow fields and states of species produced in the internal combustion engines.

- Ideal gas law
- Equation of state (gaseous phase)
- Fick's law for the mass based diffusion
- Assumption for the use of Newtonian fluid
- Fourier's law of thermal diffusion

3.2 Conservation of Transport Equations

Similar to all CFD studies as well as other transport phenomena, the conservation equations are applicable in the case of internal combustion engine problems. In this section a brief description of the conservation equations will be provided. As mentioned previously, the equations have been used to account for the changes in the composition of species, and the working fluids have been modelled in gaseous phase. It must be mentioned that the working fluids in the gaseous form have been modeled as a mixture consisting of individual gas.[13]. The composition of these species change

during different steps of the engine cycle due to different phenomenas such as convection, diffusion of molecules from denser place to other, transport, interaction of gaseous species with the liquid fuel sprays, and the combustion itself[13]. The accurate and complete consideration and realization of changes in the species during the pre-combustion, combustion, and exhaust phases is the core of modeling of internal combustion engines, and in numerical simulations the main task is related to accurately model the changes in the composition of species considering the variations in the phase and interactions of the particles. Equation 1 presents the conservation of the mass for the species k.

$$\frac{\partial \bar{\rho}_k}{\partial t} + \nabla \cdot (\bar{\rho}_k \tilde{\mathbf{u}}) = \nabla \cdot \left[\overline{\rho} D \nabla \tilde{y}_k \right] + \nabla \cdot \Phi + \dot{\bar{\rho}}_k^c + \dot{\bar{\rho}}_k^s \quad (k=1,\cdots,K) \tag{1}$$

In the above equation, ρ represents the density, k stands for the index of species, and K is the total number of species. u is the velocity vector, and y_k is the mass fraction of the species. Similarly, the continuity equation is derived from the summation of equation 1 when applied to total number of species. Equation 2 represents the gas continuity equation[13].

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\overline{\rho} \tilde{\mathbf{u}}) = \dot{\bar{\rho}}^s \tag{2}$$

The momentum equation in case of the internal combustion engines is detailed one. It considers the convection phenomena, stress due to viscous forces, pressure force, transport turbulence, and also incorporates the effects of interactions between liquid spray and body force. Equation 3 represents the momentum conservation equation

$$\frac{\partial \overline{\rho} \tilde{\mathbf{u}}}{\partial t} + \nabla \cdot (\overline{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}}) = -\nabla \overline{p} + \nabla \cdot \overline{\boldsymbol{\sigma}} - \nabla \cdot \boldsymbol{\Gamma} + \overline{\mathbf{F}}^s + \overline{\rho} \mathbf{g}, \tag{3}$$

In the above equation, F^S represents the momentum gain per unit volume, p is the pressure, g is the spray term. σ is the viscous shear stress term.

The energy conservation equation is based on first law of thermodynamics. According to first law of thermodynamics, the change in the internal energy should be balanced by the pressure work and heat transfer[13]. In case of the fluidic problems such as internal combustion engines, the energy equation is written considering the effects related to different processes taking place, such

as convection, transport and dissipation that is turbulent in nature, spray characteristics, chemical reactions, and enthalpy diffusion[13]. Equation 4 represents the internal energy equation

$$\frac{\partial \overline{\rho}\tilde{I}}{\partial t}+\nabla\cdot\left(\overline{\rho}\tilde{\mathbf{u}}\tilde{I}\right)=-\overline{p}\nabla\cdot\tilde{\mathbf{u}}-\nabla\cdot\tilde{\mathbf{J}}-\nabla\cdot\mathbf{H}+\overline{\rho\varepsilon}+\dot{Q}^{C}+\dot{Q}^{S} \tag{4}$$

In the above equation I represents the specific internal energy term, and J is the heat flux vector.

3.3 Turbulence Modelling

The main aspects that are related to the turbulence and its modeling are the length scales and extreme random variations in the flow fields. In ANSYS forte reaction design, there are two main approaches available for the modeling of turbulent flow, and the equations are used in the context of flow field variations that are produced in internal combustion engines. These two approaches are Reynolds-Averaged-Navier-Stokes (RANS) and Large Eddy Simulations (LES). The RANS method of turbulence modeling is based on considering the ensemble average of flow field from many different understanding and realization under specific conditions. The small variations and structures are not resolved in this approach that are the part of individual flow realizations, the key is to consider the turbulent effects on averaged flow fields and different characteristics of combustion.

3.4 Reynolds Averaged Navier Strokes (RANS)

As mentioned before, RANS approach simulates the ensemble average flow field. The transport phenomena of the turbulence are modelled using gradient based mass diffusion. For the momentum based equation, the assumption is made that the Reynolds's deviatoric stress components are considered directly proportional to the mean of the deviatoric strain rate. Reynolds stress tensor has been defined as

$$\mathbf{\Gamma}=-\overline{\rho}\upsilon_{T}\left[\nabla\tilde{\mathbf{u}}+\left(\nabla\tilde{\mathbf{u}}\right)^{T}-\frac{2}{3}\left(\nabla\cdot\tilde{\mathbf{u}}\right)\mathbf{I}\right]+\frac{2}{3}\overline{\rho}\tilde{k}\mathbf{I} \tag{5}$$

Where v_T = turbulent kinematic viscosity, and ǩ is turbulent kinetic energy.

The Re-Normalized Group (RNG) *k* - *ε* model was used for turbulence modeling, it must be mentioned that *k* is the same as in the standard *k* - *ε* model, yet the value of *ε* is different in RNG model. Equation 6 presents the RNG –*ε* equation. The *k* - *ε* model has been derived from the RNG formulations that were proposed by the Yakhot and Orszag [14]

$$\frac{\partial \overline{\rho}\widetilde{\varepsilon}}{\partial t}+\nabla\cdot\left(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{\varepsilon}\right)=-\left(\tfrac{2}{3}c_{\varepsilon 1}-c_{\varepsilon 3}\right)\overline{\rho}\widetilde{\varepsilon}\nabla\cdot\widetilde{\mathbf{u}}+\nabla\cdot\left[\frac{(\upsilon+\upsilon_T)}{Pr_\varepsilon}\nabla\widetilde{\varepsilon}\right] \quad (6)$$
$$+\frac{\widetilde{\varepsilon}}{\widetilde{k}}\left[c_{\varepsilon 1}\left(\boldsymbol{\sigma}-\boldsymbol{\Gamma}\right):\nabla\widetilde{\mathbf{u}}-c_{\varepsilon 2}\overline{\rho}\widetilde{\varepsilon}+c_s\overline{\dot{W}}^{s}\right]-\overline{\rho}R$$

Equations 7 and 8 provide the Favre-averaged standard form of *k*-ε form[13].

$$\frac{\partial \overline{\rho}\widetilde{k}}{\partial t}+\nabla\cdot\left(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{k}\right)=-\frac{2}{3}\overline{\rho}\widetilde{k}\nabla\cdot\widetilde{\mathbf{u}}+\left(\overline{\boldsymbol{\sigma}}-\boldsymbol{\Gamma}\right):\nabla\widetilde{\mathbf{u}}+\nabla\cdot\left[\frac{(\mu+\mu_T)}{Pr_k}\nabla\widetilde{k}\right]-\overline{\rho}\widetilde{\varepsilon}+\overline{\dot{W}}^{s} \quad (7)$$

$$\frac{\partial \overline{\rho}\widetilde{\varepsilon}}{\partial t}+\nabla\cdot\left(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{\varepsilon}\right)=-\left(\tfrac{2}{3}c_{\varepsilon 1}-c_{\varepsilon 3}\right)\overline{\rho}\widetilde{\varepsilon}\nabla\cdot\widetilde{\mathbf{u}}+\nabla\cdot\left[\frac{(\upsilon+\upsilon_T)}{Pr_\varepsilon}\nabla\widetilde{\varepsilon}\right] \quad (8)$$
$$+\frac{\widetilde{\varepsilon}}{\widetilde{k}}\left(c_{\varepsilon 1}\left(\boldsymbol{\sigma}-\boldsymbol{\Gamma}\right):\nabla\widetilde{\mathbf{u}}-c_{\varepsilon 2}\overline{\rho}\widetilde{\varepsilon}+c_s\overline{\dot{W}}^{s}\right)$$

The values of the C constants and Prandtl number are listed in table 1 for RNG $k-\varepsilon$

Table 1 Values of the C constants and Prandtl number for for RNG $k-\varepsilon$

Variable	Value
Prandtl number	0.74
Air Mu Coef. 1	1.4 e -5
Air Mu Coef. 2	110
Air lambda Coef 1	252
Air lambda Coef 2	200
Epsilon Coef 1	1.42

Epsilon Coef 2	1.68
Viscosity Coef	0.085
1/Pr (k-equation)	1.39
1/Pr (Epsilon-equation)	1.39
RNG Eta0 Parameter	4.38
RNG Beta Parameter	0.012
Epsilon Spray Coef	1.5

3.5 Initialization of Fluidic Properties

The values of the state variables and other terms in the main governing equations are initialized and determined using the fluidic properties. Initialization of the fluid is usually required for carrying out the transient simulations. In order to perform initialization, following parameters must be determined [13]

- Initial pressure value for all computational domains
- Initial temperature values for all computational domains
- The composition of species must be initialized for all computational domains in terms of mass or mole fractions. For example the composition of pure air or the composition of air in case of introduction of EGR
- Value of initial turbulent kinetic energy density in all computational regions. For the case of internal combustion engines, the initial total turbulent kinetic energy is determined as a fraction of total kinetic energy. The total kinetic energy is calculated on the basis of mean piston speed.
- Initial turbulent length scale for all computational regions.

The correct initialization of the required variables serve as a base for the determination of correct and accurate solution. The stability of the numerical solution in case of CFD and internal combustion engine simulations directly or indirectly depends upon the definition of initial values or initialization of the solution.

3.6 Discretization Methods

The governing equations are normally discretized according to the spatial coordinates on a computational mesh or grid, the finite volume approach is adopted in this case. To ensure the accuracy of solution in time based problems, operator splitting method is adopted to discretize the governing equations with respect to time.

3.6.1 Time Discretization using Temporal Differencing Method

The integration of the equations in time, a temporal differencing method is employed. For discrete time moment, t^n (n =0, 1, 2,...), the next step time interval is provided by $\Delta t^n = t^n + 1 - t^n$. the 'n' is related to the time of the cycle number. In the integration of the time step, a three step solution of each time step is done by ANSYS-FORTE [13] Operator splitting method is applied to separate the chemical source term, spray source term, and the flow transport source term in time stepping. The solution of the flow transport is done using Arbitrary-Lagrangian-Eulerian (ALE) method[15]. Amsden et al developed the numerical simulation computer program for two and three dimensional transient chemically reactive flow problems[15]. Following is the division of the each time step in three different parts[13]

- This step deals with the solution of chemical and spray source term present in the energy and specie transport governing equation. Lagrangian approach is adopted in the calculation, in which the computational cell travels along with the fluid, and the droplets of the spray undergo collision, breaking, and the repeated motions, and the mass and energy terms are also considered due to chemical interaction between gas and spray droplets.
- The second step is based on consideration and taking steps towards providing a coupled solution that is implicit in nature for the acoustic terms, momentum spray source terms, and terms related to the diffusion of mass, momentum, and energy. In the second step, the terms that were left unsolved in the turbulent transport equations are also accounted for.
- Third stage is the interesting and plays a very critical role in determining the part of solution related to wall motion. In this step, the flow field is not changed and sort of

locked and frozen, and then remapping is done on the revised mesh with the consideration of wall motion. The convection term is calculated in the transport equation as a consequence of motion of the Langrangian mesh formulated in the second step to the newly revised mesh, and the motion is relative to the fluid.

3.6.2 Space Discretization Technique

The equations of the flow fields, turbulence, and other transport properties have been discretized for spatial differencing using Arbitrary Lagrangian-Euler (ALE) method[16]. This method considers the hexahedron shaped arbitrary mesh elements when applied to 3D geometries. The conservation of the local characteristics of the differential equations is necessary, this was done by using either control volume method. The mesh is formed of spaces, and it is composed of cells, and the corners of these cells are vertices. The vertices can move in arbitrarily suggested way, in this way valve and piston motion is accounted. For differentiation of momentum equations a separate control volume called momentum cell is used. In ALE method velocities are mainly located at cell vertices. There is retention of velocities at cell vertices and momentum related too cell vertices is conserved. The normal components of velocity situated at the cell centers calculate the changes in volume of the cells in second step of time discretization, and also the volume of the fluid crossing or transporting across the cells in third stage.

SIMPLE method has been adopted for obtaining the solution of the algebraic equation that are finite volume based, these equations were produced as a result of discretization of the main governing equations. An advanced modified version of SIMPLE method is employed, in which variables associated with the flow fields are solved in two steps. Advanced time pressure in the gradient form are used to calculate the velocities during each time step, this method of computing the velocities generates the need for an iterative solution procedure, as the acceleration variables are used to find the time-advanced pressures, and the values of velocities are then further computed from the pressure values.

It must be mentioned that the spatial as well as time discretization techniques employed in simulating the EGR and Water Injection cases of the internal combustion engine problems have been marginally touched only too highlight the general techniques adopted, however, there is a detailed explanation that is required for elaboration of the techniques used. The detailed

explanation is currently not present in the scope of this document. It must be mentioned that the fundamental numerical techniques that have strong basis and verified by the researchers have not only been used directly, but also modified in such a way that presents the accurate solution to the user.

3.7 Spray Model

The spray of liquid fuel in the hot air is the man characteristic of the diesel engines. The interaction of the liquid fuel spray with the gaseous mixture determines the major outcomes of the combustion. In order to perform the numerical simulations of the internal combustion engine accurately, particularly diesel engines, the spray characteristics must be defined accurately. The spray terms are an important part of governing equations. Advance models are required for the simulation of dynamics of multi-component fuel spray and interaction of the multicomponent gaseous mixture with the spray. In reality, the molecular size of each gas is different, and the air that is composed of multiple gases is a mixture of gases with different molecular size.

The overall process of spray include sub-processes like flow from the nozzle, atomization of spray, breakdown of droplets into different sizes, collision of droplets, vaporization of the droplets and impingement of the drops with the walls. These are actually complex phenomena from modelling point of view. The vaporization aspect is important in case of water injection, as the timing of vaporization of water vapors either present in the inlet air or directly injected in the combustion chamber play an important role in lowering the temperature of the combustion products. The timing of vaporization is very important in this regard. In this section only the short description regarding the solid cone spray numerical modeling will be provided.

In case of solid cone sprays in ANSYS Forte, the initialization of spray at the nozzle exit is done by either discharge co-efficient model or nozzle flow model. For capturing the spray droplet breakup, Kelvin-Helmholtz / Rayleigh-Taylor (KH/RT) model has been employed. In order to reduce and minimize the dependence of calculated results on the size of mesh and time step, several advanced techniques have been employed related to droplet breaking, collision, and spray atomization in ANSYS FORTE[13]. For solid cone sprays, an unsteady jet model is used by default in ANSYS, and radius of influence collision model is employed for minimizing the mesh size and time dependency.

3.7.1 Discharge Coefficient Model

Volumetric mean flow velocity of the liquid fuel at the inlet of the nozzle can be determined using equation 9[13]

$$U_{mean} = \frac{\dot{m}}{\rho_f A} = \frac{4\dot{m}}{\rho_f \pi D^2} \quad (9)$$

U_{mean} is the mean volumetric flow velocity, ṕ is the density of fuel, and ṁ is the mass flow rate of the fuel. A is the cross-sectional area of the nozzle, and D is the diameter of the nozzle.

In order to account for losses in the flow a discharge co-efficient is normally defined. Figure 8 shows the ow of the fluid through the nozzle and also highlights the important zones that are formed[13].

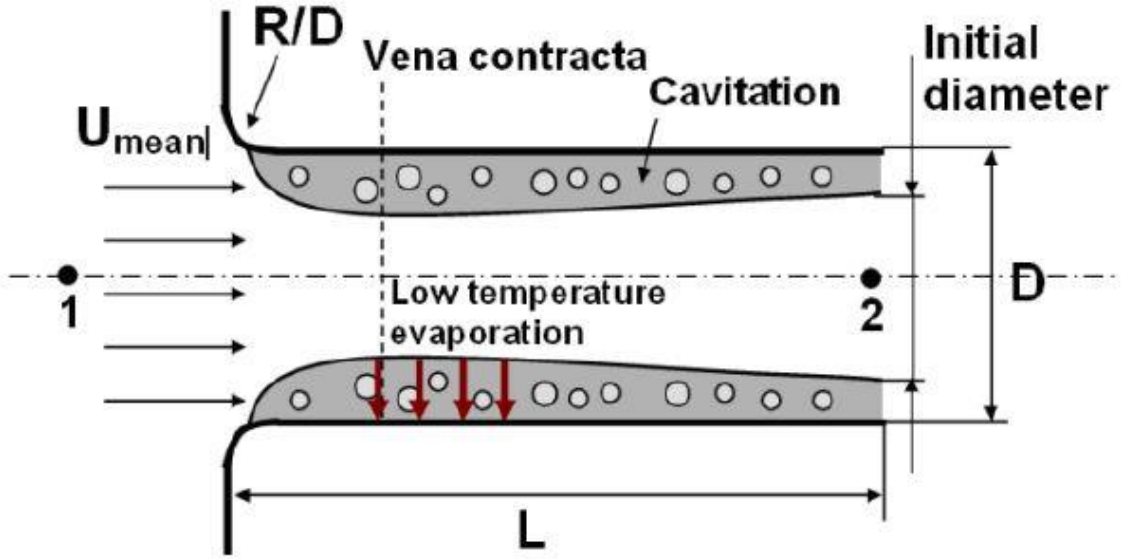

Figure 8 Flow of fluid through the nozzle. Cavitation region and Vena contracta have also been labelled

Equation 10 presents the discharge co-efficient[13]

$$C_d = \frac{U_{mean}}{\sqrt{2 \cdot (p_1 - p_2)/\rho_1}} \quad (10)$$

P_1 and P_2 corresponds to the pressures at regions 1 and 2 respectively with reference to the figure 7. It must be mentioned that in case of non-cavitatiing flows that are also turbulent in nature, the exit velocity of the liquid droplets s considered equal to mean velocity and the diameter of the jet at nozzle exit is considered equal to diameter of the nozzle[13]. In case of cavitation the effective injection velocity and the effective flow exit area are determined by a different formulation

3.7.2 Kelvin-Helmholtz / Rayleigh-Taylor (KH/RT) Breakup Model

The breakup of spray and atomization have been modeled using Kelvin-Helmholtz / Rayleigh-Taylor (KH /RT) hybrid breakup model[17]. The KH-RT model is based on the two main steps, primary breakup and secondary breakup[17]. KH breakup model is applied within a specific breakup length 'L' from the nozzle exit area 'A', the small droplets are stripped off or separated from the jet (parcels or blobs are just formed), yet jet manages to maintain it as a liquid core. After the breakup length 'B' , RT model is employed along with KH to predict the secondary breakup behavior[18]. Figure 9 presents the KH/RT breakup model for solid-cone sprays[13].

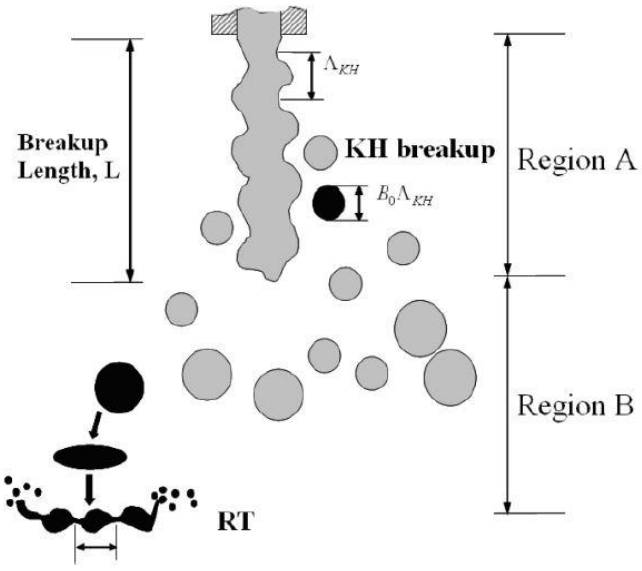

Figure 9 KH/RT breakup model for solid-cone sprays

KH model is based on the stability analysis of the liquid jet, and the model is used to predict the primary breakup of the liquid jet. From the linear stability analysis, any formulation applied at the junction of liquid gas interface can be expanded as Fourier series, and the fastest growing from is the final breakup and generation of new particles[13].

ANSYS FORTE employs the usage of concept of blob injection[19], in this concept the liquid spray jet injection is considered to be made up by parcels of blobs, the size of the blobs is initially considered to be equal to effective nozzle diameter. Utilizing this concept, primary process of break up is in which new droplets of radius r_c are formed from parent droplet having radius r_p. The new droplet is formed as per this theory, when the parent droplet loses its mass to produce the child droplet, the radius change formula can be written as per equation 11 [19].

$$\frac{r_p - r_c}{\tau_{KH}} \tag{11}$$

The timescale of breakup τ_{KH} is calculated as follows[13].

$$\tau_{KH} = \frac{3.726 C_{KH} r_p}{\Lambda_{KH} \Omega_{KH}} \tag{12}$$

3.7.3 Unsteady Gas Jet Model

In numerical simulations of spray, the mesh dependences of KH-RT breakup spray model is due to the requirement for the calculation of liquid-gas relative velocity U_{rel} given by equation (13)

$$U_{rel} = \left| \vec{V}_{gas} + \vec{V}'_{turb} - \vec{u}_d \right| \tag{13}$$

The V_{gas} velocity mentioned in the equation is taken as cell velocity of gas in CFD. Unsteady jet gas theory has been used in the ANSYS and the simulations performed in the current study to reduce the dependency on the mesh size, a gas jet model has been used for the interaction and interfacing of liquid droplet and gas. With the help of the unsteady gas jet model, the relative

axial velocities of droplet-gas can be modelled without the usage of discretization (CFD mesh). Figure 10 shows the diagram of unsteady gas jet model helpful in understanding from simulation point of view[13]

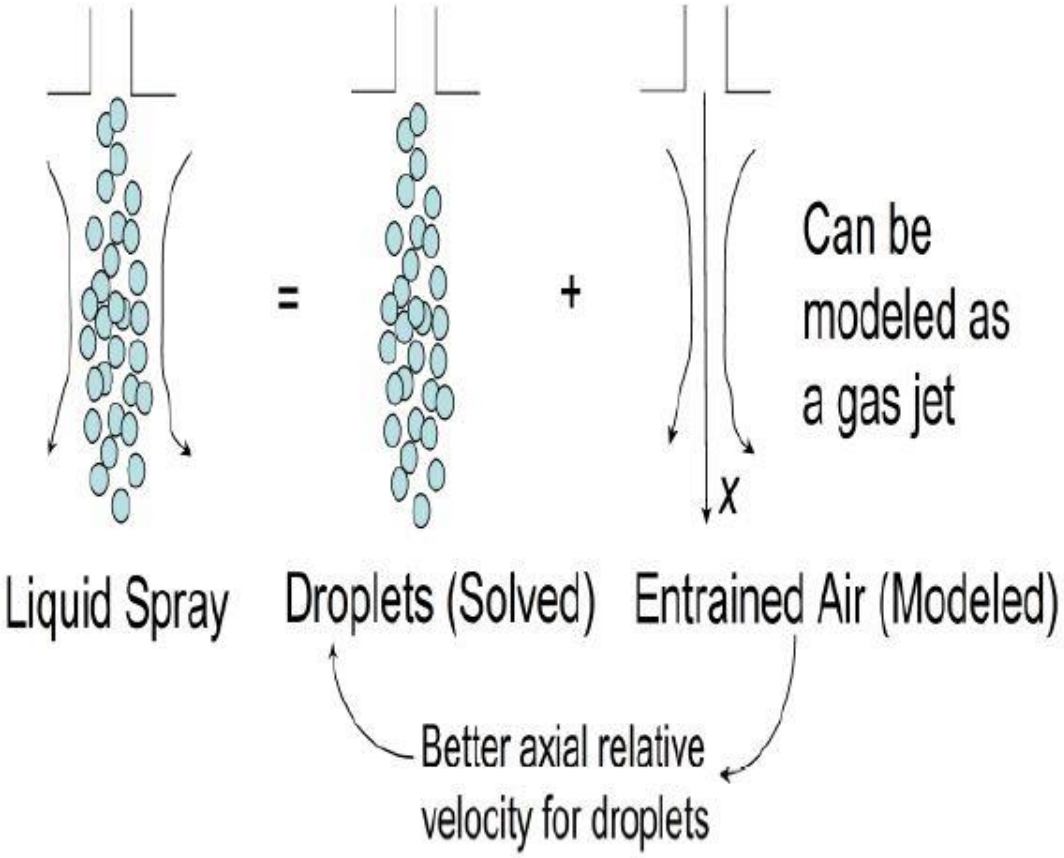

Figure 10 Unsteady Gas Jet model pictorial representation.

3.8 Wall Impingement Model

When the spray droplet hits the wall, the outcome of this interaction has been determined in the wall impingement model in ANSYS FORTE, and the outcome depends on the Reynolds number and Weber Number of the incident droplet, and the surface conditions[13]. There can be four possibilities or regimes that are possible as a result of collision of droplet with the wall. These four possibilities are, sticking, recoiling or rebounding, spreading, and flash.

Impact energy plays a critical role in deciding the outcomes of the collisions. If the impact energy of the droplet coinciding with the wet wall is very low, then stick regime occurs, and the droplet sticks to the wall. If the impact energy of the incident particle increases, the air traps between the liquid droplet and wall surface causes the slight energy loss and then the rebounding of the droplet occurs. If the impact energy of the striking particle is increased further, the incident droplet gets spread and get merges with the film. The splash occurs at very high impact energy, the incident droplet strikes back from the impact site, and breaks down into smaller droplets. Fig. 11 shows the four possible outcomes of the droplet wall interactions[13]

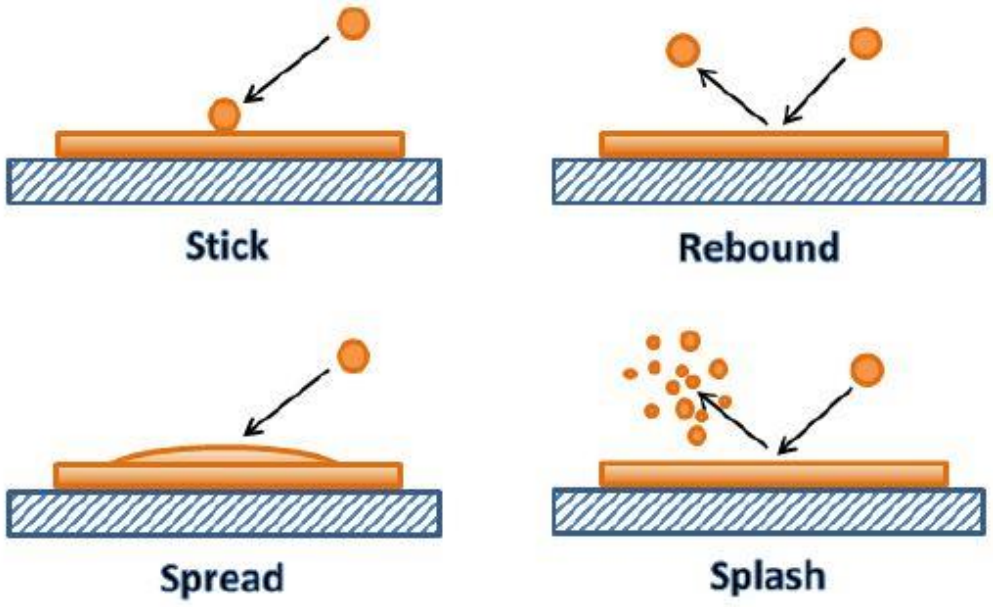

Figure 11 Wall impingement model outcomes used in ANSYS FORTE

The outcomes of the collision between droplet and wall as employed in simulation in ANSYS, and their relationship with Weber number and Reynold number is shown below[13]

Stick: $We_n \leq 5$

Rebound: $5 < We_n \leq 10$

Spread: $We_n > 10$ and $We_n Re_n^{0.5} < H_{cr}$

Splash: $We_n Re_n^{0.5} < H_{cr}$

H_{cr} stands for splash threshold

3.9 Method of Moments for Calculation of Soot and Particle Tracking

ANSYS FORTE allows the users to use the feature of particle tracking, and this particle tracking feature includes the condensed and dispersed phase matter in the form of particles. The feature is helpful in determining the properties, quantity, and size of the particulate matter.

Method of moments has been utilized to model the soot formation. In this technique the average description of properties of a particle population is used. The suspension of very fine solid or liquid particles in the gas (most of the times air) forms an aerosol system. In this method, moments of particle size distribution function is utilized to track the growth and evolution of an aerosol system. Method of moment can provide significant details about the properties of a particulate system such as number density, density of particle surface area, volume fraction of the particle etc. without making any assumptions about the particle size distribution function. Frenklach and associated coworkers first reported the soot formation as an application of method of moments[20].

CHAPTER 4: EXPERIMENTAL VERIFICATION OF NUMERICAL MODEL

A Peugeot Citroën Dw-10b Diesel Engine was used in the experimentation for six zone combustion model development[21].The operating conditions of the engine were provided as input in the software. Table 2 presents the specifications of the engine.

Table 2 Specifications of the engine used in the current study

Engine	**Peugeot Citroën Dw-10b**
Bore	8.5 cm
Stroke	8.8 cm
Connecting Rod length	15.2 cm
Compression Ratio	18
Number of holes per injector	7
Injector hole Diameter	0.01 cm
RPM	1661
Displacement Volume	2000 cc
Fuel Quantity (Diesel)	25.4 mg

4.1 Simulation Steps

The simulation of the combustion engine in Forte consist of various steps. The first step is the formation of geometry. The second step is based on the chemical formulation, defining the chemical properties of the species and fuel involved in the chemical reactions. Third step is the Definition of various properties of the turbulence, flame propagation model, and properties of the fluid that will be used in the transport equations. In this step, the spray and injection characteristics of the fuel are also defined. Mean cone angle and discharge co-efficient is also

defined for the initialization of spray. Fourth step consisted of application of boundary conditions. Fifth step was the definition of initial conditions. Finally, simulation controls and output controls are defined and various parameters regarding the running of the simulation and solvers are defined. Figure 12 shows the simulation steps.

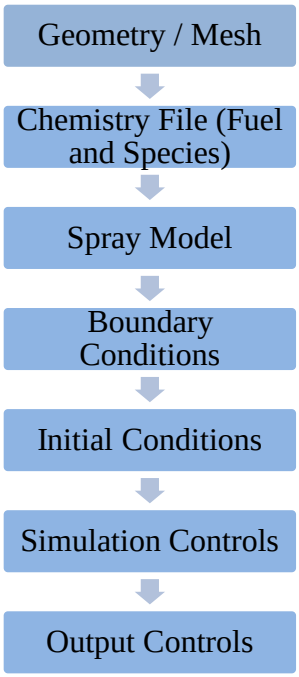

Figure 12 Simulation steps used in the current study

4.1.1 Geometry/ Mesh

The engine cylinder is divided into sector, and the sector angle is dependent upon no of holes per injectors. For the present case, the fuel injector had seven holes, therefore

Sector angle=360/7=51.4 degrees

A sector can represent the full geometry, since we can take advantage of the periodicity of the cylinder and injector nozzle-hole pattern. The sector was generated in Ansys Forte Sector Mesh generator. The compression ratio was achieved by adjusting the bowl depth and bowl diameter. X and Y coordinate points are provided to define the bowl depth and diameter. Ansys Forte compression ratio calculator was used to check the compression ratio. Fig 13 shows the injector hole and spray pattern visual, $1/7^{th}$ of geometry of a single cylinder has been selected.

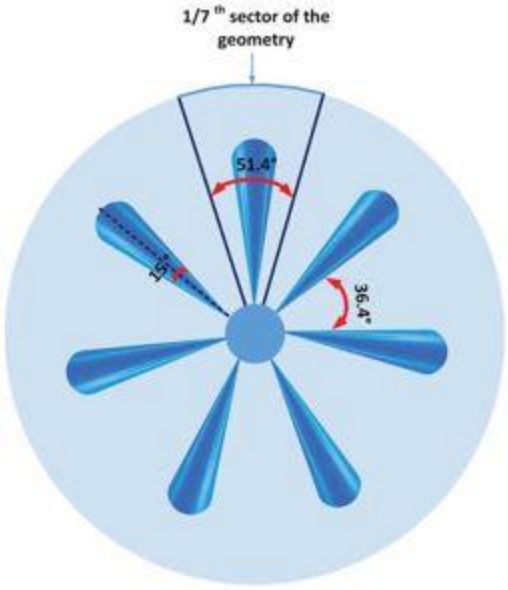

Figure 13 Geometry injector hole pattern and selection of sector

For the formation of sector following parameters are required

- Bore
- Stroke
- Connecting Rod Length
- Piston Profile
- Compression Ratio
- Sector Angle

Cell count has to be defined in the radial, axial, and circumferential direction.

Figure 14 and 15 present the 3D views of sector generated and meshed sector respectively

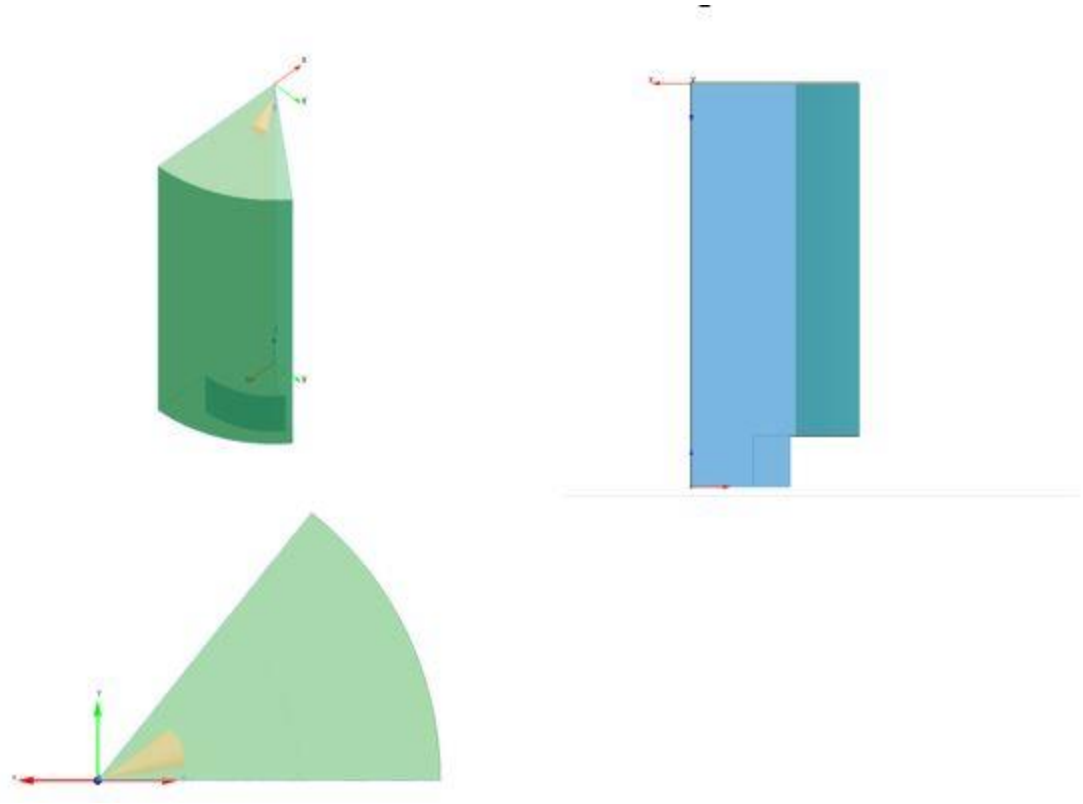

Figure 14 3D and side view of the sector of the diesel engine used for modeling.

Figure 15 View of meshed sector.

4.1.2 Chemistry and Chemical Reactions

The sub-module of FORTE, CHEMKN was used for the solution of chemical reactions. Chemkin is a very good package for solving chemical reactions. It also utilizes Arrhenius equation for calculating the concentration and reaction rates of chemical reactions. Equation 14 represents the Arrhenius equation.

$$k = Ae^{\frac{Ea}{RT}} \quad (14)$$

k= Rate constant, A= Pre-exponential factor (collision frequency factor), Ea= Activation Energy

R= Gas Constant, and T= Temperature

Chemkin model with 243 species soot particle tracking was selected. Chemkin considers the thermodynamic data, surface chemistry, and surface kinetics of the species while solving the chemical reactions. Properties of n-decane were assigned to fuel. Chemkin has the capability of calculating the ignition delay by the reaction reduction mechanisms.

4.1.3 Spray Model

The solid cone injector was selected under the tab of spray models. Nozzle direction, nozzle location, and nozzle hole diameter was defined. Table 3 shows the different parameters that were defined regarding the solid injector

Table 3 Solid Injector Parameters

Solid Injector Nozzle Parameters		
Nozzle Location		
Coordinate system	**Cylindrical**	**Units**
R	0.1	cm
θ	22.5	degrees
A	9.8	cm
Spray Direction		
θ	110	degrees

φ	22.5	degrees
Nozzle Diameter	0.1	mm

The spray atomization and droplet breakup of solid-cone sprays are modeled by the Kelvin-Helmholtz/ Rayleigh-Taylor (KH /RT) hybrid breakup model. Table 4 presents the parameters that were selected for injection and spray initialization.

Table 4 Parameters for spray and Injection initialization

Number of Parcels	3000
Inflow Droplet Temperature	320
Discharge co-efficient	0.7
Mean Cone Angle	15 degrees
Type of Injection	Pulsed
Wave Form of Injection	Square
Start of Pilot Injection	-10.8 CAD
Start of Main Injection	3.2 CAD
Duration of Injection	17.138

4.1.4 Boundary Conditions

Temperatures of the piston, head and liner were specified. The conditions of periodicity was defined. Motion type of slider crank was selected. Sector angle was specified again. Forte sector mesh generator automatically specifies different regions as required by naming them as head, liner, and piston based on the input parameters. This makes the problem setup very easy.

4.1.5 Initial Conditions

The initial conditions were defined on the basis of composition of gas mixture. The composition of gas mixture used for EGR is shown

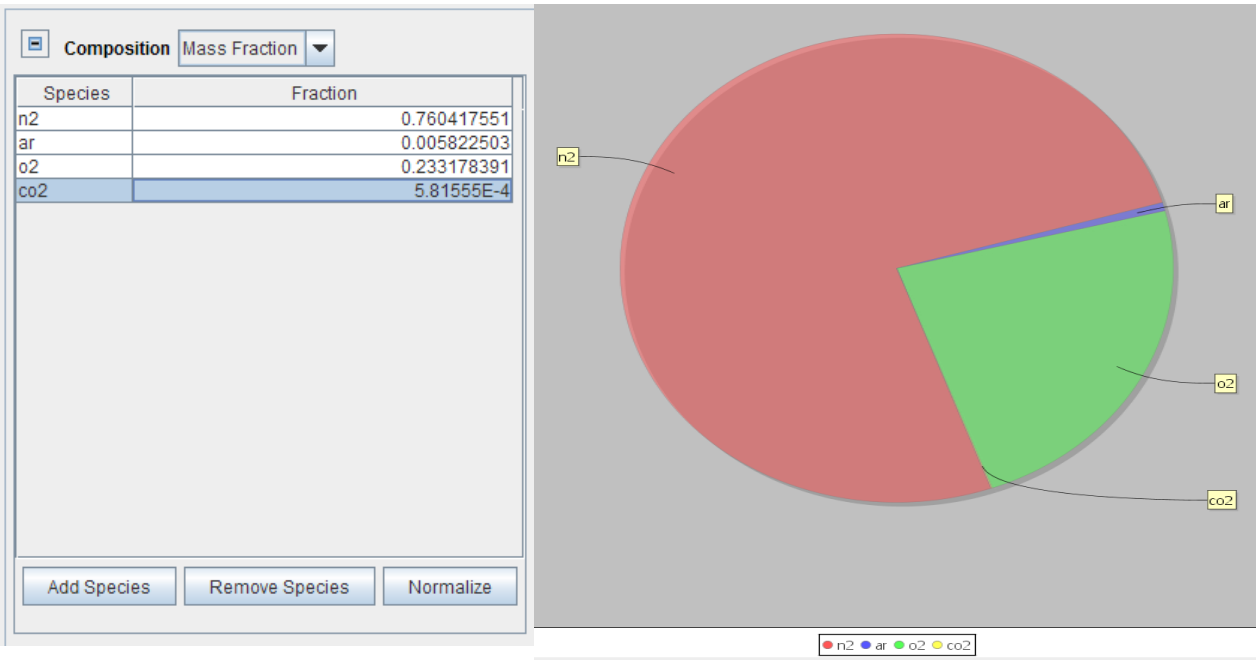

Figure 16 Composition of Gas mixture used in EGR

Temperature of gas mixture was set to 470K. Pressure of Gas mixture was set to 1.2 bar.

4.1.6 Simulation Controls

In simulation controls initial crank angle from where the cycle should start is provided. And final crank angle is also defined. Engine RPM (revolutions per minute) and final and initial time step of the simulation were also defined. The parameters set for the simulation are mentioned below

- Initial Crank Angle= -165 CAD
- Engine RPM = 1664
- Final Crank Angle= 130 CAD
- Initial simulation time step= 5.0E-7 sec
- Final simulation time step= 5.0E-6 sec
- The technique of dynamic cell clustering was used to reduce the run time for chemistry intensive simulations

4.2 Comparison of Experimental and Numerical Data

The basic benchmarking technique used in the research is based on the estimation of Accumulated Chemical Heat release rate (ACHR). ACHR is the primary indicator that can be used to evaluate the status of combustion and fuel burning. Equation 15 shows the formula for ACHR

$$\text{ACHR (Joules)} = (Mf).(LHVf) \quad (15)$$

Mf= mass of fuel, LHVf = Lower heating value of fuel

4.2.1 Water Injection Case Benchmarking

The benchmarking for the water injection was done in two steps. In first step, the ACHR value obtained from the formula and numerical solution were compared. In second step, the pressure curves obtained from experiment and numerical solution were compared. The first step is shown below

$M_f = 25.45$ mg, $LHV_f = 44.56$ MJ/kg

ACHR=25.45 (mg).44.56 (MJ/kg) = 1134.052 Joules

Numerically calculated value of ACHR for WI case= 1111.52 Joules

Fig. 17 shows the plot of ACHR for the water injection case

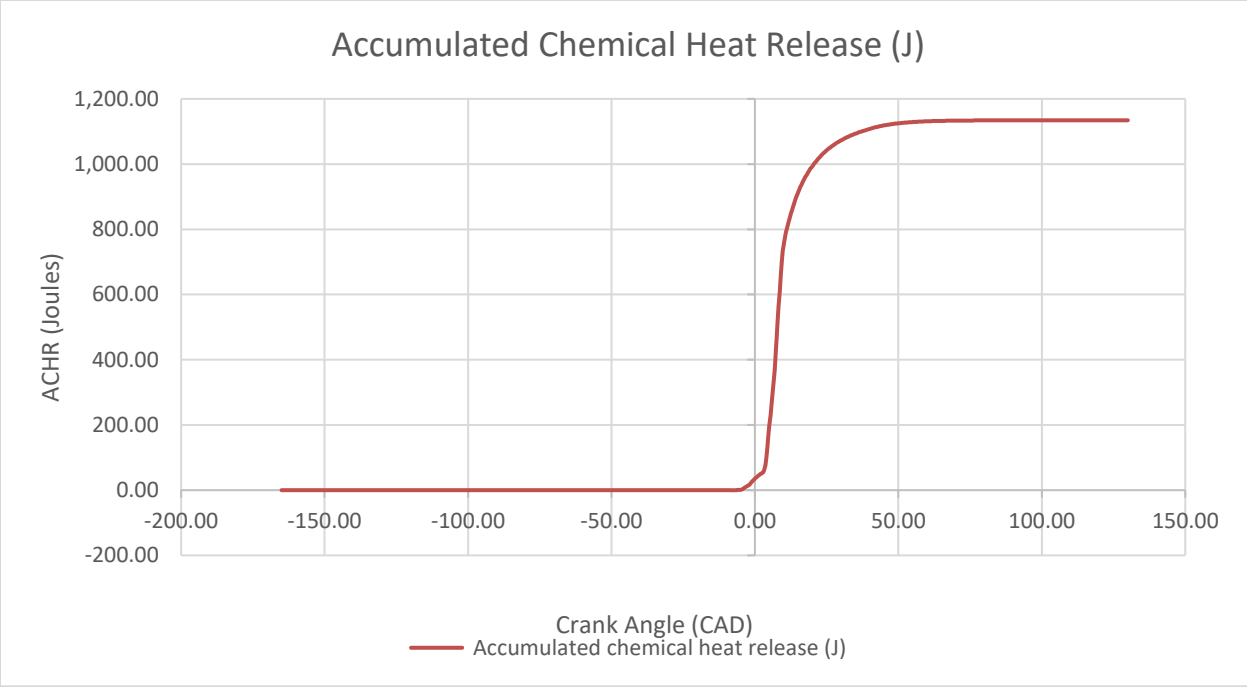

Figure 17 Plot of ACHR for the water injection case

Figure 18 shows the experimental and numerical pressure plots

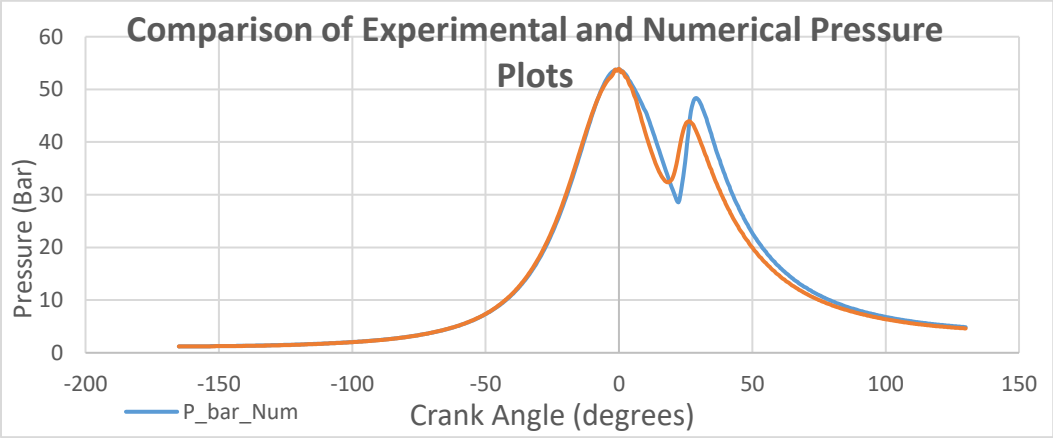

Figure 18 Experimental and numerical pressure plots

4.2.2 EGR Case Benchmarking

Theoretically ACHR should also be equal to the sum of work done and wall heat transfer. The formula for this proposition is shown below

$$ACHR \approx WD+WHT$$

Using this approach the EGR benchmarking was done in addition to the comparison of numerically calculated ACHR value and analytically calculated value (from formula). Fig. 19 shows the plot of ACHR and sum of work done and wall heat transfer.

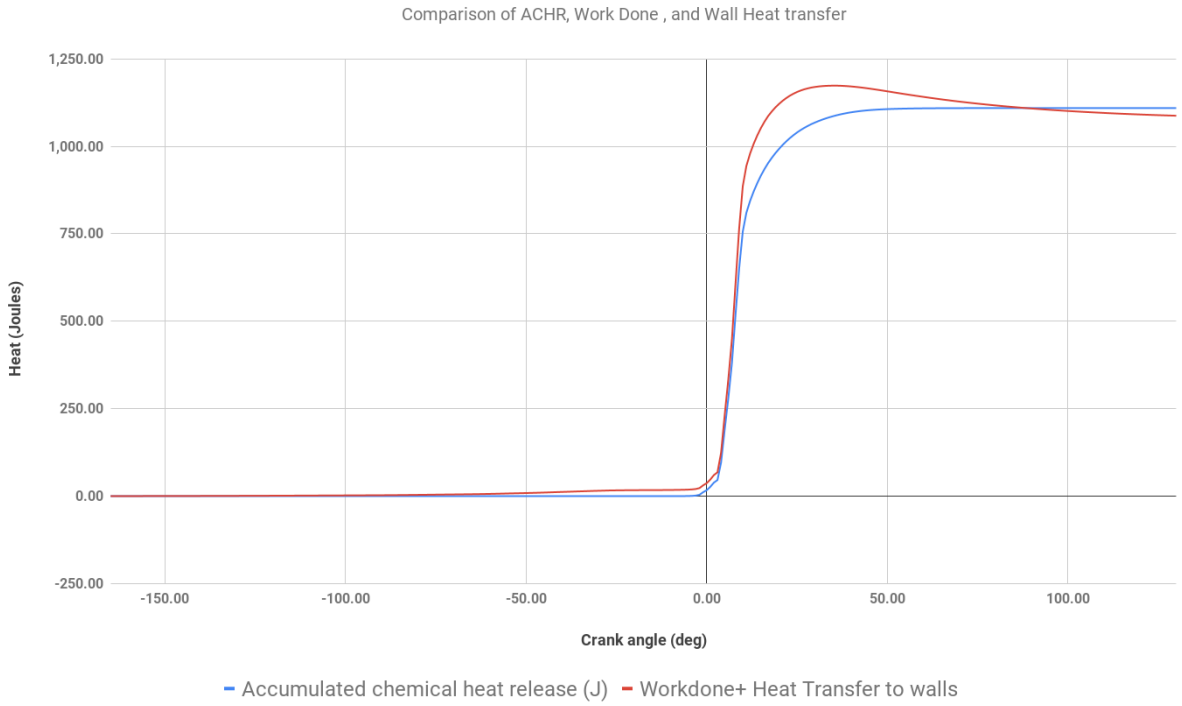

Figure 19 Plot of ACHR and sum of work done and wall heat transfer.

There is a very close agreement between the experimental and simulation results and the percentage error or difference is very less for both EGR and WI cases. This leads to the conclusion that the numerical model and approach used for the simulation of EGR and WI process in ANSYS Forte is correct. As the bench marking was complete, the next step was to perform the parametric study.

CHAPTER 5: PARAMETRIC STUDY AND CONCLUSION

Both EGR and water injection reduce the temperature of the combustion chamber, which directly or indirectly reduce the peak combustion temperatures. The reduction of temperatures play a critical role in the formation of emission quantities. In order to properly compare which technique reduces the combustion temperatures more effectively, equal concentration by volume or mass should be injected. Figure 20 shows the reduction of temperatures when 0.058 percent of EGR and 3 percent of water is used for WI.

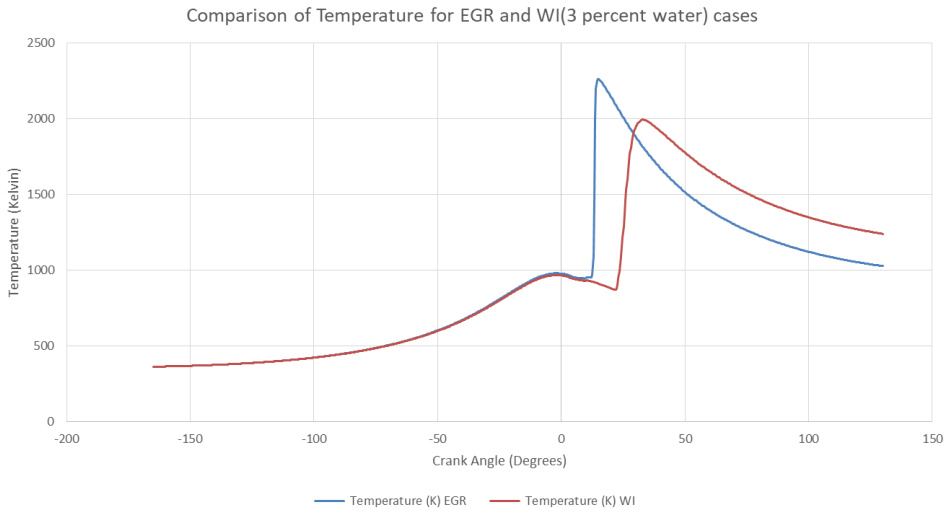

Figure 20 Reduction of temperatures when 0.058 percent of EGR and 3 percent of water is used for WI.

For the parametric study performed, four important parameters were studied. These parameters are

- Temperature of Gas Mixture (intake air temperature)
- Temperature of Fuel Injected
- Start of Injection (SOI)
- Duration of Injection (DOI).

5.1 Effect of Gas Mixture Temperature on Emissions

The gas mixture temperature is actually the temperature of intake air mostly, however, the determination of exact temperature if the cycle is started at any position of the crank angle other that zero is a complex task. In such cases it is better to refer the temperature as 'gas mixture temperature'. And in this case especially when EGR is used a mixture of gases is formed. Three different temperatures for the gas mixture have been simulated. During simulation of the each temperature case, all other parameters were kept unchanged. The temperatures that were selected for the parametric study of gas mixture temperatures were 480 K, 500 K, and 600 K. Figure 21, 22, 23, and 24 show the effect of three different gas mixture temperatures on the formation of CO, NO, NO_2, and Soot formation respectively.

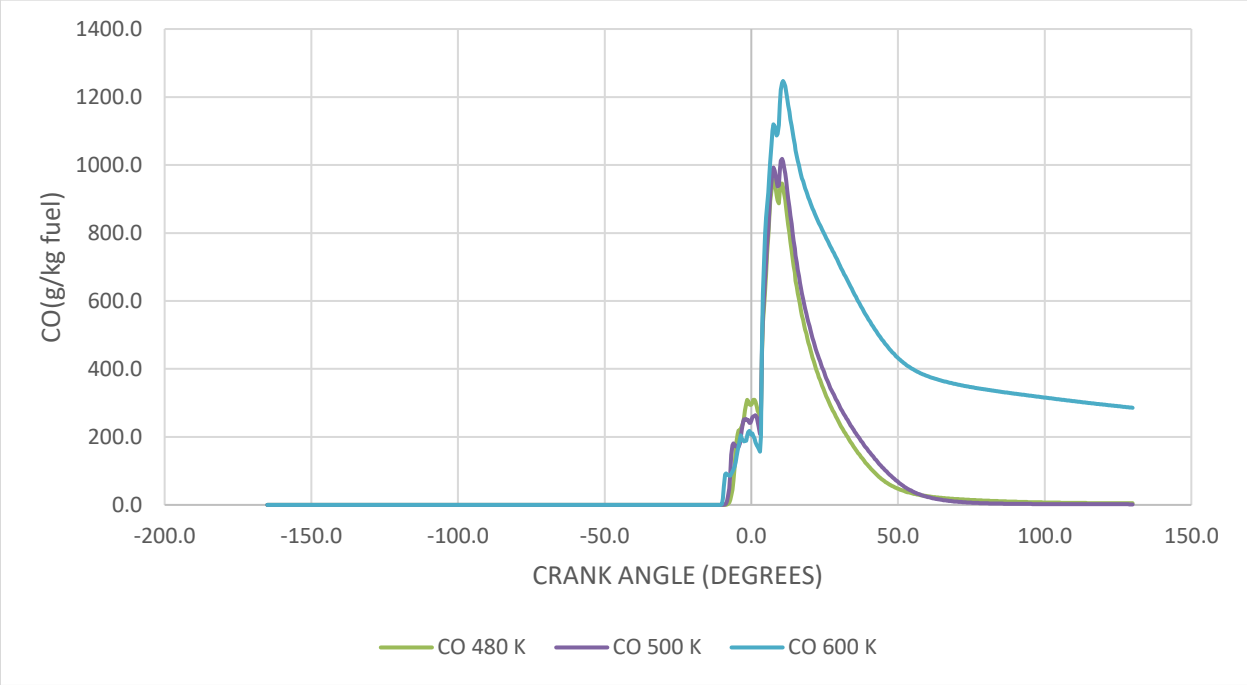

Figure 21 Effect of gas mixture temperature on CO emission

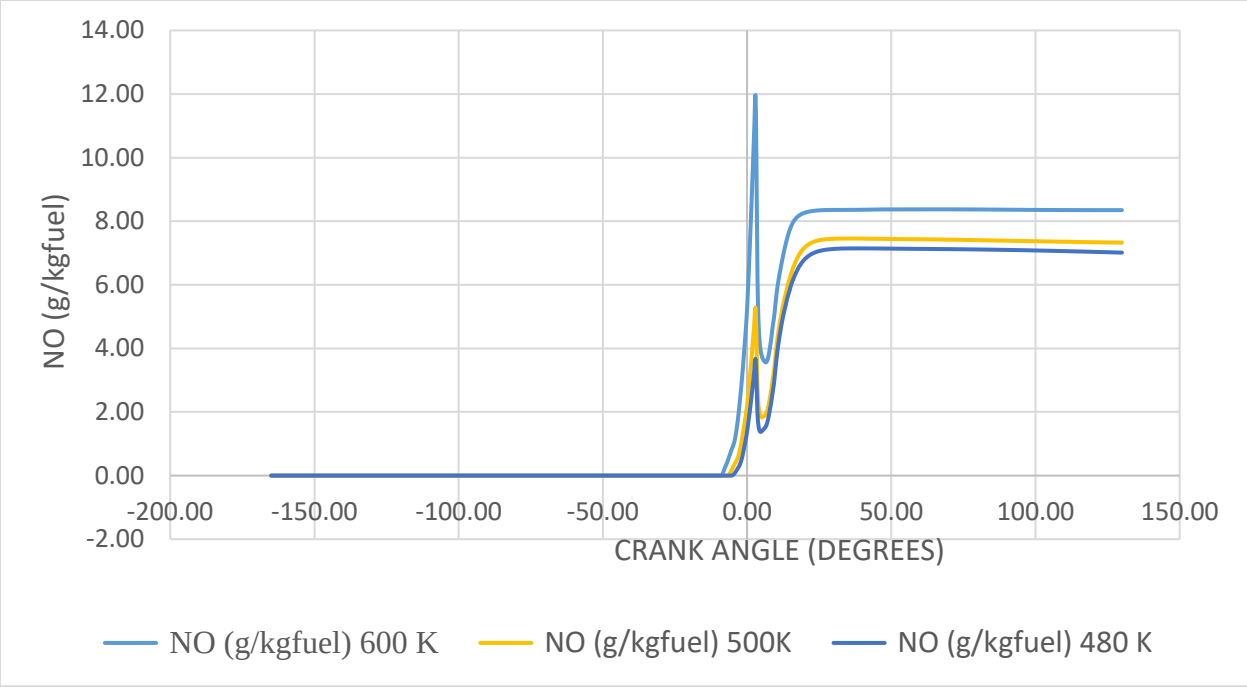

Figure 22 Effect of gas mixture temperature on NO emission

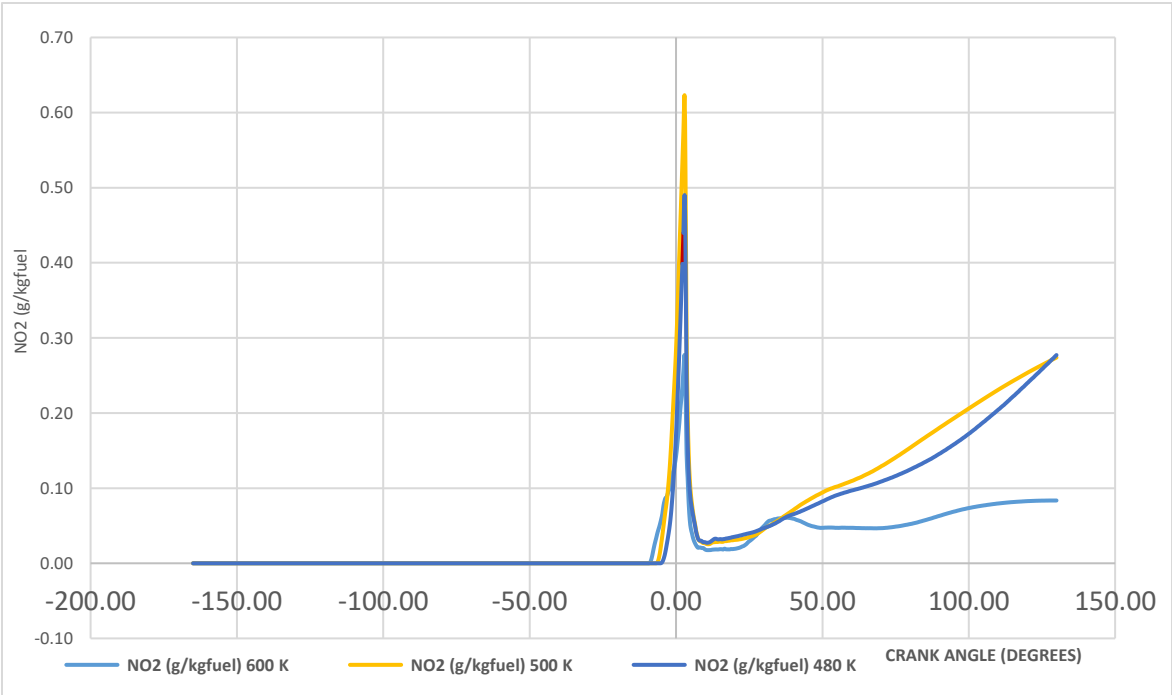

Figure 23 Effect of gas mixture temperature on NO2 emissions

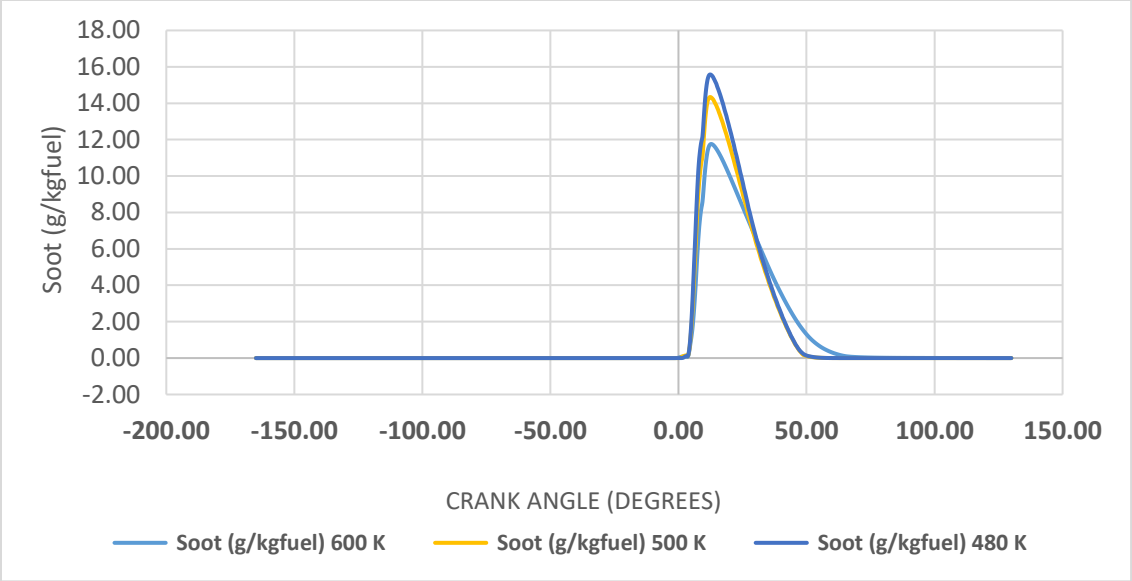

Figure 24 Effect of gas mixture temperature on soot formation

There is an increase and decrease in the emission quantities observed, as the gas mixture temperature changes. Table 5 shows the increment and decrement trend of quantities of the emissions as the temperature of the gas mixture changes

Table 5 Trend of variation in quantities with the variation of gas mixture temperature

Emission Parameter	**Effect**
CO	Increases
NO	Increases
NO2	Normally increases but decreases when temperature is rapidly increased
SOOT	Decreases

The percentage change helps in the exact quantification on the basis of which we can infer how much the quantity of emission has increased or decreased. It would be useful for understanding purposes to study the change in percentages of the emissions as per 20 K increase

in temperature. Table 6 shows the percentage change in the quantities of the emissions as per 20K increase in the gas mixture temperature

Table 6 Percentage change in the quantities of the emissions as per 20K increase in the gas mixture temperature

Increment in Intake Air Temperature	**20 K**
CO	4.587 % Increase
NO	2.74 % Increase
NO2	25.64 % Increase
SOOT	5.96 % decrease

5.2 Effect of Fuel Droplet Temperature on Emissions

There is a limited extent up to which the temperature of the fuel in the diesel engines can be varied due to the compression ignition. Therefore a very small difference in the variations of fuel temperatures were studied. Effect of increase in temperature of the fuel on emissions was studied by simulating three different temperatures. These temperatures are, 300 K, 305K, and 320 K. Figure 25, 26, 27, and 28 show the effect of temperature increase on the formation of CO, NO, NO_2, and Soot formation respectively.

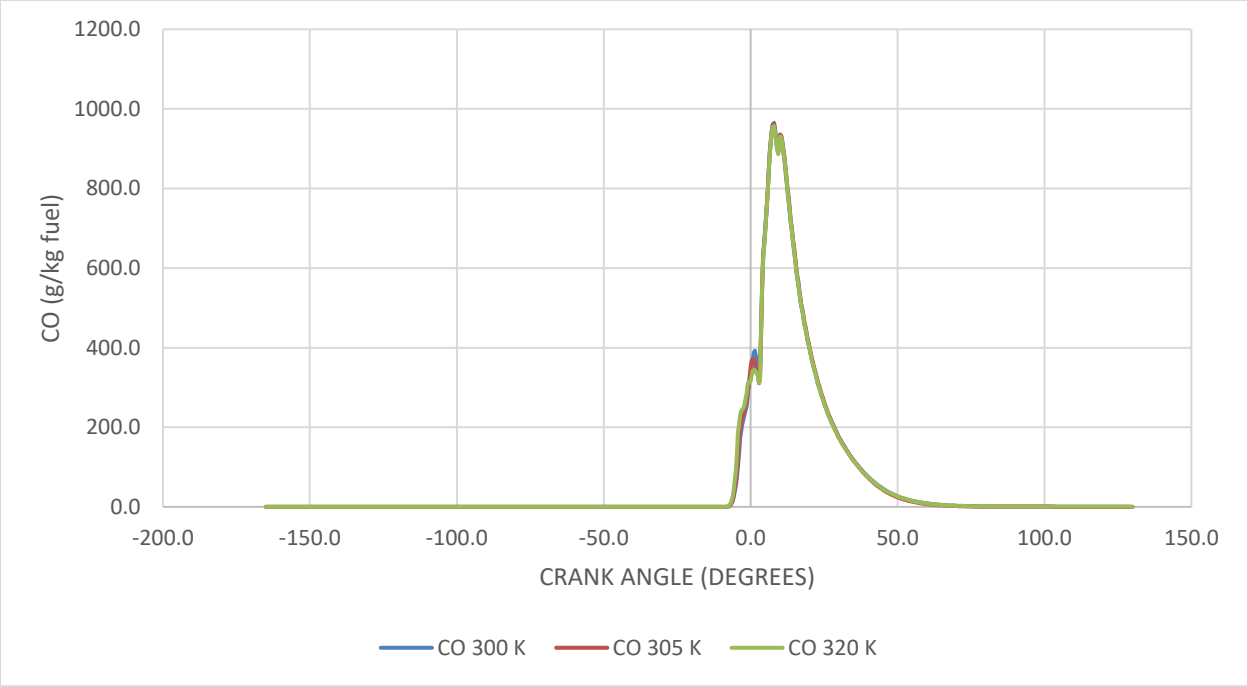

Figure 25 Effect of Increase in the fuel temperature on CO formation

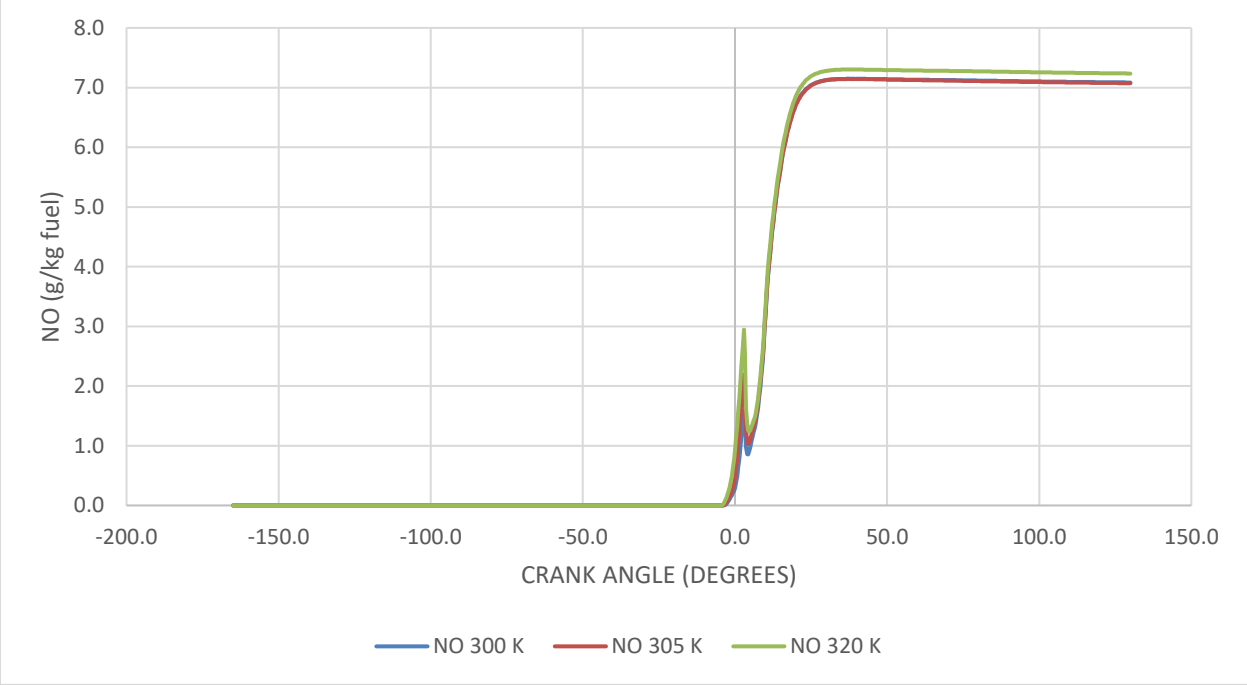

Figure 26 Effect of Increase in the fuel temperature on NO formation

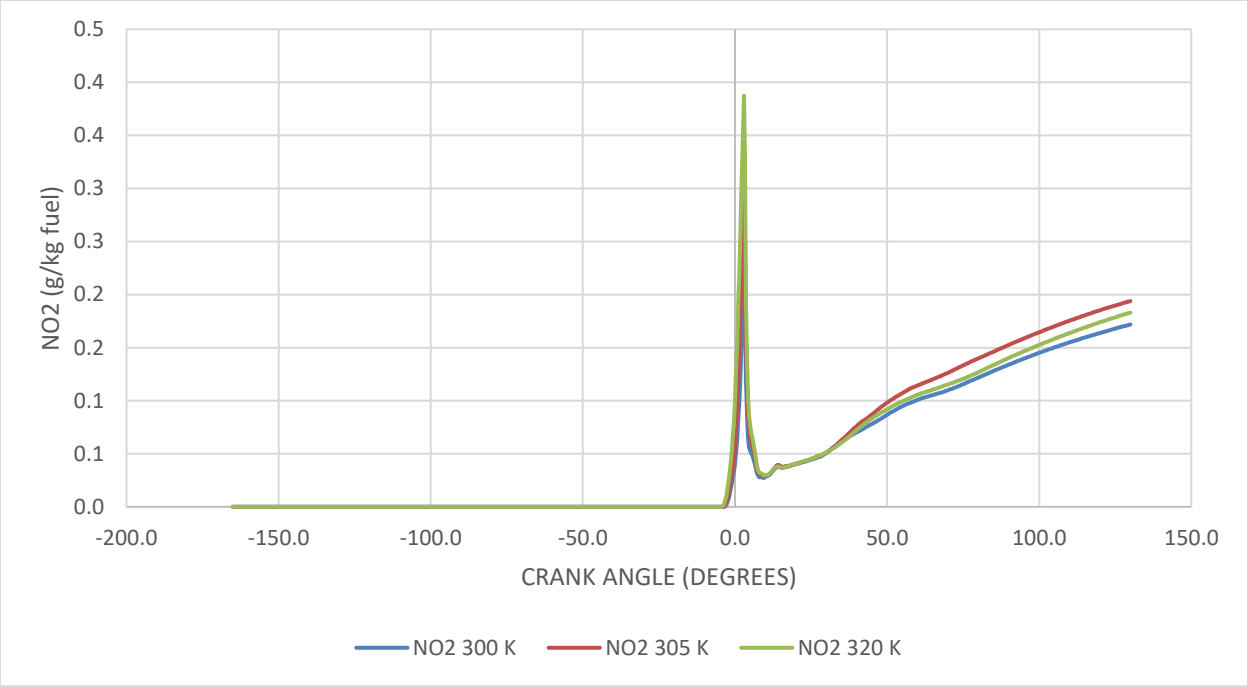

Figure 27 Effect of Increase in the fuel temperature on NO2 formation

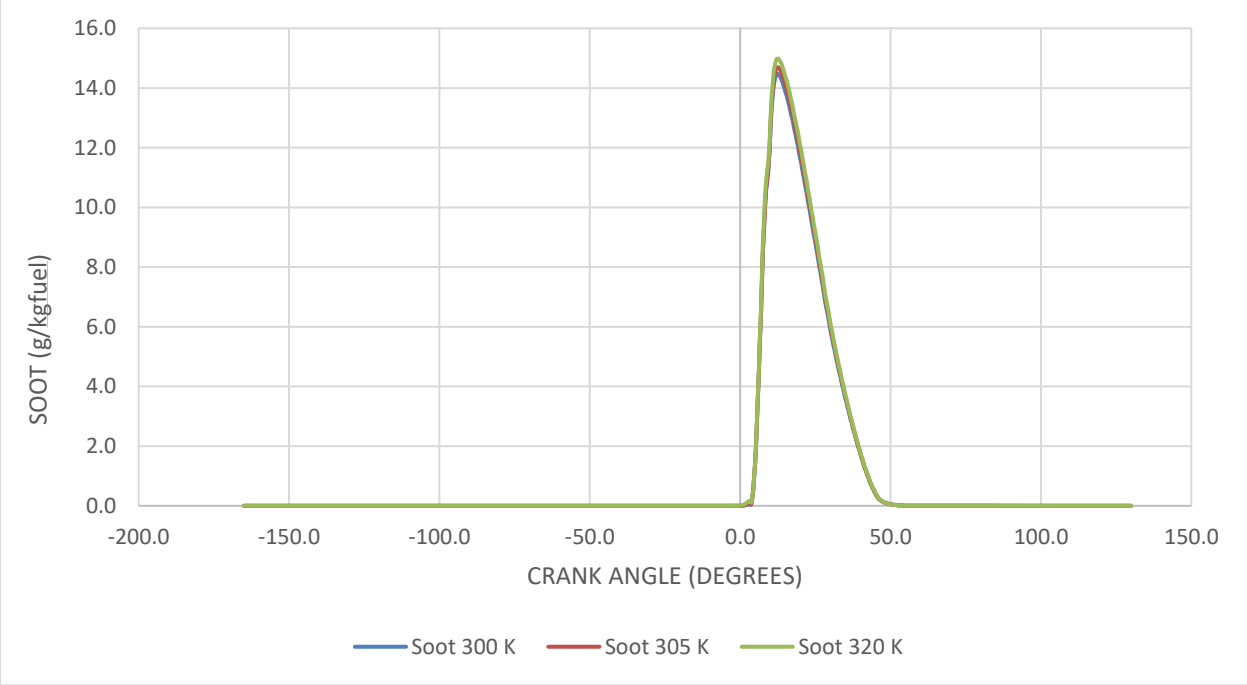

Figure 28 Effect of Increase in the fuel temperature on soot formation

Table 7 and 8 present the effect of increase in fuel droplet temperature of 10 K and 15 K on the emissions respectively.

Table 7 Effect of increase in fuel droplet temperature of 10 K on emisssions

Increment in Fuel Droplet Temperature	**10 K**
CO	0.41 % Decrease
NO	0.05 % Increase
NO2	36.36 % Increase
SOOT	1.8 % Increase

Table 8 Effect of increase in fuel droplet temperature of 15 K on emissions

Increment in Fuel Droplet Temperature	**15 K**
CO	0.44 % Decrease
NO	2.26 % Increase
NO2	77.27 % Increase
SOOT	1.97 % Increase

5.3 Effect of SOI on Emissions

SOI is an important operating parameter in the diesel engines. The start of combustion, ignition, and burning of the fuel depends upon the timing of fuel injection. If the fuel is injected

very early, then it may result in no combustion or misfire, because the gas mixture would not be heated enough to support the compression ignition. As the present case involves two injection events, that are pilot and main injection, it was challenging to study the effect of start of both injections on the quantities of emissions. For the present case, effect of change in start of both main and pilot injections on the emissions was studied. Following four cases of the start of injection were studied.

- Start of pilot injection at -25 CAD, start of main injection at -10 CAD
- Start of pilot injection at -15 CAD, start of main injection at 0 CAD
- Start of pilot injection at -10 CAD, start of main injection at 3.2 CAD
- Start of pilot injection at 0 CAD, start of main injection at 12 CAD

Figure 29, 30, 31 and 32 show the effect of start of injection on the formation of CO, NO, NO_2, and Soot formation respectively.

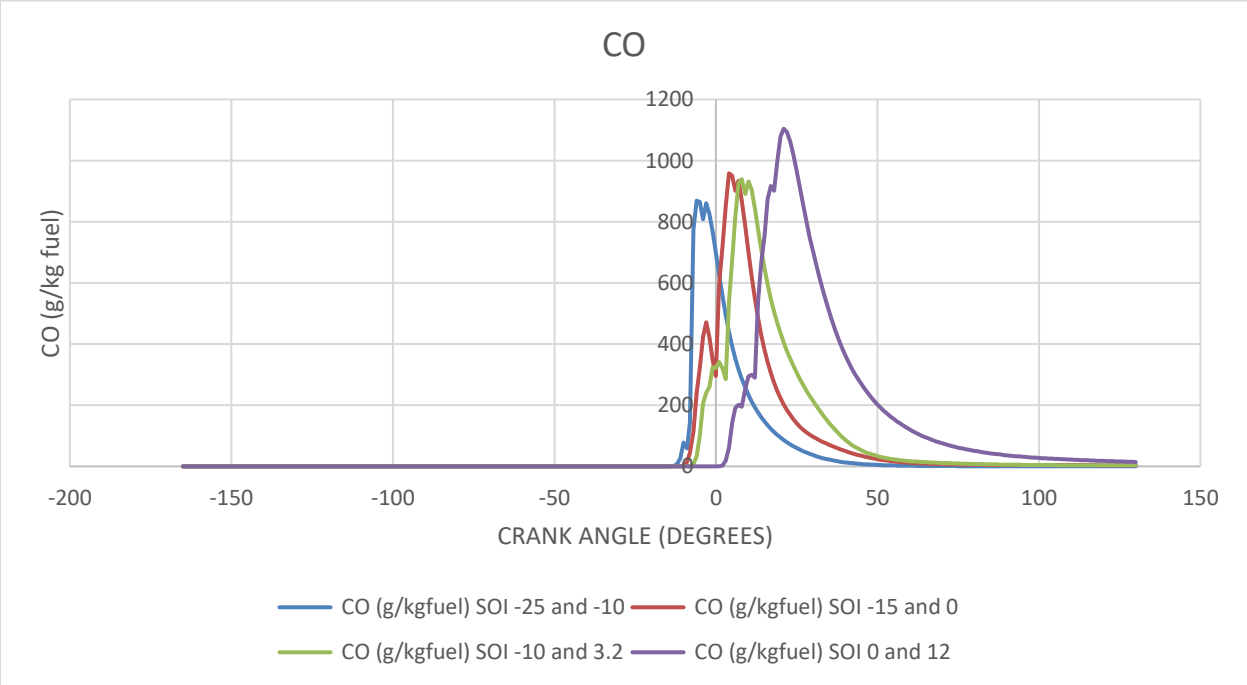

Figure 29 Effect of SOI on the formation of CO

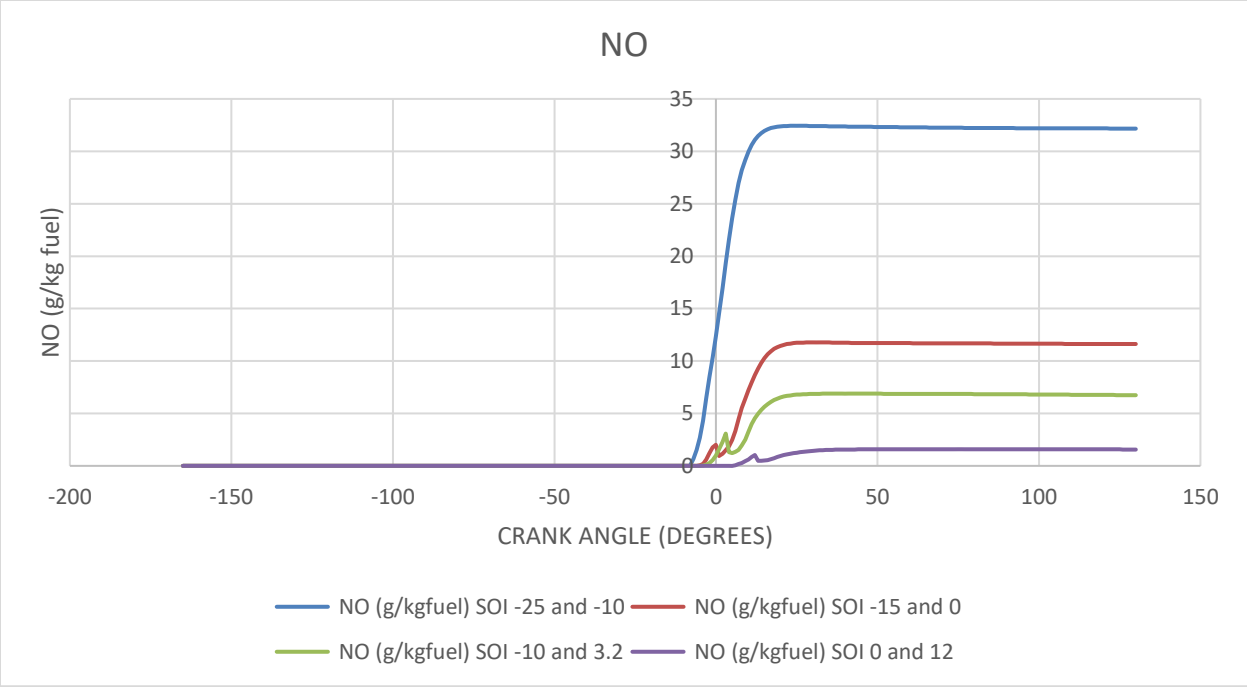

Figure 30 Effect of SOI on the formation of NO

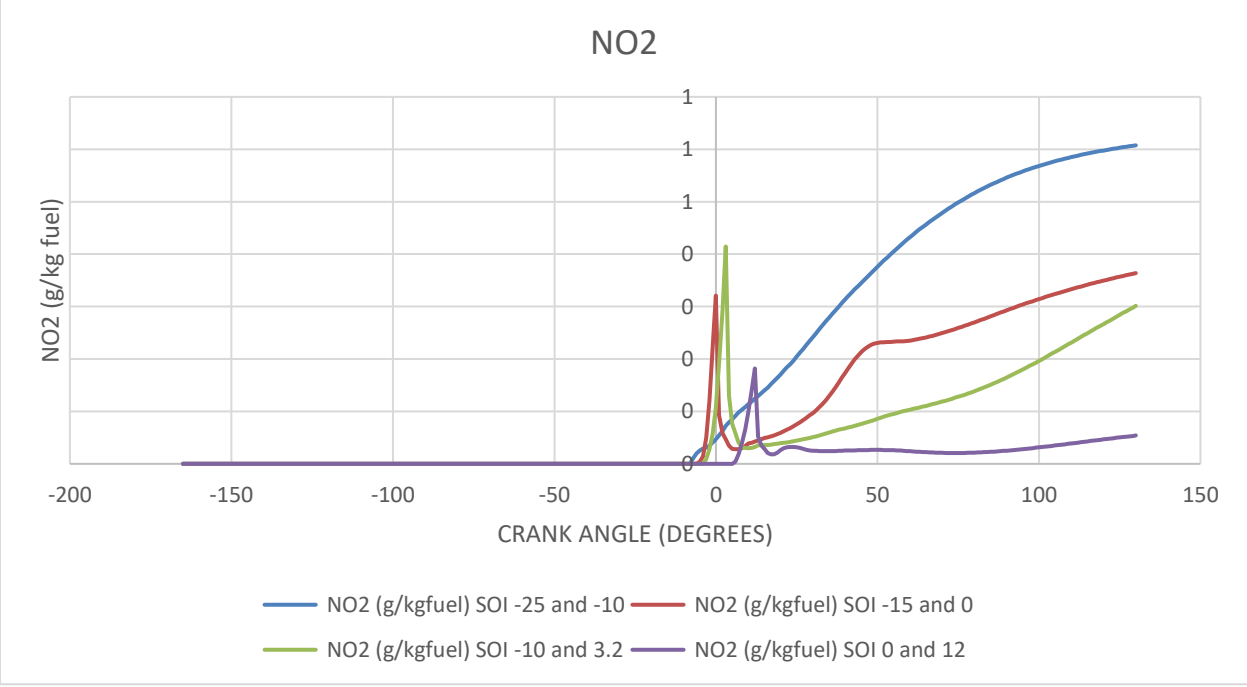

Figure 31 Effect of SOI on the formation of NO2

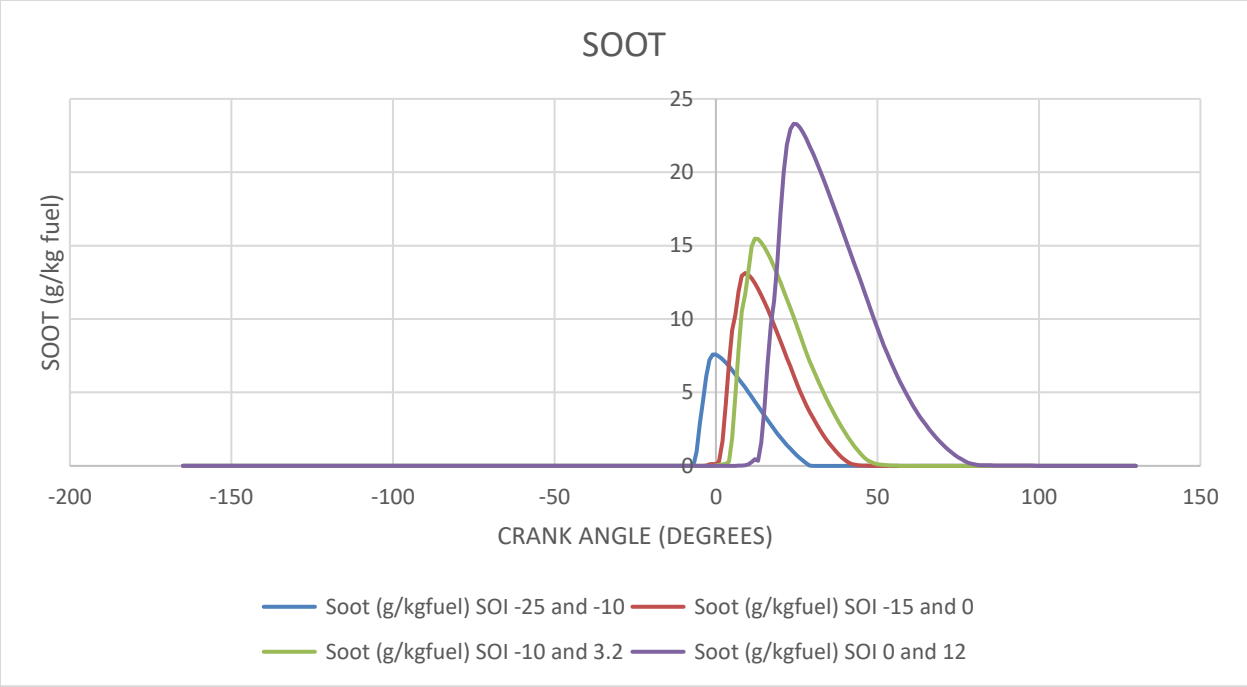

Figure 32 Effect of SOI on the formation of Soot

Table 9 shows the maximum value of the emission recorded at four cases of the SOI

Table 9 Maximum value of the emission recorded at four cases of the SOI

EMISSION PARAMETER	SOI Pilot (CAD)	SOI Main (CAD)	Maximum Value (g/kg fuel)
CO	-25	-10	869
	-10	3.2	931
	0	12	1104
NO	-25	-10	32
	-10	3.2	7
	0	12	2
NO2	-25	-10	0.181
	-10	3.2	0.414
	0	12	0.607
SOOT	-25	-10	8
	-10	3.2	15
	0	12	23

5.4 Effect of DOI on Emissions

Three cases for the duration of injection has been considered. The three values of DOI against which emissions were studied are, 10 CAD, 15 CAD, and 17 CAD. Figure 33, 34, 35, and 36 present the trend of formation of CO, NO, NO_2, and soot formation.

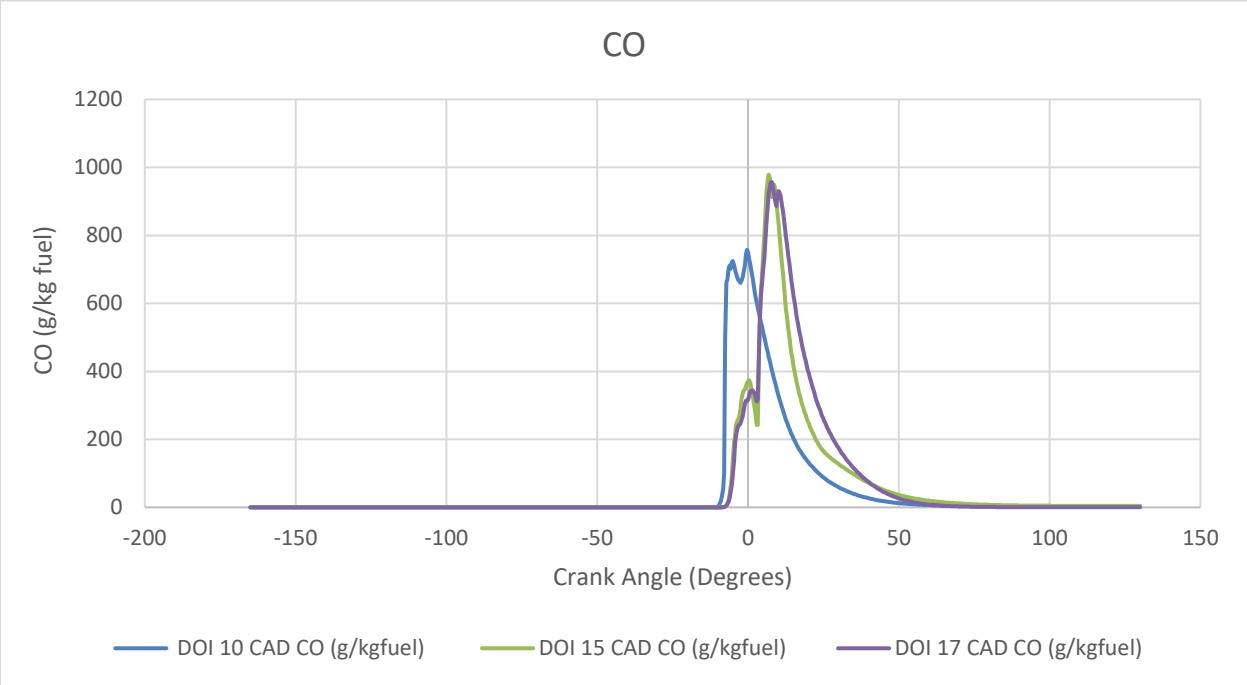

Figure 33 Effect of change in DOI on CO formation

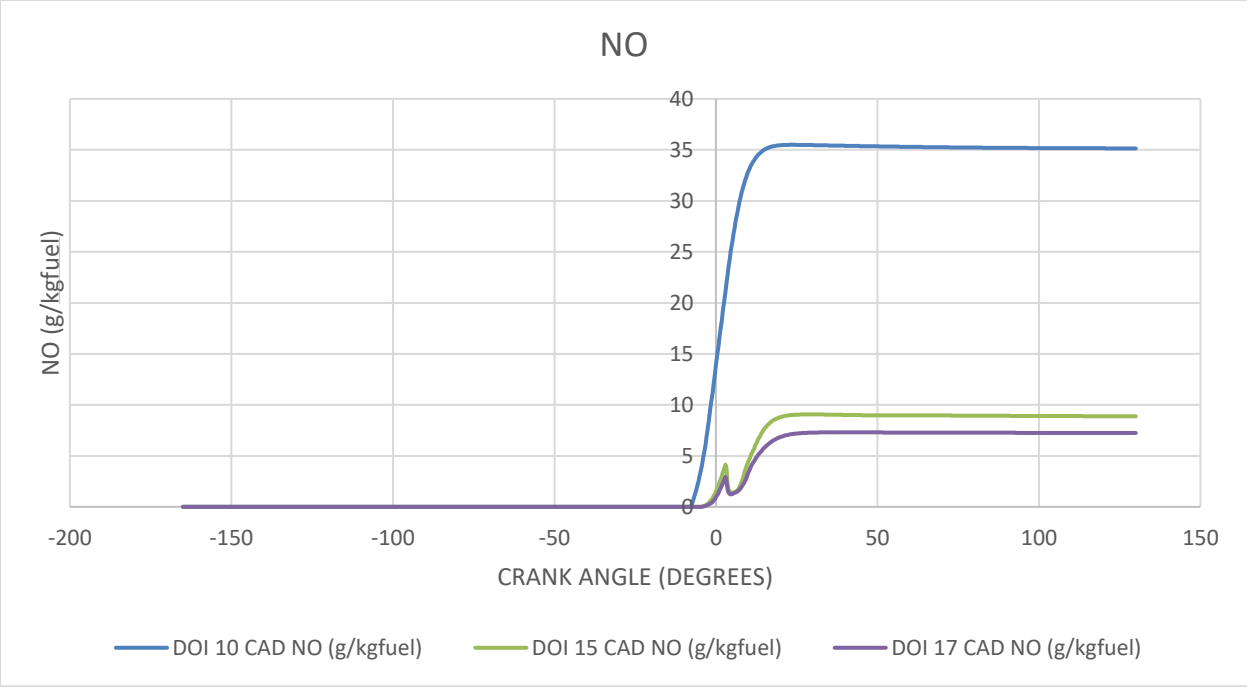

Figure 34 Effect of change in DOI on NO formation

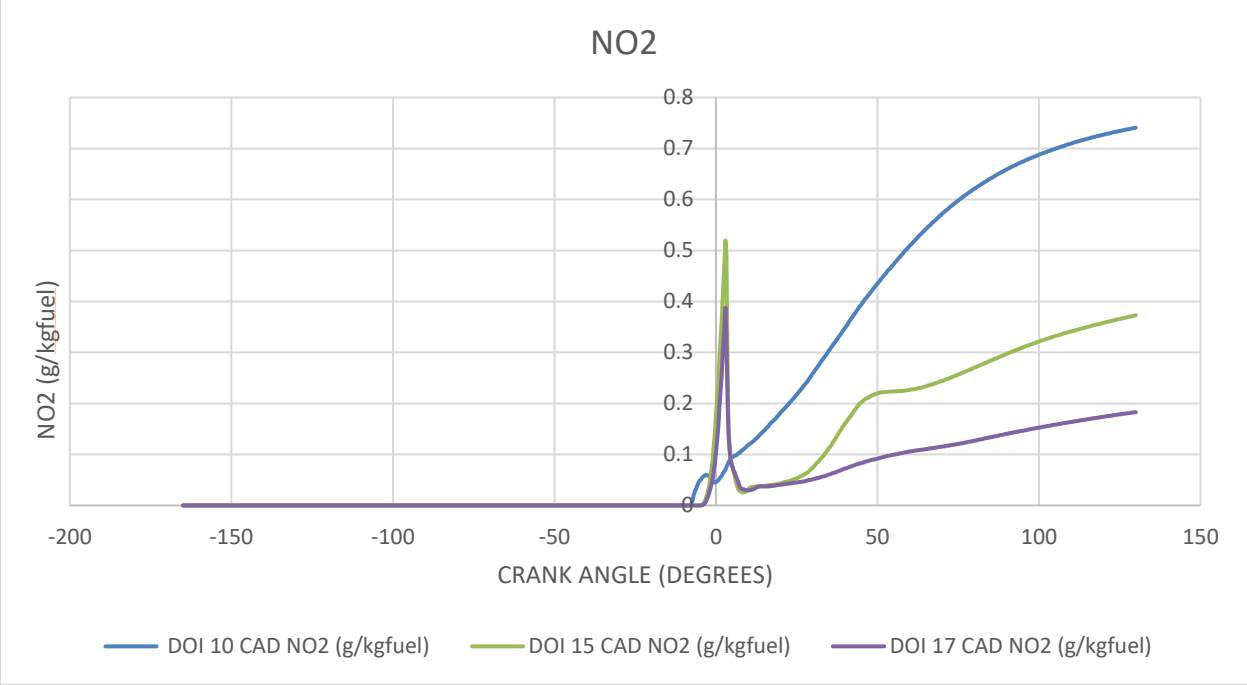

Figure 35 Effect of change in DOI on NO2 formation

Figure 36 Effect of change in DOI on soot formation

Table 10 shows the effect of increase in duration of injection on the formation of emissions.

Table 10 Effect of increase in duration of injection on the formation of emissions.

Emission Parameter	**Effect**
CO	Increases
NO	Decreases
NO2	Decreases
SOOT	Increases

Table 11 and 12 show the percentage increase and decrease in the quantity of emissions when an increase in duration of injection of 5 CAD and 7 CAD was done.

Table 11 The effect of increase in duration of injection of 5 CAD on percentages of emissions

Increment in Duration of Injection	**5 CAD**
CO	29.42 % Increase
NO	74.52 % Decrease
NO2	31.08 % Decrease
SOOT	19.85% Increase

Table 12 The effect of increase in duration of injection of 7 CAD on percentages of emissions

Increment in Duration of Injection	**7 CAD**
CO	27.47 % Increase
NO	79.48 % Decrease
NO2	47.7 % Decrease
SOOT	82.05 % Increase

5.5 Concluding Remarks

Start of injection and duration of injection have significant effect on the emission characteristics

Intake air temperature affects the soot production. Normally soot production is reduced with increase in temperature

Fuel droplet temperature has very significant effect on NO2 emissions, while it has a little impact on other emissions. Cold air is less dense and contains higher oxygen concentration

Increased oxygen in combustion chamber leads to complete combustion and oxidation of CO and hydrocarbon emissions. The higher intake temperature reduces the oxygen availability that leads to incomplete combustion and misfires, resulting in more emissions and increased fuel consumptions. Injection timing directly affects the engine performance and emissions

The injection duration directly affects the flow rate and injection pressures of the fuel. Increase in the injection duration decreases the flow rate of the fuel injected

Start of injection influences the emissions due to changes in premixing ratios. The emissions' quantities are dependent upon the reaction rates and the quantity of the fuel injected during the premixing and combustion processes.

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