Numerical Simulation of Evaporation in Fuel Spray Droplets in a Diesel Engine

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Thesis Supervisor's Signature: _____

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Abstract

The objective of present thesis is to model thermophysical process of evaporation of diesel fuel spray in the combustion chamber of diesel engine numerically. Evaporation of fuel droplets has an impact on the efficiency and exhaust of engine that is quiet obvious in the literature. In this work evaporation of diesel fuel is modeled numerically in Ansys. Presents work takes into account the turbulence effects generated into the engine cylinder due to high pressure and high temperature inside. In the this work evaporation of different diesel fuels is modelled numerically taking into account the turbulence effects present in the cylinder due to high temperature and pressure using the RANS turbulence model. A realizable RANS turbulence model is applied to analyze the effects of turbulence. RANS model is used in the present study due to its low computation cost and an appreciable accuracy for the present problem. Evaporation of n-heptane and n-decane is governed by the conservation equations of mass, energy, momentum and species transport. Heat transfer to drop and mass lost by the drop is governed by the discrete phase model equations. Results are plotted by varying the droplet diameter and temperature. Results include the vapor mass fraction of droplet, decay in droplet diameter, and increase in the droplet temperature, effect on the velocity of droplet and temperature changes in the cylinder due to evaporation of fuel. It is observed that size of droplets, temperature of droplets, ambient temperature, injection pressure and velocity, and turbulence intensity have an acceptable effect on the evaporation time of diesel fuel droplets in the engine cylinder. Small droplets need short time to evaporate and droplets with larger diameter require more time to evaporate completely. Droplets having high temperature have short evaporation time and high evaporation rate. High ambient temperature also shows a good effect on the evaporation rate of droplets. Finally proposed evaporation model is implemented on the diesel engine and results are described.

Key Words: *Evaporation, RANS, Droplet, Diesel Fuel*

Table of Contents

List of Figures

x

List of Tables

CHAPTER 1:

INTRODUCTION

1.1   Overview

Automobiles manufacturing companies aim to develop the internal combustion   engines with high output power and appreciable high efficiency keeping in mind the highly sophisticated emission standards that are becoming rigorous day by day. To achieve the high emission standards a lot of work has been done in past few decades by developing some new techniques [1, 2]. There are different thermal and chemical processes in the engine cylinder that control the exhaust and power output of internal combustion engine. Efficiency is also affected by these processes. These includes the air-fuel mixture preparation, spray breakup, evaporation, and combustion and exhaust gas after treatment. Air-fuel mixture preparation is the most important phenomenon inside the engine cylinder that controls the engine efficiency and output power. After that injection type, penetration length, and evaporation of fuel droplets are the processes that are related to the complete combustion of fuel in the internal combustion engine [3]. From afore mentioned phenomena the importance of evaporation of fuel droplets is very well known from the literature and is not fully understood at high operating conditions [4]. The distribution and concentration of vapors of fuel in the engine cylinder directly affects the combustion performance, engine efficiency and exhaust gas control in the DI engines that are being developed by the automobile makers currently [5]. Although new techniques are being developed by the automakers to aid in the reduction of emissions but this is still a continuous subject of environmental care. Exhaust emissions of diesel fuel internal combustion engines are the main causes of air pollution. Nitrogen oxides are emitted from the exhaust of internal combustion engines and make nitric oxide when mix with air present in the atmosphere that is a major pollutant in atmosphere. Evaporation of diesel fuel droplets has been investigated thoroughly in the recent past decades both numerically and experimentally. Evaporation phenomenon has many important industrial and commercial applications and hence it is a topic much interest and importance [6-8]. One of the

prominent example is the evaporation of fuel droplets in the engines during the fuel combustion to produce power. Evaporation also finds it vast applications in the working of gas turbines. Some worthy investigations about droplet vaporization are presented in [9-12]. Evaporation of multi-component diesel fuel droplets began with Landis and Mills [13] followed by Sirignano and Law [14-15]. Evaporation of diesel fuel droplets occurs at high operating conditions i.e. high temperature and pressure. When fuel is injected in form of spray in the engine cylinder at the temperature greater than its saturation temperature then it becomes superheated and its temperature and pressure exceeds the critical value [16, 17]. Evaporation of supercritical droplets has been investigated by many researchers numerically and experimentally in [18-23]. In this work a new droplet vaporization model is presented that takes into the turbulence effects present in the combustion chamber.

1.2   Applications of Evaporation

Evaporation is an important phenomenon and finds it various applications for commercial and industrial purposes. It also has many practical applications in our daily life. Some of the important applications of evaporation are given below.

i.   Steam jacketed kettle.
ii.   Horizontal and vertical tube evaporators.
iii.   Evaporation process is used to manufacture the different biological products e.g. insulin enzymes and hormones.
iv.   Evaporation process is used in the preparation of bulk drugs in pharmaceutical industry.
v.   Evaporation is used in the demineralization of water.
vi.   Evaporation is used in domestic refrigerators to produce the cooling effect.
vii.   Cooling of water in earthen pots in hot summer.
viii. Drying of wet clothes in sunshine.
ix.   In working process of desert coolers.
x.   In wilting of plants.
xi.   Evaporation of fuel in engine cylinder.

Figure 1.1: Steam jacketed kettle
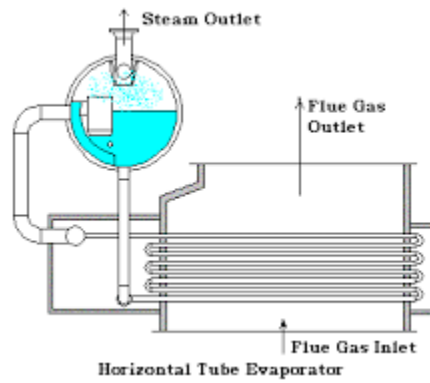
Figure 1.2: Horizontal tube evaporator
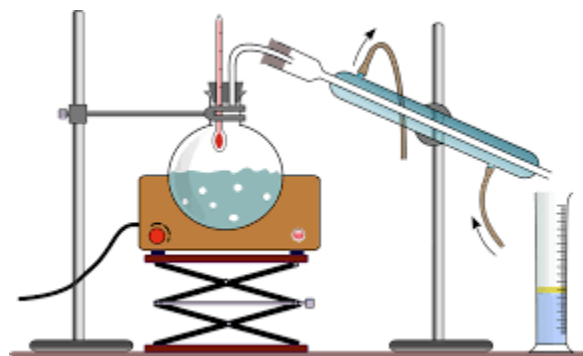
Figure 1.3: Demineralization of water
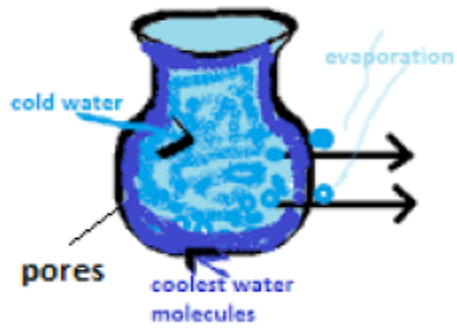
Figure 1.4: Evaporation of water in earthen pots
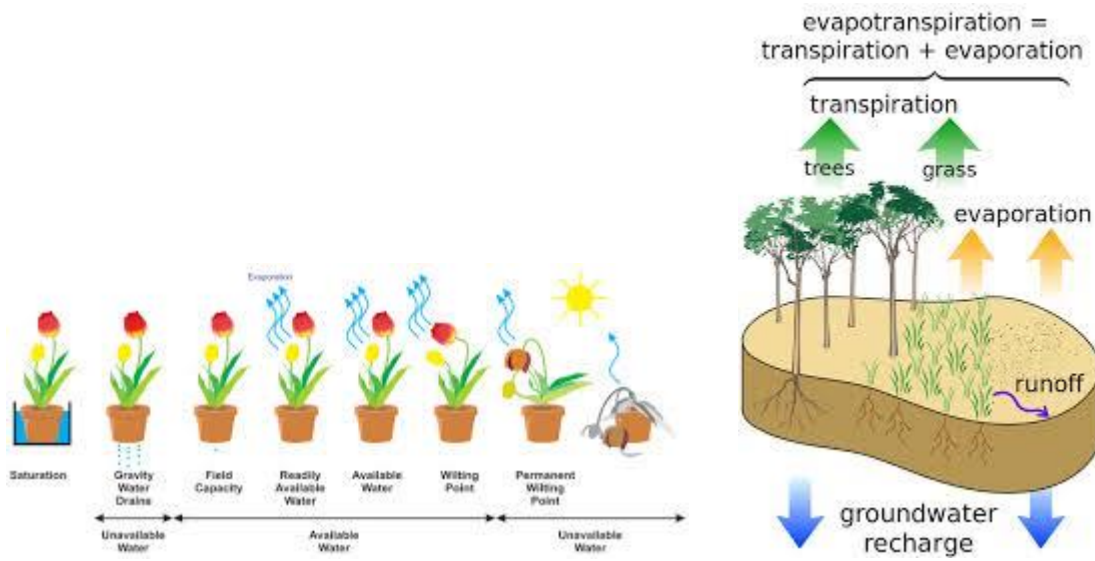
Figure 1.5: Wilting of plants
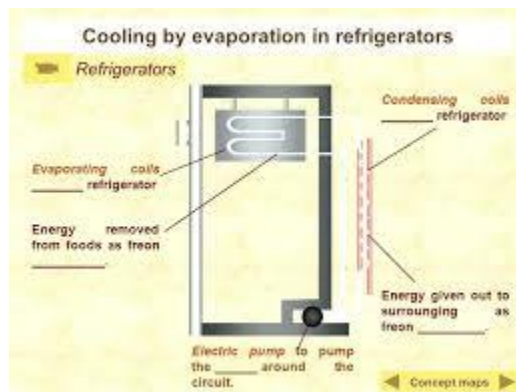
Figure 1.6: Evaporation in refrigerator
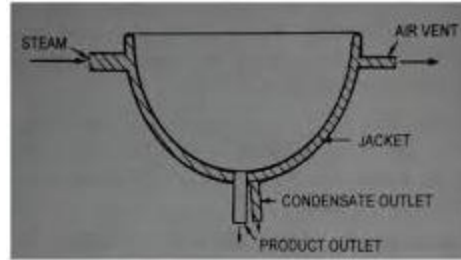
Figure 1.7: Evaporation in pan

1.3 Motivation

Automobile industry is growing day by day and enormous improvements have been seen in the development of engines in the past few decades. Improvements in the diesel engine are taking place constantly to achieve high efficiency and better fuel emissions to clean the environment from the pollution of burnt gases that emits from the engines exhaust. Diesel engines are being used extensively in the daily life for most commercial and industrial purposes due to its high power and torque. There are different applications where high power and torque is required to perform the work e.g. cranes and heavy duty trucks and buses. Due to application of high loads and to get the better fuel economy and emissions developments in the diesel engine is a constantly growing subject to achieve the high efficiency of engine. There are different thermodynamic and chemical processes that take place in the combustion chamber of I.C engines. Efficiency of engine highly depends upon the process and many factors affect these processes. One of them is evaporation of fuel droplet before combustion in the engine cylinder. Efficiency of engine is directly affected by the evaporation of fuel droplets in the engine cylinder. Evaporation of fuel is a subject of much importance and a handsome work has been done on it. But a complete picture of evaporation processes in the engine cylinder is very difficult to observe due to high operating conditions experimentally. There are many factors upon which evaporation of fuel depends in the engine cylinder e.g. velocity of spray, droplet size, ambient temperature and pressure, injection pressure and droplet temperature. Turbulence is produced in the engine cylinder due to high temperature and pressure of fuel. This an important parameter that also affects the evaporation of fuel spray. Incomplete evaporation in the combustion chamber results in the improper combustion of fuel that reduces the efficiency of engine and increases the pollution level in atmosphere due to

5

emission of unburnt gases in the environment. The present dissertation is motivated by the above considerations to improve the evaporation process in the diesel engine to achieve the better fuel economy, efficiency and improved emissions.

1.4   Contribution

In modelling of diesel fuel evaporation effects of turbulence are taken into account using RANS turbulence model coupled with the discrete phase model and the species transport equation for particle mass diffusion. This model is coupled with the conservation equations of mass, energy and momentum. A novel approach is considered here by solving the discrete phase that is fuel droplets into the continuous phase present in the engine combustion chamber which is air. Decay of droplet diameter and increase in temperature is observed rigorously against the injection time. Complete evaporation time is predicted by the model for different droplet sizes. Droplet size is also predicted for the better evaporation to produce the efficient combustion. Furthermore, a parametric study is carried out predict the droplet behavior under different temperatures and sizes. The main objective of this parametric study is to achieve a practically acceptable size of droplet to completely evaporate in the engine cylinder for better combustion to achieve high efficiency.

1.5   Thesis outline

Present dissertation is comprised of six chapters that are described below.

Chapter one consists of the overview and applications of evaporation process in different fields. In chapter two a detailed literature view is presented for evaporation of diesel fuel droplets. In chapter three detailed mathematical modelling of model is described. Chapter four consists of the model validation and verification. In chapter 5 detailed results and discussions are presented for diesel fuel droplet vaporization. Chapter 6 consists of conclusion and future work that can be performed from this research work. The objective of this thesis is to simply model the evaporation process of diesel fuel droplets under high operating conditions i.e. high temperature and pressure by considering the turbulence present in the engine cylinder.

CHAPTER 2:

LITERATURE REVIEW

During the diesel cycle air is injected into the combustion chamber at nearly close to atmospheric temperature and pressure and then compressed to pressure of about 4 MPa and temperature of 800K in the compression stroke [1]. At the end of compression stroke liquid fuel is injected in the engine cylinder. The fuel is atomized in form of droplets and penetration occurs into the cylinder. Injection pressure of fuel varies from 20 to 170 Mpa that depends upon the type of engine, size and power output [1]. When fuel is atomized is in form of fine droplets then it is heated and mixes with high temperature and pressure air to form the air-fuel mixture. When the fuel droplets are injected into the engine cylinder the temperature and pressure of air present in the combustion chamber is above the critical point of fuel droplets and thus a spontaneous ignition is occurred after the delay period. Combustion process in the diesel engine is heterogeneous and unsteady. The present thesis is focused on the modelling of diesel fuel droplet evaporation in a turbulent environment at high temperature and pressure.

Classical Models of Droplet Evaporation

In the following section classical models of droplets evaporation are presented.

Maxwell and Stefan-Fuchs model

This is the simplest model for droplet evaporation given by the Maxwell in 1877 [25]. This model explains that evaporation rate of diesel fuel droplet is governed by the diffusion process. This model takes into account the only effects of diffusion process and ignores the convective effects due the high operating conditions present in the cylinder and also vapor away from the surface of the fuel droplets.

Abramazon and Sirignano model

This model is just a refinement of the evaporation model presented by Maxwell and Stefan-Fuchs. In the previous model the effects of convection were not taken into account and this model refines the calculation by taking into account the convection effects caused by the droplet motion relative to the ambient gas. In this classical model film theory is employed that is discussed in [26, 27].

Yao, Abdel–Khalik, and Ghiaasiaan Model

This model is also an extension of the evaporation model presented by the Abramazon and Sirignano. In this model thermal and mass thickness are introduced and effects of Stefan flow are also taken into account. Boundary conditions used in this model are same as in the previous two models.

Tonini and Cossali Model

A new evaporation model was developed by Tonini and Cossali [28] for heat and mass transfer from a spherical droplet suspended in the stagnant air. This model assumes that there are no temperature gradients inside the fuel droplet i.e. thermal conductivity of liquid phase is infinitely large. The main focus of this model was on the vapor phase. The analysis is based on the conservation equations of steady state mass, momentum and energy for the both vapor phase and gas phase that surrounds the spherical droplet. All the above presented classical models are discussed in details in [29].

2.1 Models of Droplet Heating and Evaporation

Evaporation of multi-component diesel fuel droplets began with Landis and Mills [13] followed by Sirignano and Law [14-15]. Steady state evaporation characteristics of hydrocarbon fuel droplets were examined by J.S Chin & Lefebvre in [24]. Evaporation of fuel droplets into engine cylinder is an important phenomenon to make a proper air/fuel mixture for complete combustion in the diesel engines. Evaporation of fuel droplets into engine cylinder involves simultaneous heat and mass transfer processes occurring at high temperature and pressure. The temperature of surrounding gas is as higher to evaporate the fuel droplet after atomization in the combustion chamber. Heat is absorbed by the droplet from surrounding by the process of convection and radiation. When a droplet absorbs the heat then it starts to decay and mass is lost during this process. Then mass transfer from droplet to ambient gas takes place by the process of diffusion from the surface of droplet. J.S. Chin and A.H. Lefebvre modelled the evaporation of different fuel droplets in a quiescent environment. The influence of gas temperature and pressure was seen by analytical model on the vaporization rate of droplet [24]. In this model it was observed that pressure dependence is more on the vaporization rate of fuel droplet for high pressure conditions than the low pressure environment. Temperature dependence is also correlated with the pressure. If ambient temperature is high then pressure dependence would be positive and negative at lower temperatures. In [30] the role of heat up period of fuel droplet is described analytically.

In this work an equation of heat up period is derived analytically. It was observed that heat up period is proportional to the square of fuel droplet diameter. If the ambient pressure is increased heat up is also increased. But it decreases with the increase in ambient temperature. Evaporation rate of diesel fuel droplet can be increased by increasing the ambient temperature and decreasing the heat up period. Droplet life time largely depends upon the heat up period. At high temperature and pressure conditions role of heat up period cannot be ignored [30]. A.P. Watkins and Khaleghi modelled the diesel fuel spray evaporation using the non-iterative implicit scheme [31]. J Tamim developed a model for multicomponent liquid fuel droplets in [32] by using the continuous thermodynamics approach. Transport equations describing the mixture composition are solved numerically. It is demonstrated that for modeling evaporation of diesel fuel droplet for complex mixtures, continuous thermodynamics approach is practical. This model showed that for commercial diesel fuels this approach is pretty realistic. In [33] a droplet vaporization model was developed by E. W. Curtis for high operating conditions spray fuel modeling. This model is an advancement of common Spalding vaporization model in which phase equilibrium effects at high temperature and pressure are accounted for. The new is developed in the KIVA code and gives the better results for surface temperature of droplet, density of droplet and surface tension. This model for tested for single droplet at high ambient conditions and found a good agreement with experimental values. This model showed an improvement in the penetration length and droplet evaporation of fuel spray. Hiroshi Miyagawa and Makoto Nagaoka studied the vaporization of multicomponent gasoline fuel vapor for port injection system [34]. In this study it was observed that evaporation of gasoline droplet that contain more than one hundred components can be observed by using a fuel that have at least three representative components. It was observed that mass fraction left in the intake port was smaller than the n-heptane diesel fuel. A multicomponent droplet evaporation model was developed by Yangbing Zeng in [35] for high pressure spray calculations and combustion computations. Turbulent boundary layer assumption and mixing-length theory were employed for the gas phase to determine the vaporization rate. Surface temperature and surface mass fractions are the important parameters that governs the rate of evaporation of a fuel droplet. Species concentration and increase in temperature profiles were evaluated using a third order polynomial for accurate predictions. Governing equations were reduced to ordinary differential equations for film evaporation by using this method. This new reduced the computational cost effectively instead of solving the conservation equations directly

and an acceptable accuracy was achieved. The results obtained were also in a good agreement with infinite-diffusion model. The new model was also employed to the wall impingement case and gained a better physical insight for fuel spray. Guang-sheng Zhu and Rolf D.Reitz presented a comprehensive model for transient evaporation of liquid fuel droplet in the complex mixtures that contain complex mixture compositions by using the continuous thermodynamics approach. Vapor liquid equilibrium was also considered in this model with the mixture properties at high temperature and pressure. Vapor liquid equilibrium was considered using the cubic equation of state in conjunction with the general transport equations. It was showed that an intrinsic evaporation was seen for vapor liquid mixture at high temperature condition regardless of the sub or supercritical pressure. Evaporation rate of liquid fuel droplet is increased by increasing the heat up period. S. Hohmann and U. Renz studied the effects of real gas and gas solubility on the evaporation rate of diesel fuel droplets at high temperature and pressure [37]. Evaporation of fuel was modelled by solving the conservation equations of mass, momentum and energy numerically at high pressure and temperature. This model included the effects of real gas on the droplet and concentration of species through the species transport equation. Equation of state was employed to perform the unsteady droplet calculations. This evaporation model was based on an Eulerian/Lagrangian approach. It was showed that for evaporation at high operating conditions distribution of diameter was mostly influenced by the secondary breakup. A.P. Kryukov and V.Yu. Levashov presented a comparative analysis between the kinetic approach and hydrodynamic approach to solve the problems regarding the diesel fuel evaporation for diesel engine [38]. It was observed that at high ambient conditions kinetic effects on the droplet evaporation cannot be neglected. This showed the limitations of employing the hydrodynamic models for the diesel fuel evaporation. Hydrodynamic models are used widely for droplet evaporation in computational fluid dynamics code. The prediction of droplet temperature and evaporation rate is longer in the kinetic models as compared to the hydrodynamic models. Smaller droplets are more affected by the kinetic effects than the larger ones. Effect of evaporation coefficient was also discussed on the droplet regression rate and increase in droplet temperature. It was observed that by decreasing the evaporation coefficient droplet evaporation time and droplet temperature increased. Then S Sazhin modelled the droplet evaporation using the combined analytical, asymptotic and numerical analysis in [39]. In this work new approach was introduced by taking into account the convection and radiation effects from hot gas in surrounding by using combined analytical and numerical

modelling of heating and evaporation of diesel fuel droplets. In this analysis semitransparency of fuel droplet was also taken into account. It was evident that this new model had clear advantages over the conventional approaches used in CFD codes in terms of CPU efficiency and accuracy. A brief summary of modelling of several processes in the diesel is presented by S Sazhin in [40]. It included the different processes i.e. liquid penetration length and heating and evaporation of diesel fuel droplet. It was observed that dynamic decomposition methods are an effective tool to solve the system of differential equations for modeling heating and evaporation for fuel droplets. A validated comprehensive droplet vaporization model was presented by Hongtao Zhang and Vasudeva Raghavan in [41]. This model included the high pressure transient effects, different theosophical properties and solubility of inert species in the gas phase. Fuel droplet was allowed move in a zero gravity environment at different velocities and pressures. Fuel used for the numerical model was n-heptane. It was observed that at low ambient pressures the constant of evaporation becomes almost constant at the end of droplet lifetime. When ambient pressure is high transient effects of fuel droplet cannot be ignored with passage of droplet heating and evaporation throughout. Youngchul Ra and Rolf D. Reitz developed a multicomponent droplet vaporization model for diesel fuel sprays in [42]. A discrete multi-component approach was used to model the evaporation characteristics of gasoline and diesel fuels. Unsteady evaporation for single and multicomponent fuel droplets was modelled using normal and flash point boiling conditions. A quasi-steady energy equation was employed take into account the effects of heat flux from hot ambient gas to the droplet surface. Change in density of fuel droplet was also considered interphase species equations. S Sazhin discussed various unresolved problems some effective results regarding droplet heating and evaporation in [43]. New methods to solve the problems relating modeling the heating and evaporation of multicomponent fuel droplet are discussed in [44]. In these methods effective thermal conductivity and effective diffusivity models are included. In these models analysis is reduced to few components instead of many. It was observed that in case of evaporation of both gasoline and diesel fuel analysis is based on at least five components. In [45] recent advancements and other future challenges are described. The main focus is on the Lagrangian and fully Lagrangian approaches to solve the challenges in spray modeling. Fully Lagrangian (Osiptsov) is applied to solve the general engineering problems including heating and evaporation of non-spherical and spherical fuel droplets in internal combustion engines, ignition and combustion of fuel drops. Future challenges include the development of fully Lagrangian

approach to solve the realistic fuel sprays in turbulent environment, heating and evaporation of deformed drops, heating and evaporation of fuel droplets in trance and supercritical conditions. Modelling of sprays has been studied extensively over the past 100 years results are summarized briefly in [46-48].

2.2   Evaporation of Diesel Fuel Droplets

The evaporation of diesel droplets has been little studied as compared to the spray of diesel fuel droplets Due to the relatively high importance of the spray in the combustion process. Diesel varies physically from one region to another depending on the refining process [49].The published work on the evaporation of diesel droplets will be revised with respect to two Conditions free convection and forced convection, where the later can be broken down In two categories; ambient temperature and pressure.

2.3   Effect of ambient temperature on the evaporation

Experimental Studies

Experimental studies that focus on the evaporation of diesel droplets are mainly limited due to the variety of composition that exists between diesel fuels from different regions of the world. The experimental studies that exist have shown drop of diesel fuel Evaporation only under atmospheric pressure and normal gravity [50, 51, and 52]. The reported results of [50] have shown diesel fuel to follow the D^2-law (for example, [53]) after an initial Heating period at ambient temperatures that varied from subcritical (684 K) to supercritical (917 K), where the critical temperature of diesel fuel is commonly taken to be approximately 450 Celsius or 723 K. A heat-up period was observed for all of these ambient temperatures. The evaporation rate in contrast to the heat-up period showed a strong Dependence on the ambient temperature where it increased monotonically with the environment temperature. The high ambient temperature helps the evaporation of diesel drops by providing greater heat transfer to the surface of the drop while allowing a faster evolution of Components of diesel fuel from the liquid phase to the gas phase (i.e. gasification).Diesel fuel requires a high ambient temperature to produce fuel vapors [54].Experimentally, 200 degrees Celsius or 473 K, represents a relatively low environment temperature compared to the boiling range of diesel fuel, 150-330 ° C, which can evaporate a drop of diesel fuel completely. Yupo et

al. [52] explored the evaporation of diesel drops in ambient temperatures of 448 K and 473 K under atmospheric pressure. Diesel fuel was purposely preheated to the approximate ambient temperature before the drop was formed; this in turn guarantees that there will not be a heat-up period that allows the experiment only focus on the rate of evaporation. It was found that the evaporation of diesel droplets follows a linear decrease in the projected surface area of the drop and follows the D^2-law. This latter allowed the determination of the evaporation rate, which was found to be 0.19 and 0.33 mm2/ s for ambient temperatures of 448 K and 473 K, respectively. One comment that must be made about its experimental results refers to what is reported Evolution of the square diameter of the droplets with respect to time, particularly in the case of 175C (448 K), where the final square diameter used in the calculation of the evaporation rate did not coincide with the value used for 200 C (473 K).

The final value in the question was greater than the final value for 200 ° C, which implies diesel fuel was still present at this time. Whether the diesel droplet continues or not to follow the D^2-law beyond this diameter, a law is unknown. The overall shape (i.e., Linear, etc.) the surface regression comes into the question due to the work by Promvongsa et al. [51] where diesel droplet evaporation was also carried out at 200 ° C below Atmospheric pressure, the only difference between the two attempts was preheating of diesel fuel by [52]. Attempts to Evaporate Diesel Droplets by [51] produced a nonlinear decrease in the projected surface of the droplet. This nonlinear behavior does not correspond to D^2-Law; this in turn prevents the determination of the evaporation rate, although Promvongsa has tried to get the best possible fit through the Dates. The main reason for this nonlinear behavior was the Multi-component nature of diesel fuel and the wide range of volatilities inside the diesel fuel. The authors do not indicate that the broad spectrum of components contained therein exists in the Diesel fuel, which is obvious given the boiling point range of diesel fuel.

This shows that there are some very heavy components (i.e., high molecular weight) as well as some relatively light components (i.e., low molecular weight). Diesel droplet evaporation had no observable heating period for this relatively low ambient temperature due to Evaporation of the lighter components to allow time for the droplet surface temperature than the evaporation of relatively heavier components. Unfortunately, the environment the temperature in this case was not sufficient to allow a gradual transition from one Component to another, to facilitate evaporation, which would follow the D^2-Law.

Kobayasi [55] experimentally investigated the evaporation of light diesel under Atmospheric pressure for ambient temperatures from 475 K to almost 1000 K. Surface regression profiles were reported only for ambient temperatures of 198, 300, and 305 C. The development of the surface regression profile shows an initial heating period followed by a steady decline, in particular the surface decreases non-linearly for 198 C. The author decided to quantify drop evaporation using medium evaporation rate for all tested ambient temperatures at which this value was derived from slope of a straight line connecting the beginning and ending point of the droplet life. It was found that the average evaporation rate rose steadily with the ambient temperature. These method for calculating the evaporation rate does not agree with the D^2-Law however the work was done around the time the D^2-law was first proposed by Godsave [56].From the aforementioned works it is obvious that there are some ambiguities There is still evidence of the vaporization of diesel fuel droplets, especially in view of the Evaporation behavior at relatively low ambient temperatures, where it remains uncertain if diesel follows the D^2-law, as well as the existence or nonexistence of a heat up period.

Numerical studies

The evaporation of diesel droplets has been studied mainly numerically under the presence of relatively high ambient temperatures (i.e., temperatures above critical) temperature) [57, 58 and 8]. Zhang and Kong [57] simulated the evaporation of diesel drops to ambient temperatures of 858, 912 and 1019 K under atmospheric pressure, reported that the associated life times for a drop with a diameter of 1 mm were 5.53, 4.51 and 3.86 seconds, respectively. Interestingly, the authors chose to report the life of the droplets instead of evaporation rate despite having the regression profiles of the drop surface that follow the D^2- Law after a period of initial heat-up. Unlike other authors, Zhang and Kong validate their model with experimental droplet data for n-heptane, n-decane and biodiesel from [59].The use of biodiesel to validate their numerical work shows that the model can produce however, reliable results with respect to the evaporation of droplets of multiple components, although biodiesel can be a multi-component droplet; has a significantly narrower range of Component compared to diesel fuel.

Lippert and Reitz [58] simulated the evaporation of diesel droplets at ambient temperature (973 K) at atmospheric pressure. They found that while an initial the heat-up period was present, it was quickly followed by a linear decrease in the square Diameter of the drop indicative of D^2-law. His

simulation predicted an evaporation rate of 0.32 mm2/ s, this value showed a close agreement with the previous numeric.

However, the works compare the life of the droplets with the previous numerical work of Tamim and Hallett [8] showed a remarkable difference of around 30 percent. Zhang and Kong [60] simulated the evaporation of diesel droplets under the same conditions like Lippert and Reitz [58], and found a similar behavior with respect to the evolution of the superficial regression profile of the drop. However, Zhang and Kong [60] conducted this simulation in the evaporation of drops without comparing the results with previous works by Lippert and Reitz. These mentioned numerical works only focused on evaporation of diesel droplets for an ambient temperature while the work of others has focused on a wider range of ambient temperatures. Hallett [61] simulated the evaporation of diesel droplets and compared the predicted ones evaporation rates with the experimental data of Kobayasi [55] over the entire environment temperature range, which was investigated in [55]. The range of ambient temperatures ranges from subcritical to supercritical, the evaporation rate being logarithmic frame. This scale shows the temperature dependence of the vaporization of diesel droplets for both sub- and supercritical temperatures. The numerical results showed good agreement with the experimental data on the evaporation rate despite the associated uncertainties with the fuel specifications used by [55]. The numerical models showed that over the entire range of ambient temperatures followed by the evaporation of the diesel droplets of the D^2-Law after an initial heating period however, the relative size of the heating season could not compared with [55] because this information was not available. Comparatively, the numerical work by Daho et al. [50] compared not only the evaporation rate, but also compared the length of the heating period with their own experimental data for ambient temperatures from 684 K to 917 K. in the numerical models used by [50] the duration of heating and the lifetime of the droplets were constantly overestimated for diesel fuel as compared to experimental data. On the other hand, the evaporation rate was consistently underestimated by the numerical models except one model numerical model that only considers the effects of natural convection. The authors concluded that the heating period had little effect on the evaporation rate in comparison with the presence of natural convection over the ambient temperature range studied. The influence of the ambient temperature on the evaporation of diesel droplets was short-lived examined by Ra and Reitz [42] for an ambient pressure of 4 MPa, the environment the temperature was varied from 500 K to 1000 K. The authors found this for the ambient temperatures above the critical temperature of the diesel

fuel droplets is the temperature of the surface of the droplet reached the critical value and evaporated immediately. Comparatively subcritical ambient temperatures led to longer drop durations, where droplet life significantly increased with decreasing ambient temperature. From the above discussion it can be seen that the evaporation of diesel droplets has taken place With some models numerically examined over a range of ambient temperatures direct comparisons with available experimental data while others only Compared to previous numerical works due to lack of compositional knowledge in terms of fuel. The evaporation rate was simulated for ambient temperatures from subcritical to supercritical where a good match has been found with experimental However, there is still a problem with the data to get an accurate estimate of the heat-up period and therefore the droplet life. The limited works examine the effect of the ambient temperature at elevated ambient pressure is also worth mentioning, as explained below.

2.4   Effect of ambient pressure on the evaporation

Numerical Studies

Numerical studies have so far been the only method for studying diesel droplets evaporation at elevated ambient pressure. Chin and Lefebvre [24] investigated diesel droplets evaporation, where the simulation focused only on the quasi-stationary part of the evaporation rather than his entire life. The results of the diesel droplet evaporation rate were compared with experimental data at temperature and pressure of 2000 K and 1 atm in the engine cylinder respectively. The calculated evaporation rate was less than 2% of experimental value; Unfortunately, further validation of the vaporization of diesel droplets at conditions with elevated ambient pressure were missing due to missing experimental data. The authors studied five ambient temperatures, 500, 800, 1200, 1600 and 2000 K and varied the ambient pressure from 0.1 MPa to 2 MPa at rest surroundings. It should be noted that the critical temperature and pressure of the diesel were assumed to be 725.9 K and 2.089 MPa, respectively. The evaporation rate was found too at supercritical ambient temperatures, the ambient pressure increases the behavior reverses at subcritical ambient temperatures. Further examination for the pressure dependence of the evaporation rate of diesel fuel shows a relationship in which the evaporation is directly proportional to the pressure to the power of n, where the value of n is varies as ± 0.25. Interestingly, the value of n at 750 K is zero for all environments while the n values for subcritical and supercritical temperatures follow a similar behavior in relation to the ambient pressure to what for the observed evaporation rate. Diesel droplet evaporation undergoes

this subcritical-supercritical behavior was recently investigated by Ra and Reitz [42]. Ra and Reitz [42] investigated the vaporization of diesel droplets for various environmental temperature and pressure conditions as well as the initial drop temperature. One of the specified test conditions were for the operating conditions of 500 K and 0.1 MPa in connection with an initial temperature of the droplet at 360 K. Diesel fuel droplet evaporation under these ambient conditions shows a nonlinear decrease in surface of the drop where the simulation showed the lightest components Initially evaporated so that the heaviest components of the drop can control the final result stages of evaporation. They showed that a reduction in ambient pressure is below 0.1MPa combined with the above ambient temperature and the initial drop the temperature reduces the life of the droplets. No heating period was found for in cylinder pressures below 0.1 MPa, while for elevated cylinder pressures heating takes place period was not only available, but also important in terms of the environment. At an ambient temperature of 800 K, the ambient pressure was increased from 0.1 MPa to 4 MPa to find that the droplet surface decreased nonlinearly. The droplet life increased with pressure up to 2 MPa, beyond that the droplet surface temperature could reach the critical temperature immediately evaporated. Zhu and Reitz [62] investigated the evaporation of diesel droplets at various pressures spans from 0.186 MPa to 13.02 MPa at an ambient temperature of 950K. The model was used to simulate the entire droplet life. It was found a heating period for all ambient pressures. This was attributed to the initial surface vapor fraction Evaporation rate with small values due to the low volatility of diesel fuel. The effect of the increase in ambient pressure had minimal impact on the heating period; anyway, it reduced the droplet life by increasing the evaporation rate. It has been found that both the enthalpy of vaporization and the liquid density are reduced due to increased gas absorption; these two effects were probably responsible for reducing the effect Droplet life at elevated ambient pressures. The reviewed literature revealed that the effects of ambient pressure on diesel Drop evaporation was studied primarily at supercritical ambient temperatures. The only study that examined subcritical temperatures looked only at the quasi-stationary fraction associated with the evaporation rate while the potential is ignored effects of the heating period on the droplet life. The heating season gets longer significant as the ambient pressure increases while the general non-linearity is associated with it the time course of the droplet surface shows a general trend of conformism to the classic D^2-Law. The developed numerical models were not validated using experimental data (or compare with it). This is due to the lack of experiments Data / studies.

2.5   Effect of forced convection on the evaporation

Numerical Studies

The effect of forced convection on the vaporization of diesel droplets was investigated economical with the main focus of these studies with supercritical environment temperatures below atmospheric pressure [63, 64]. Barata [63] simulated injection of diesel droplets into a hot convective cross-flow, where the cross-flow velocity was reached 10 m / s and the ambient temperature was 800 K. The evaporation of the diesel droplet is subjected to a noticeable heating period before evaporation. Neither the evaporation rate nor was the droplet life mentioned. On the other hand, Saha et al. [64] also simulated diesel fuel droplet vaporization under the same ambient conditions as Barata [63], where the evolution of droplet size was shown for two initial droplet sizes, 20 μm and 400 μm around. The normalized drop diameter decreased linearly with time for the 400 micron droplet, whereas the 20 micron droplet is non-linear decrease in normalized diameter. Similar to [34], there was no quantification in terms of evaporation rate or droplet life for both drop diameters and there was also no indication whether the droplet followed the D^2-Law. Unlike before mentioned authors, Saha et al. [65] simulated the vaporization of diesel droplets for 100 μm droplets injected in a hot, stagnant environment with an initial velocity of 5 m / s. diesel drop evaporation started with a relatively short heating period, followed by an approximately linear decrease of the droplet surface with respect to time. The linear regression of the surface area of the drop was associated with the maintenance of a constant wet bulb temperature, where the authors affirm that the temperature of the humid bulb represents the thermal temperature equilibrium for a drop whose boiling point is lower than the ambient temperature. Chin and Lefebvre [30] simulated the evaporation of diesel droplets in the presence of forced convection. The focus of his simulation was on the relationship of the heat-up period to life of the droplet. They observed that the warm-up period did not change with the velocity of the flow; however, it was described that the rate of evaporation increased with the velocity of the flow, which in turn, the relationship between the time of the heating period and the life of the droplets increased. Interestingly, it was found that the temperature of the surface of the drop remained constant as the flow varied speed. Simulations were carried out for operating conditions of 500 K and 2000 K as well as environmental pressures of 0.1 MPa and 2 MPa. The ratio of the heating period to the drop was found that the service life increased with the flow velocity at a high ambient pressure, where

the It was found that the heating period increased with ambient pressure. In the previous literature it can be seen that the evaporation of the diesel droplets in the presence of forced convection has not yet been examined in relation to the applicability of the D^2- Law and therefore the focus was more on heating period to determine the rate of vaporization. On the other hand, the literature revealed that experimental investigations of the evaporation of diesel droplets in the presence of forced convective flow is still missing.

2.6   Problem statement

The main focus of this thesis is to model the evaporation of different diesel fuels at high temperature and pressure by taking into account the turbulence produced in the engine cylinder due to high operating conditions. Evaporation and ignition of fuel droplets in the combustion chamber is an important phenomenon in the I.C engines.

1) An appreciable work is done on different aspects of evaporation for I.C engines. But a little work is shown for high torque low speed diesel engines in the literature.

2) Different evaporation models are described in literature using the different aspects that affects the evaporation process. One important thing in the evaporation is to take into account the turbulence effects. A little work is done on turbulence with respect to evaporation process especially in the high torque low speed diesel engine.

3) In the present work evaporation of two different diesel fuels is modeled by considering the turbulence effects using Realizable k-epsilon turbulence model.

2.7   Objectives

Following are the objectives of this research

1. Achievement of efficient fuel evaporation in the heavy duty high torque low speed diesel engine.

2. Achievement of better fuel economy.

3. Analysis of turbulence induced in the evaporation process due to break up regimes.

4. Achievement of an overall efficient evaporation model considering the different effects.

5. Recommendations for Nozzle Design.

CHAPTER 3:

NUMERICAL METHODOLOGY

GOVERNING EQUATIONS

In modelling of evaporation of diesel fuel spray following governing equations are used.

3.1 Continuity Equation

The general continuity equation can be written as

$$\frac{\partial \rho}{\partial t} + \nabla \bullet \left(\rho \vec{v} \right) = S_m \tag{1}$$

Mass of liquid fuel droplet is conserved by following the above equation. This equation is valid for the both compressible and incompressible flows. Source term indicates the mass is added by the discrete phase to the continuous phase.

3.2 Momentum Equation

Momentum of droplet particle is conserved by the following momentum equation.

$$\frac{\partial}{\partial t} \left(\rho \vec{v} \right) + \nabla \bullet \left(\rho \vec{v} \vec{v} \right) = -\nabla p + \nabla . \left(\overline{\overline{\tau}} \right) + \rho \vec{g} + \vec{F} \tag{2}$$

Where

$$\overline{\overline{\tau}} = \mu [(\nabla \vec{v} + \nabla \vec{v}^T) - \frac{2}{3} \nabla . \vec{v} I] \tag{3}$$

$\overline{\overline{\tau}}$ Is a stress tensor where I is unit tensor.

3.3 Energy Equation

$$\frac{\partial}{\partial t} (\rho E) + \nabla \bullet \left(\vec{v} (\rho E + p) \right) = \nabla \bullet \left(k_{eff} \nabla T - \sum_j h_j \vec{J}_j + (\overline{\overline{\tau}}_{eff} \bullet \vec{v}) \right) + S_h \tag{4}$$

Where

$$E = h - \frac{p}{\rho} + \frac{v^2}{2} \tag{5}$$

h Is the sensible enthalpy and it can be represented as

$$h = \sum_j Y_j h_j \tag{6}$$

And h_j is given by

$$h_j = \int_{T_{ref}}^{T} c_{p,j} dT$$

3.3 Species Transport Equation

Local mass fraction of species is conserved by the solution of following convection-diffusion equation of species j

$$\frac{\partial}{\partial t}(\rho Y_j) + \nabla \cdot (\rho \vec{v} Y_j) = -\nabla \cdot \vec{J}_j + R_j + S_j \tag{8}$$

Where

$$\vec{J}_j = -(\rho D_{j,m} + \frac{\mu_t}{Sc_t})\nabla Y_j - D_{T,j}\frac{\nabla T}{T} \tag{9}$$

And Sc_t is gives as follows

$$Sc_t = \frac{\mu_t}{\rho D_t} \tag{10}$$

Typically Sc_t is taken as 0.7

3.4 Discrete Phase Model Equations

1) **Particle force balance**

The trajectory of evaporating droplet is predicted by the integration of forces balance on the droplet in Lagrangian frame of reference. Inertial force of particle is balanced by the other forces on it which is given in the following form.

$$\frac{dv_p}{dt} = F_d\left(v - v_p\right) + \left(\rho_p - p\right)\frac{g_x}{\rho_p} + F_x \qquad (11)$$

Where F_d is particle drag force that is given below as

$$F_d = \frac{18\mu}{\rho_p d_p^2} \cdot \frac{C_d \, \mathrm{Re}}{24} \qquad (12)$$

And particle relative Reynolds is defined as

$$\mathrm{Re} = \frac{\rho d_p}{\mu}\left|u_p - u\right| \qquad (13)$$

Drag Coefficient is taken from [19] and it is defined as

$$C_d = \frac{24}{\mathrm{Re}}(1 + b_1 \, \mathrm{Re}^{b_2}) + \frac{b_3 \, \mathrm{Re}}{b_4 + \mathrm{Re}} \qquad (14)$$

$$b_1 = \exp(2.3288 - 6.8541\Phi + 2.4486\Phi^2)$$

$$b_2 = 0.0964 + 0.5565\Phi$$

$$b_3 = \exp(4.905 - 13.8944\Phi + 18.422\Phi^2 - 10.2599\Phi^3)$$

$$b_4 = \exp(1.4681 + 12.2584\Phi - 20.7322\Phi^2 - 15.8855\Phi^3) \qquad (15)$$

And Φ is the shape factor of particle that is given by the following relation

$$\Phi = \frac{s}{S} \qquad (16)$$

2) **Heat Transfer to the Droplet**

After the injection in the engine cylinder fuel droplets disperse into the continuous phase and heat transfer between droplets and the air present in the chamber takes place by the following equation.

$$m_p c_p \frac{dT_p}{dt} = hA_p(T_\infty - T_p) + \frac{dm_p}{dt} h_{fg} \tag{17}$$

3) **Mass Transfer Equation**

When droplet is placed in the hot environment then mass of the droplet is reduced according to the following mass transfer equation.

$$m_p(t + \Delta t) = m_p(t) - N_j A_p M_{\omega,j} \Delta t \tag{18}$$

And

$$N_j = k_c(C_{j,s} - C_{j,\infty}) \tag{19}$$

In above equation k_c is calculated by the following Nusselt correlation.

$$Nu_{AB} = \frac{k_c d_p}{D_{j,m}} \tag{20}$$

3.4 Turbulence Modelling

Turbulence theory is a difficult subject area and it is probably too much to expect a universal solution for the turbulent flows. There are models and each model has its own area of applicability.

The main turbulence modelling techniques are:

- DNS (Direct Numerical Simulation)
- Reynolds average Navier Stokes Equation (RANS)

    K-e Turbulence Model (Standard, RNG, Realizable)

- Large Eddy Simulation (LES)

A realizable k-epsilon turbulence model is used in the present calculation to account for the turbulence effects generated in the engine cylinder due to high operating conditions. High temperature and pressure present in the cylinder generates turbulence. When droplets are injected into this hot environment with high injection pressure then effects of turbulence on the particle trajectory becomes vital.

These turbulence effects are taken into account by the following equations of realizable k-epsilon turbulence model.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial X_j}(\rho k u_j) = \frac{\partial}{\partial X_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial X_j}\right] + G_k + G_b - \rho\varepsilon - Y_M + S_k \tag{21}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial X_j}(\rho\varepsilon u_j) = \frac{\partial}{\partial X_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial X_j}\right] +$$

$$\rho C_1 S\varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{v\varepsilon}} + C_{1\varepsilon}\frac{\varepsilon}{k}C_3 G_b + S_\varepsilon \tag{22}$$

Where

$$C_1 = \max[0.43, \frac{\eta}{\eta+5}], (\eta = S\frac{k}{\varepsilon}), (S = \sqrt{2S_{ij}S_{ij}}) \tag{23}$$

Turbulent Eddy viscosity in the (21) and (22) is computed as follows.

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{24}$$

And C_μ is given by

$$C_\mu = \frac{1}{A_o + A_s \dfrac{kU^*}{\varepsilon}} \tag{25}$$

Model constants are given below.

$$C_{1\varepsilon} = 1.44, C_2 = 1.9, \sigma_k = 1.0, \sigma_\varepsilon = 1.2, A_o = 4.04 \tag{26}$$

3.4 Numerical Model

Above presented model is applied to simulate the droplets of n-heptane and n-decane fuels in Ansys. Conservation equations of mass, momentum and energy are coupled with the realizable k-e turbulence model and species transport equation to model the evaporation of fuel droplets in high temperature and pressure conditions. DPM is applied to solve the discrete phase i.e. fuel droplet into the continuous phase present in the combustion chamber. In coupled calculation continuous

phase is solved before introduction of discrete phase into the engine cylinder. Then discrete phase is introduced by calculating the particle trajectories for discrete phase injection. Then continuous flow phase is recalculated after the injection of discrete phase using interphase exchange of mass, momentum and heat determined by the previous calculation. Finally discrete phase is recalculated using the modified continuous phase flow field. The present model is applied to the following engine specifications.

The above numerical model is applied to a heavy duty high torque diesel engine operating at low speed. The evaporation if two different diesel fuels is modelled at high temperature and pressure conditions under a turbulent environment. Engine specifications are given in the following table.

Engine Specifications		Injection specifications	
Bore	150 mm	Injection type	single
Stroke	180 mm	Droplet velocity	35 m/s
Max Torque	295 kg-m	Droplet temperature	300 K
Ambient Pressure	4 MPa	Fuel type	n-heptane & n-decane
Nozzle Diameter	0.29 mm	Flow rate	0.003 kg/s
Injection pressure	20 MPa	Injection duration	4 ms

Table 2.1 Engine Specifications

3.5 Solution Methods

Following solution schemes are used in numerical calculations.

Pressure velocity coupling: SIMPLE

Gradients: Least Square Cell Based

Pressure: Second Order

Momentum: Second Order Upwind

Turbulent Kinetic Energy: First Order Upwind

Turbulent Dissipation Rate: First Order Upwind

Energy: Second Order Upwind

3.6 Fuel Properties

Properties of n-decane fuel are given below.

Density	730	kg / m^3
Specific heat	2090	$J/ kg - k$
Latent heat	277000	J / kg
Vaporization temperature	341	K
Boiling point	447	K
Volatile fraction	100%	
Binary diffusivity	3.79E-06	m^2 / s

Properties of n-heptane fuel are given below.

Density	684	m^2 / s
Specific heat	2219	$J/ kg - k$
Latent heat	320096	J / kg
Vaporization temperature	271	K
Boiling point	371	K
Volatile fraction	100%	
Binary diffusivity	6.31E-06	m^2 / s

CHAPTER 4:

RESULTS AND DISCUSSIONS

Model Validation and Verification

The droplet evaporation model presented in this research is implemented in the Ansys Fluent and obtained numerical results are compared with the most accurate vaporization experiments by Chauveau et al. [66]. The numerical results of present of model are also compared with the evaporation of model of Abramzon and Sirignano [67] and also with the earlier work in [68]. Results including droplet regression rate and increase in droplet temperature are in a good agreement with the numerical results presented in [69] for n-heptane and n-decane fuel droplets at different temperatures. Comparison of droplet regression rate are plotted for n-decane and n-heptane fuels with the results of Chauveau et al. [66] and Abramzon and Sirignano [67]. In figure 4.1 results of present model for n-decane droplet vaporization are compared with the experimental results of Chauveau et al. [66] and numerical model of Abramazon and Sirignano [67]. Obtained results are in a good agreement with the experimental and numerical values. In figure 2 and 3 present vaporization model is compared with the experimental work of Chauveau et al. [66] and numerical results presented in [69] for n-heptane fuel droplets at temperatures of 973K and 823K. Present results for the vaporization of n-heptane are close to the experimental work. Results are plotted by using the classical D^2 law with respect to normalized time.
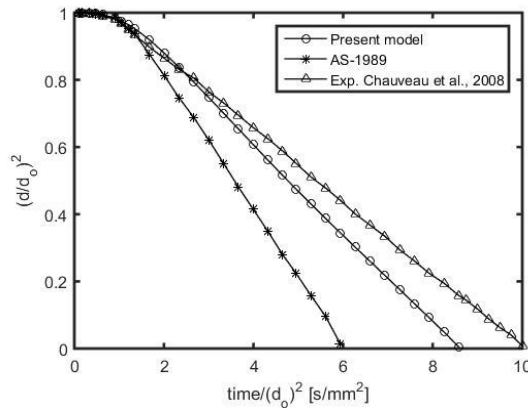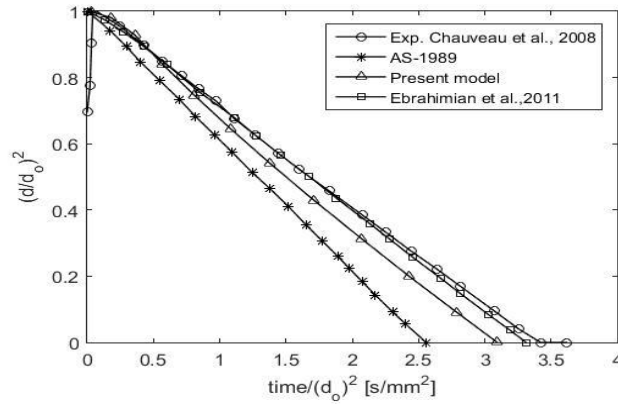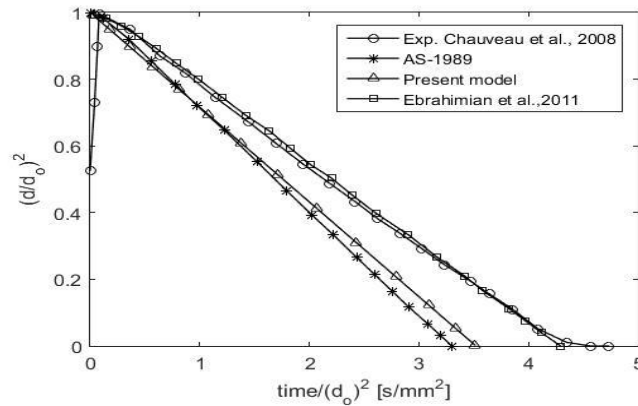

Figure 4.1: Comparison of Present model for n-decane droplet vaporization with experiment of Chauveau et al. and Numerical results of AS-989 at 623K

In figure 4.1 results of present model are compared with the experimental and numerical data. It can be seen clearly that the present model gives the better prediction of droplet diameter against the normalized time than the numerical model of AS-1989. In figures 4.2 and 4.3 results of n-heptane are compared with the experimental and numerical results and again it is observed that present model gives the better evaporation time of fuel droplet and is close to the experimental values than the AS-1989.

Figure 4.2: comparison of Present model for n-heptane droplet vaporization with experiment of Chauveau et al. and Numerical results of AS-989 at 973K

Figure 4.3: comparison of Present model for n-heptane droplet vaporization with experiment of Chauveau et al. and Numerical results of AS-989 at 823K

RESULTS AND DISCUSSIONS

In the following section results for n-decane and n-heptane fuel droplets are presented at different ambient conditions. Normalized droplet diameters are plotted using D^2-law against the normalized time. Three different sizes of droplet are taken to observe the effects of change in ambient temperature. Increase in droplet temperature is plotted with respect to the injection duration. It can be seen clearly that droplet of same sizes behave differently at different ambient conditions. it is clear that n-decane droplet of 10 micron diameter evaporates completely in a short period of time at high ambient temperature of 973K as compared to the other lower ambient temperatures of 623K and 823K.

Case-01

n-decane fuel

In this section results of n-decane fuel droplets are given. In this section droplets of size 10, 20 and 25 micron are considered. It is observed that droplets having small size are evaporated in a short time than the droplets of larger sizes. Ambient temperature also affects the evaporation of diesel fuel droplets. At high ambient temperature evaporation occurs faster than the lower ambient temperature. At temperature of 973K the droplet life time is much shorter than the temperature of 623K.

  i)   D=10 micron T=623,823,973 K
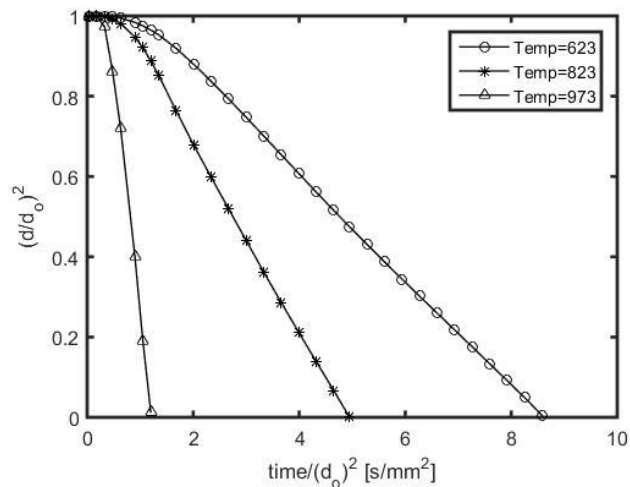
Figure 4.4: Vapourization of 10 micron n-decane dropelt at diffferent ambient temperatures

In figure 4.4 regression in diameter of droplet of size 10 micron is plotted using D^2-law against the normalized time. It is obvious that at lower temperature of 623K droplet life is higher than the temperatures of 823 and 973k. At lower temperature of 623K evaporation of time is approximately 45 percent more than the temperature at 823K. While at a higher temperature of 973K evaporation time and droplet life is much short as compared to the other two cases.
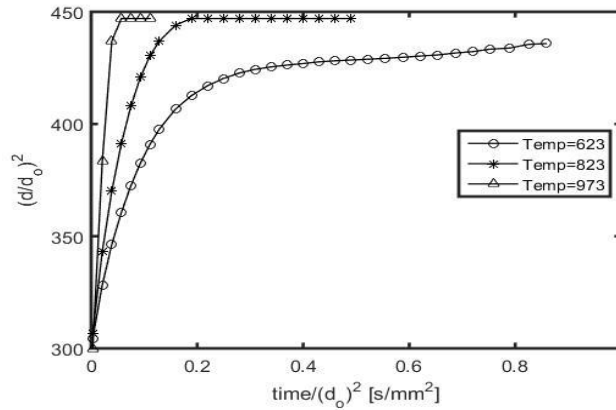

Figure 4.5: Droplet Temperature of 10 micron

In figure 4.5 Temperature profiles of 10 micron droplet is plotted against the normalized time and it is observed that a similar trend can be seen as in case of droplet regression with time. At higher temperature of 973K droplet lifetime is much short than the 623K. For the temperature of 623K droplet residence time is more than the temperatures of 823K and 973K. When ambient temperature is high droplet absorbs the temperature more rapidly and evaporates in a short interval of time. But in the low ambient temperature cases of 823K and 623K droplet residence time is obviously higher than the 973K ambient temperature. Heat up period is also an important parameter which plays an appreciable role in the evaporation time and droplet life. At higher ambient temperatures heat up period is also short and due to this evaporation time reduces to a large extent. At smaller temperatures heat up period of droplet is slightly more than the higher ambient temperatures thus droplet takes more time to evaporate.
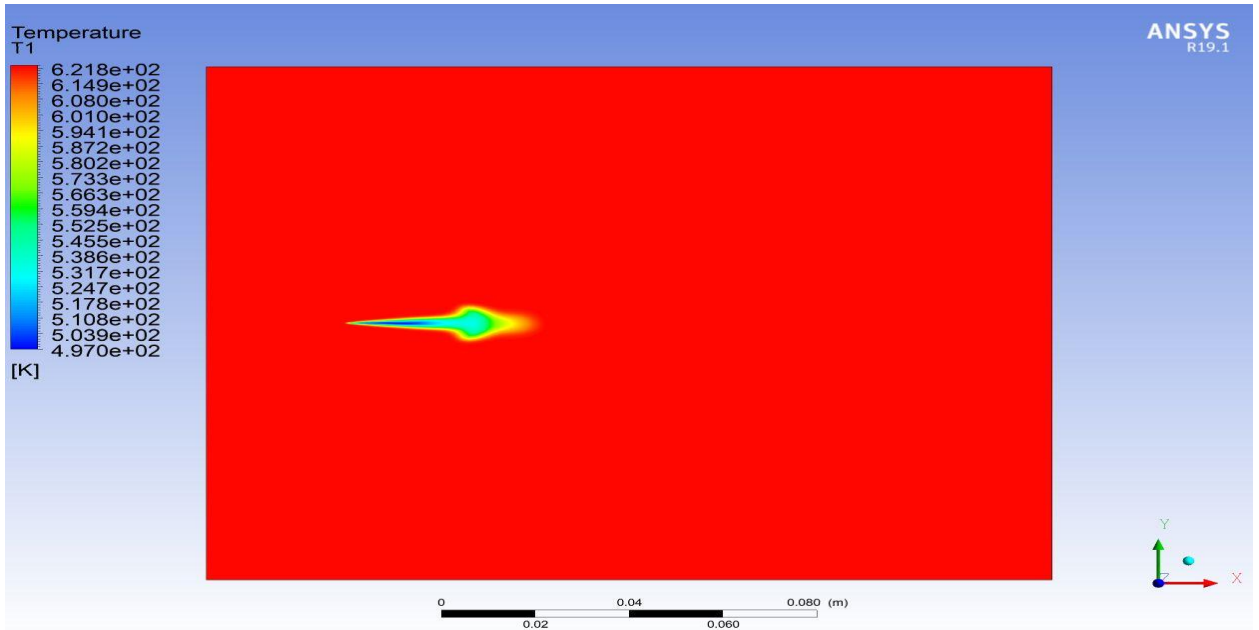
Figure 4.6: Contours of temperature at 623K

In above figure contours of temperature is shown for the engine cylinder. Ambient temperature is 623K and when droplet is injected into the cylinder it travels along the cylinder and a jet is formed. It absorb the temperature from ambient and evaporates as temperature reaches the critical value. The evaporation temperature of n-decane fuel is 371K. When droplets attain the critical temperature evaporation starts. Evaporation starts from surface and travels inside the droplets. Finally droplet evaporates completely and jet is vanished.
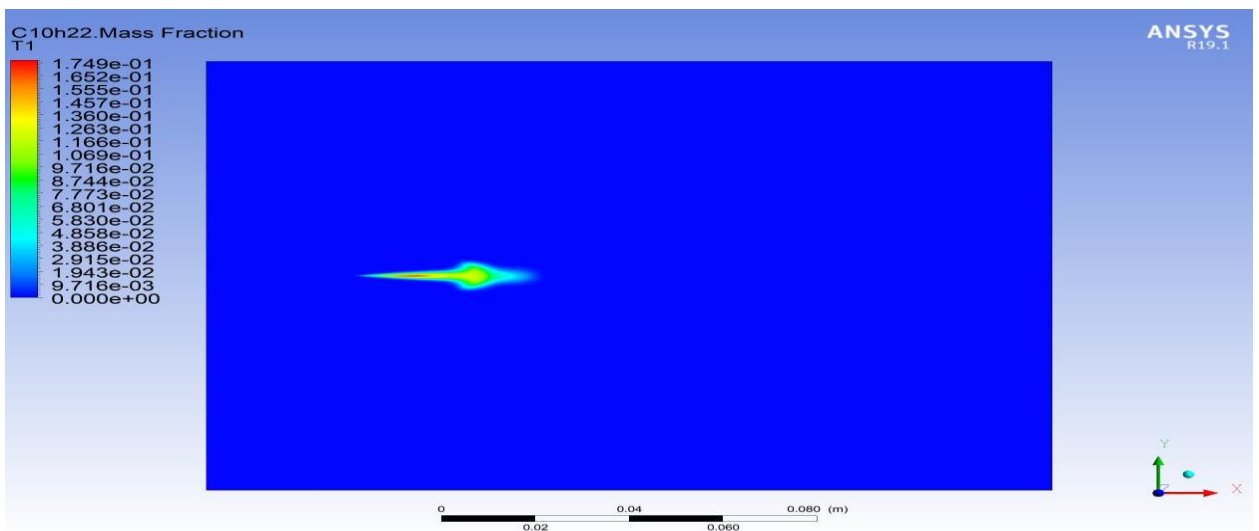
Figure 4.7: Contours of mass fraction at 623K

In figure 4.7 mass fraction contour of droplet is shown. Droplets are injected with a given initial flow rate. A calculated flow rate is given in the injection and then it is divided into droplets. For the current geometry case first the mass fraction is less in the start then it starts increasing. When evaporation of droplets is started then mass fraction is start decreasing. It can be seen clearly that in the end of plume mass fraction becomes zero because all the mass is evaporated and plume is vanished.

ii)   D=20 micron T=623,823,973 K
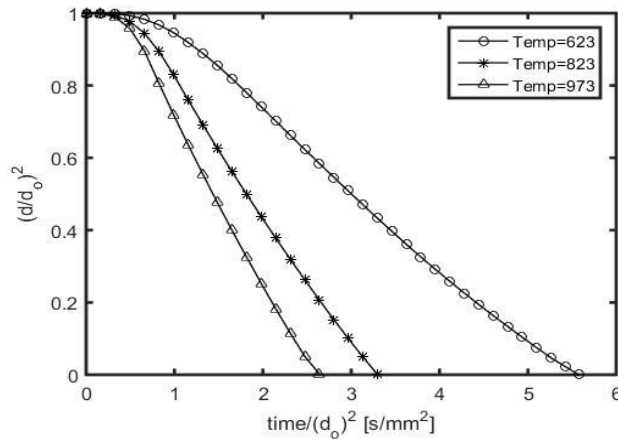
Figure 4.8: Vapourization of 20 micron n-decane dropelt at diffferent ambient temperatures

In fig 4.8 evaporation of 20 micron droplet is plotted against the normalized time. In this figure it can be seen clearly that by increasing the size of size of droplet evaporation time of droplet also increased. In above figure regression rate of 20 micron droplet is plotted at three different ambient temperatures. Evaporation time at high ambient temperature is low and vice versa.
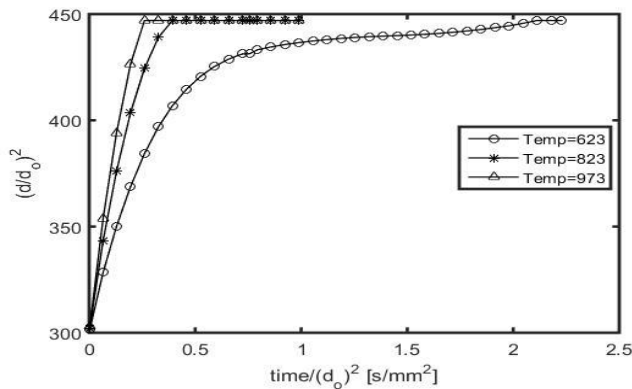

Figure 4.9: Droplet Temperature of 20 micron

In figure 4.9 temperature profiles of 20 micron droplet are plotted against the normalized time. Same trend is observed for the different ambient temperatures. For lower temperature droplet of larger diameter is evaporated in a large time as compared to the higher temperatures.
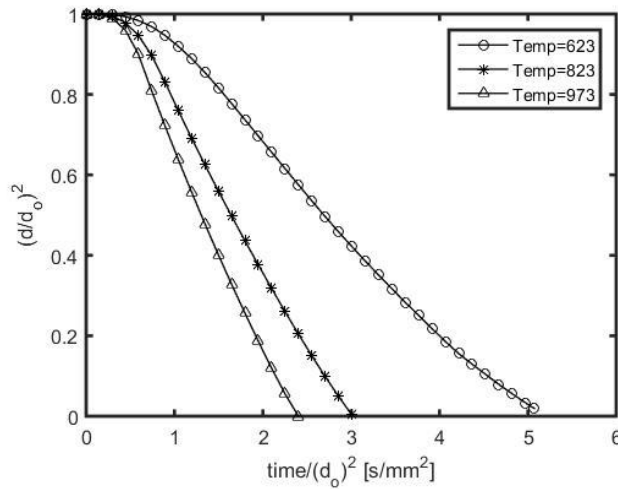
i)   D=25 micron T=623,823,973 K

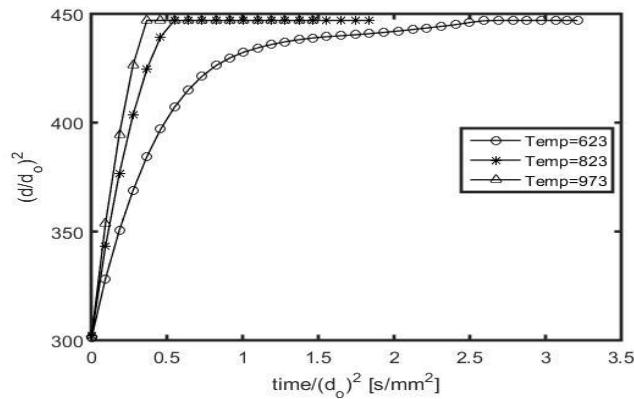*Figure 4.10: Vapourization of 25 micron n-decane dropelt at diffferent ambient temperatures*

Figure 4.11: Droplet Temperature of 25 micron

In figures 4.10 and 4.11 evaporation rate and temperatures profiles of 25 micron droplet are shown. It is evident that as the droplet size is increased heat up period, droplet lifetime and evaporation time is increased at the same ambient temperatures. In above figure it can be seen that when size of droplet is increased droplet lifetime is increased appreciably. It is due to the fact that when size is increased mass is also increased. Evaporation starts from the surface and it is a surface

phenomenon. Due to increases mass and surface area heat up period is also increased and eventually droplet life time and evaporation time is also increased.

Analysis of velocity at same temperature for different size droplets

In this section velocity profiles of droplets of different sizes are plotted at the same ambient temperature. It is observed that at same velocity and same ambient temperature residence time of small droplets is short and for large droplets it's pretty high. Drag force plays an important role in the residence time of time droplets. Large size droplets face the lower drag force as compared to smaller ones and hence their residence time is greater than the smaller ones. Thus evaporation time of larger droplets is greater than the smaller ones at same temperature and velocity.
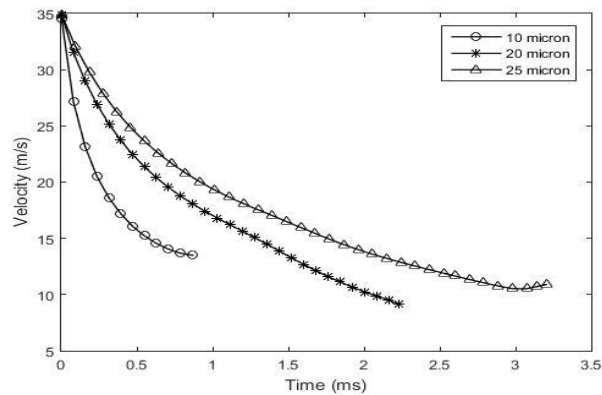

Figure 4.12: Velocity regression at 623K

In above figure velocity profile of droplet diameter is plotted for 10 micron droplet at 623K. Droplet of 25 micron remains alive for a long time. It is due to fact that because of large size its evaporation time is increased than the smaller droplets. While smaller droplets are vanished in a small time. Velocity profiles of all droplets at all temperatures are approximately same.
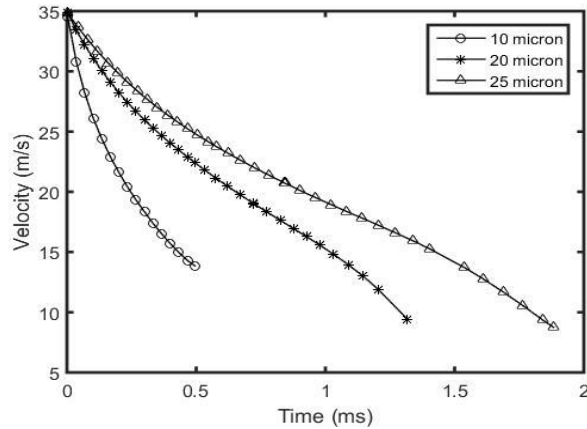
Figure 4.13: Velocity regression at 823K

In figure 4.13 velocity profiles of different diameters are plotted at same ambient temperature. Same trend is observed as in case of temperature at 823K. Only difference is at higher temperature evaporation time is decreased for the droplet.
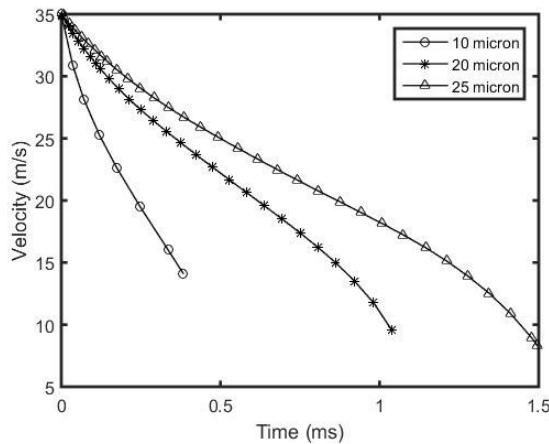

Figure 4.14: Velocity regression at 973K

In figure 4.14 velocity profiles of 10, 20 and 25 micron droplet are plotted at higher temperature of 973K. It is observed that by increasing temperature to 973K evaporation time is decreased appreciably.

DPM Summary

In this section DPM summary is given for various cases of n-decane fuel droplets. DPM summary is a report that groups together particles with each possible fate, and reports the number of particles, the time elapsed during trajectories, and the mass and energy transfer. This information can be very useful for obtaining information such as where particles are escaping from the domain, where particles are colliding with surfaces, and the extent of heat and mass transfer

35

to/from the particles within the domain. Additional information is reported for combusting particles.

Elapsed Time

The number of particles with each fate is listed under the Number heading. (Particles that escape through different zones or are trapped at different zones are considered to have different fates, and are therefore listed separately.) The minimum, maximum, and average time elapsed during the trajectories of these particles, as well as the standard deviation about the average time, are listed in the Min, Max, Avg, and Std Dev columns. This information indicates how much time the particle(s) spent in the domain before they escaped, aborted, evaporated, or were trapped.

Mass Transfer Summary

For all droplet or combusting particles with each fate, the total initial and final mass flow rates and the change in mass flow rate are reported in the Initial, Final, and Change columns. With this information, you can determine how much mass was transferred to the continuous phase from the particles.

Energy Transfer Summary

For all particles with each fate, the total initial and final heat content and the change in heat content are reported in the Initial, Final, and Change columns. This report tells you how much heat was transferred from the continuous phase to the particles.

1) D=10 micron, T=623K,Td=300K

Fate	Number	Elapsed Time (s)			
		Min	Max	Avg	Std Dev
----	------	----------	----------	----------	----------
Evaporated	714	6.089e-04	8.610e-04	8.184e-04	0.000e+00

(*)- Mass Transfer Summary - (*)

Fate	Mass (kg)		
	Initial	Final	Change
----	----------	----------	----------
Evaporated	6.426e-06	0.000e+00	-6.426e-06

(*)- Energy Transfer Summary - (*)

| Fate | Energy (J) | | Change of Energy (J) | | |
	Initial	Final	Sensible	Latent	Total
Evaporated	-1.943e+00	0.000e+00	-2.485e-02	1.968e+00	1.943e+00

Case-02

n-heptane fuel

In this section results of n-heptane fuel droplets are given. In this section droplets of size 10, 20 and 25 micron are considered. It is observed that droplets having small size are evaporated in a short time than the droplets of larger sizes. Ambient temperature also affects the evaporation of diesel fuel droplets. At high ambient temperature evaporation occurs faster than the lower ambient temperature. At temperature of 973K the droplet life time is much shorter than the temperature of 623K. Also it is observed that evaporation time of n-heptane fuel droplets is lower than the n-decane.

i)   D=10 micron T=623,823,973 K

In figure 4.40 regression in diameter of n-heptane fuel droplet of size 10 micron is plotted using D^2-law against the normalized time. It is obvious that at lower temperature of 623K droplet life is higher than the temperatures of 823 and 973k. At lower temperature of 623K evaporation of time is approximately 45 percent more than the temperature at 823K. While at a higher temperature of 973K evaporation time and droplet life is much short as compared to the other two cases.
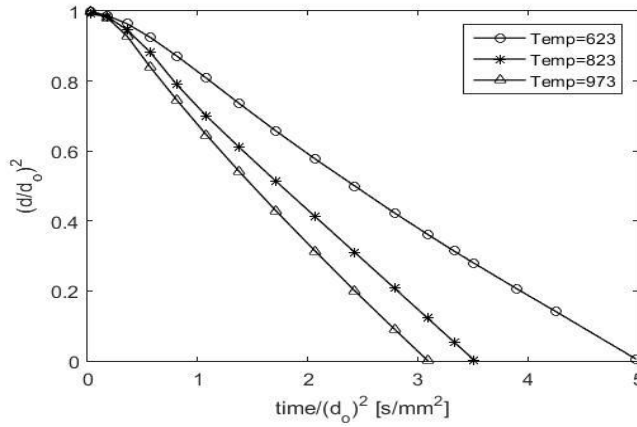
Figure 4.15: Vaporization of 10 micron n-heptane droplet at different ambient temperatures

In figure 4.15 Temperature profiles of n-heptane 10 micron droplet is plotted against the
normalized time and it is observed that a similar trend can be seen as in case of droplet
regression with time. At higher temperature of 973K droplet lifetime is much short than the
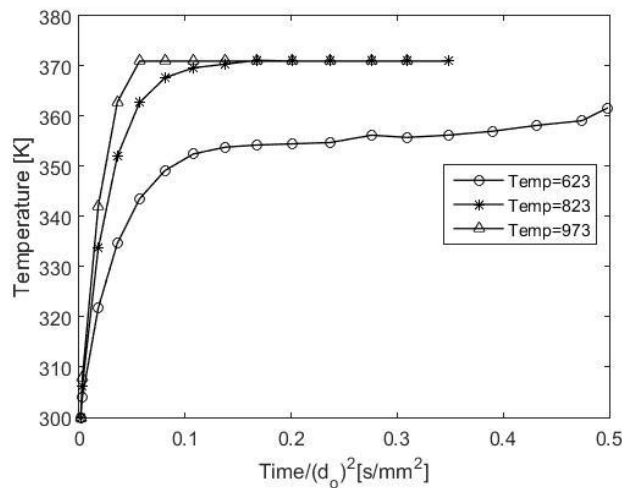623K. For the temperature of 623K droplet residence time is more than the temperatures of 823K
and 973K.

Figure 4.16: Droplet Temperature of 10 micron
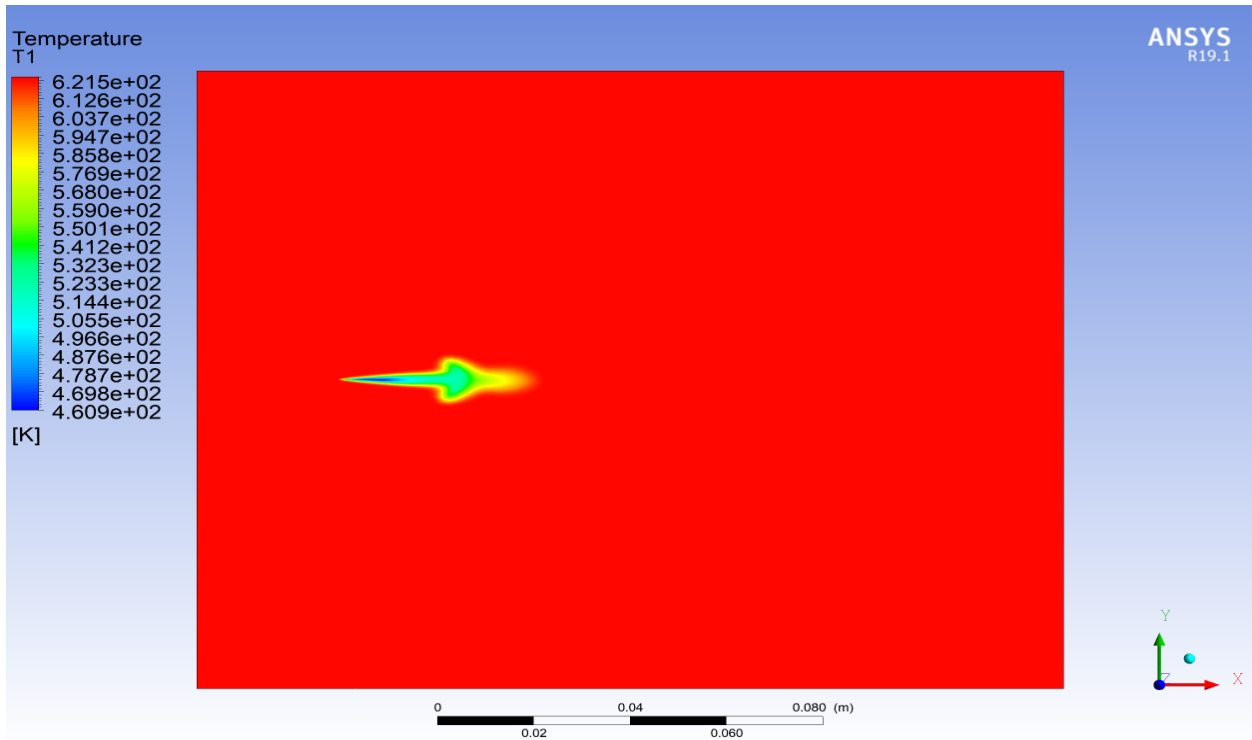
Figure 4.17: Contour of temperature at 623K
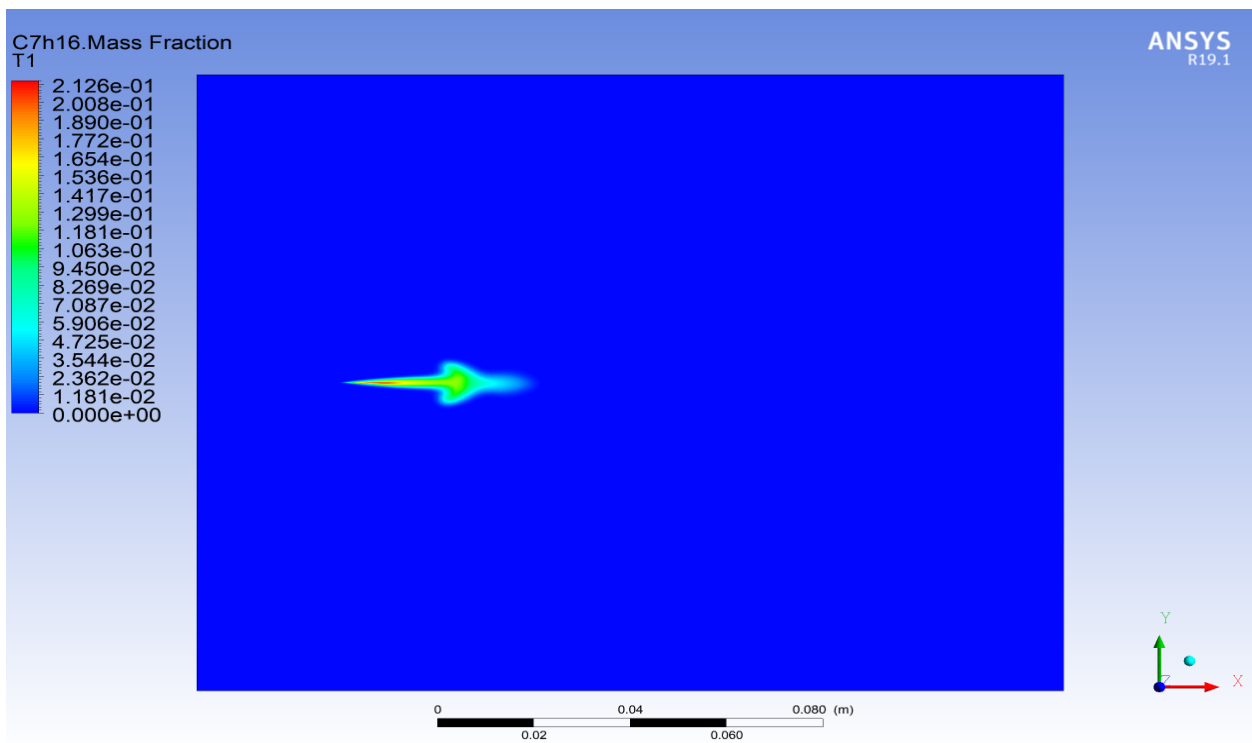
Figure 4.18: Contour of mass fraction at 623K

i) D=20 micron T=623,823,973 K

In fig 4.19 evaporation of 20 micron droplet is plotted against the normalized time. In this figure it can be seen clearly that by increasing the size of size of droplet evaporation time of droplet also increased. In above figure regression rate of 20 micron droplet is plotted at three different ambient temperatures. Evaporation time at high ambient temperature is low and vice versa.

In figure 4.20 temperature profiles of 20 micron droplet are plotted against the normalized time. Same trend is observed for the different ambient temperatures. For lower temperature droplet of larger diameter is evaporated in a large time as compared to the higher temperatures.
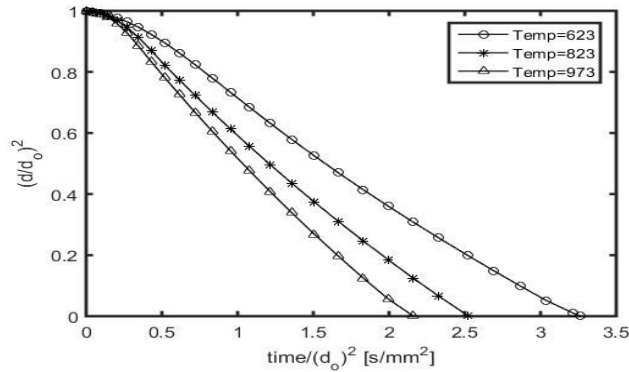

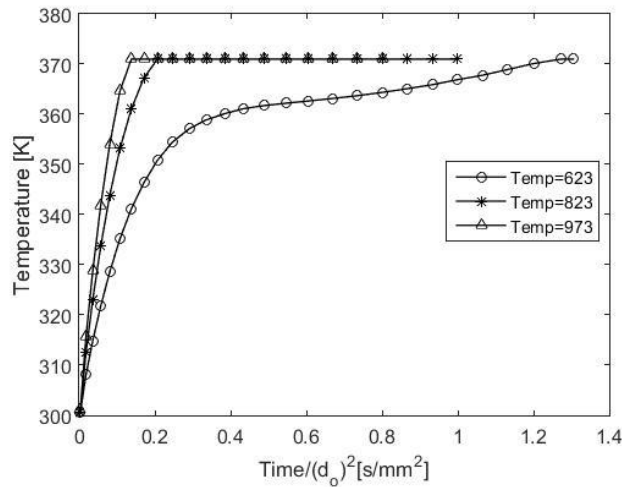*Figure 4.19: Vaporization of 20 micron n-heptane droplet at different ambient temperatures*

Figure 4.20: Droplet Temperature of 20 micron

i) D=25 micron T=623,823,973 K

In figures 4.21 and 4.22 evaporation rate and temperatures profiles of 25 micron n-heptane diesel fuel droplet are shown. It is evident that as the droplet size is increased heat up period, droplet lifetime and evaporation time is increased at the same ambient temperatures. In above figure it can be seen that when size of droplet is increased droplet lifetime is increased appreciably. It is due to the fact that when size is increased mass is also increased. Evaporation starts from the surface and it is a surface phenomenon. Due to increases mass and surface area heat up period is also increased and eventually droplet life time and evaporation time is also increased.
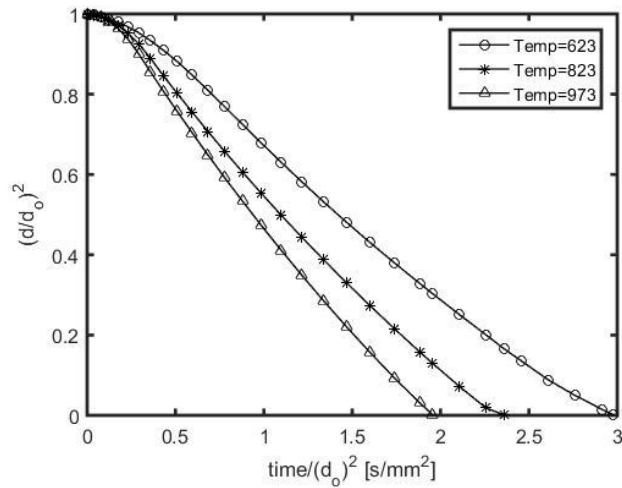

Figure 4.21: Vaporization of 25 micron n-heptane droplet at different ambient temperatures
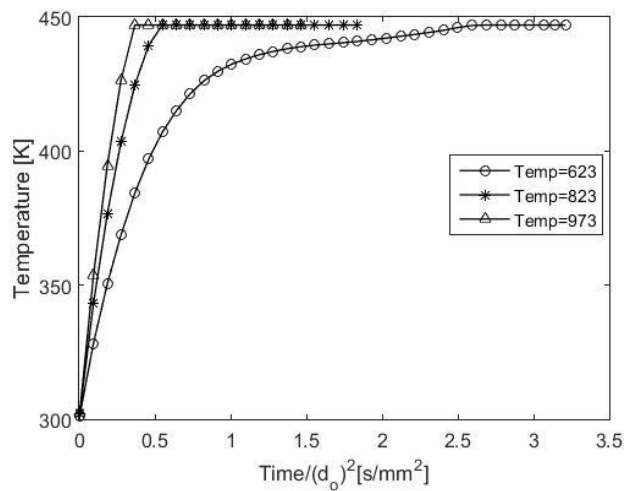

Figure 4.22: Droplet Temperature of 25 micron

Analysis of velocity at same temperature for different size droplets

In this section velocity profiles of droplets of different sizes are plotted at the same ambient temperature. It is observed that at same velocity and same ambient temperature residence time of small droplets is short and for large droplets it's pretty high. Drag force plays an important role in the residence time of time droplets. Large size droplets face the lower drag force as compared to smaller ones and hence their residence time is greater than the smaller ones. Thus evaporation time of larger droplets is greater than the smaller ones at same temperature and velocity.

In figure 4.23 velocity profile of droplet diameter is plotted for 10 micron droplet at 623K. Droplet of 25 micron remains alive for a long time. It is due to fact that because of large size its evaporation time is increased than the smaller droplets. While smaller droplets are vanished in a small time. Velocity profiles of all droplets at all temperatures are approximately same.

In figure 4.24 velocity profiles of different diameters are plotted at same ambient temperature of 823K. Same trend is observed as in case of temperature at 623K. Only difference is at higher temperature evaporation time is decreased for the droplet.

In figure 4.25 velocity profiles of 10, 20 and 25 micron droplet are plotted at higher temperature of 973K. It is observed that by increasing temperature to 973K evaporation time is decreased appreciably.
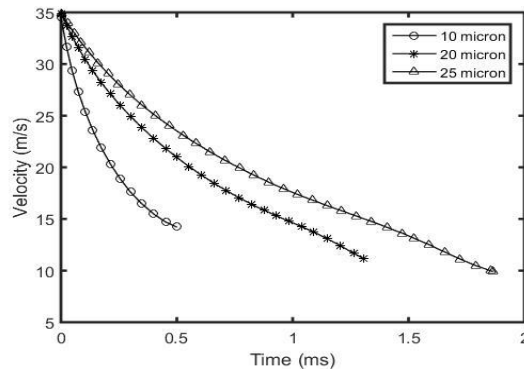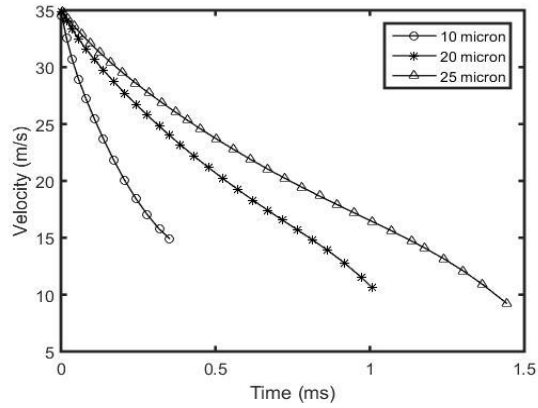

Figure 4.23: Velocity regression at 623K
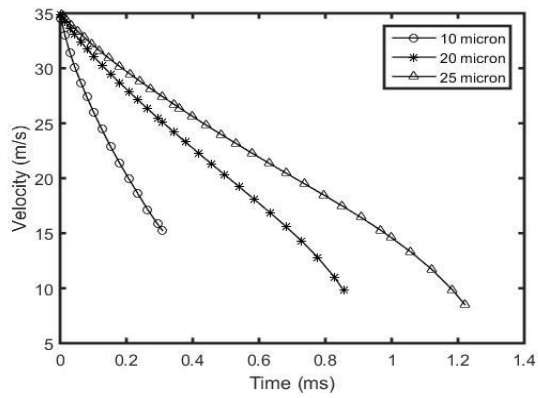
Figure 4.24: Velocity regression at 823K

Figure 4.25: Velocity regression at 973K

DPM Summary

In this section DPM summary is given for various cases of n-heptane fuel droplets.

2) **D=10 micron, T=623K,Td=300K**

Fate	Number	Elapsed Time (s)			
		Min	Max	Avg	Std Dev
----	------	----------	----------	----------	----------
Evaporated	834	3.562e-04	5.010e-04	4.804e-04	2.041e-05

(*)- Mass Transfer Summary - (*)

Fate	Mass (kg)

	Initial	Final	Change
----	----------	----------	----------
Evaporated	7.506e-06	0.000e+00	-7.506e-06

(*)- Energy Transfer Summary - (*)

Fate	Energy (J)		Change of Energy (J)		
	Initial	Final	Sensible	Latent	Total
----	----------	----------	----------	----------	---------
Evaporated	-2.598e+00	0.000e+00	-3.081e-02	2.629e+00	2.598e+00

Comparison of Fuels

In figure 4.26 comparison of two fuels is shown. It can be seen clearly that n-heptane droplets evaporates in a short span of time than the n-decane fuel droplets. It is due the fact that composition of n-heptane is different from the n-decane and its properties vary in some manners i.e. density, vaporization temperature and boiling point. Vaporization temperature of n-heptane is lower than the n-decane thus evaporation time of n-heptane is shorter than the droplets of n-decane at same temperature and pressure conditions and it is evident from the figure 4.26.
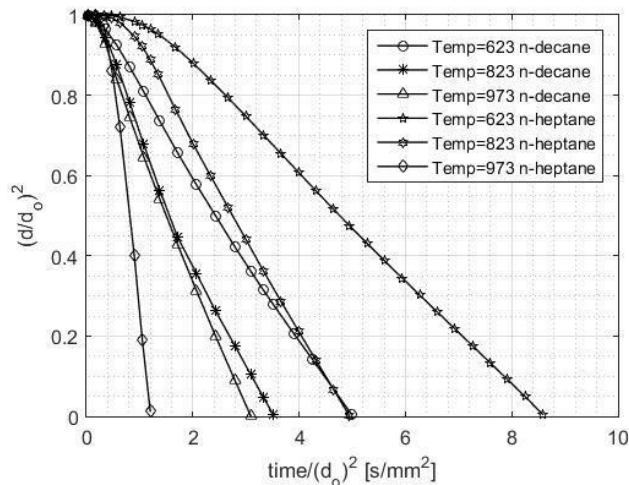

Figure 4.26: Vaporization of 25 micron n-heptane and n-decane droplet at different ambient temperatures

Application of the proposed evaporation model in Diesel engine

The present evaporation model applied to model the evaporation of n-decane diesel fuel droplets in diesel engine. This engine is operating on rpm of 2000. In the present calculation only one sixth sector of engine cylinder is taken.

Detail of the methodology of the calculation

Above presented model is applied to simulate the droplets of n-decane fuel in Ansys. Conservation equations of mass, momentum and energy are coupled with the realizable k-e turbulence model and species transport equation to model the evaporation of fuel droplets in high temperature and pressure conditions. DPM is applied to solve the discrete phase i.e. fuel droplet into the continuous phase present in the combustion chamber. In coupled calculation continuous phase is solved before introduction of discrete phase into the engine cylinder. Then discrete phase is introduced by calculating the particle trajectories for discrete phase injection. Then continuous flow phase is recalculated after the injection of discrete phase using interphase exchange of mass, momentum and heat determined by the previous calculation. Finally discrete phase is recalculated using the modified continuous phase flow field. The present model is applied to the one sixth sector of the engine cylinder. A 3D geometry is used for the calculations. Different views of one sixth sector are shown below. Symmetry is applied on the geometry to avoid any inconvenience. Cone injection with two streams is taken for 3D geometry. A 30 degrees cone angle is applied on the injection. Velocity of droplet is taken 35 m/s. Primary and secondary breakup effects are ignored in order to visualize the evaporation of fuel droplets only. Diameter of droplet is taken 10 micron. Results of mass fraction and temperature are shown for the present calculation.
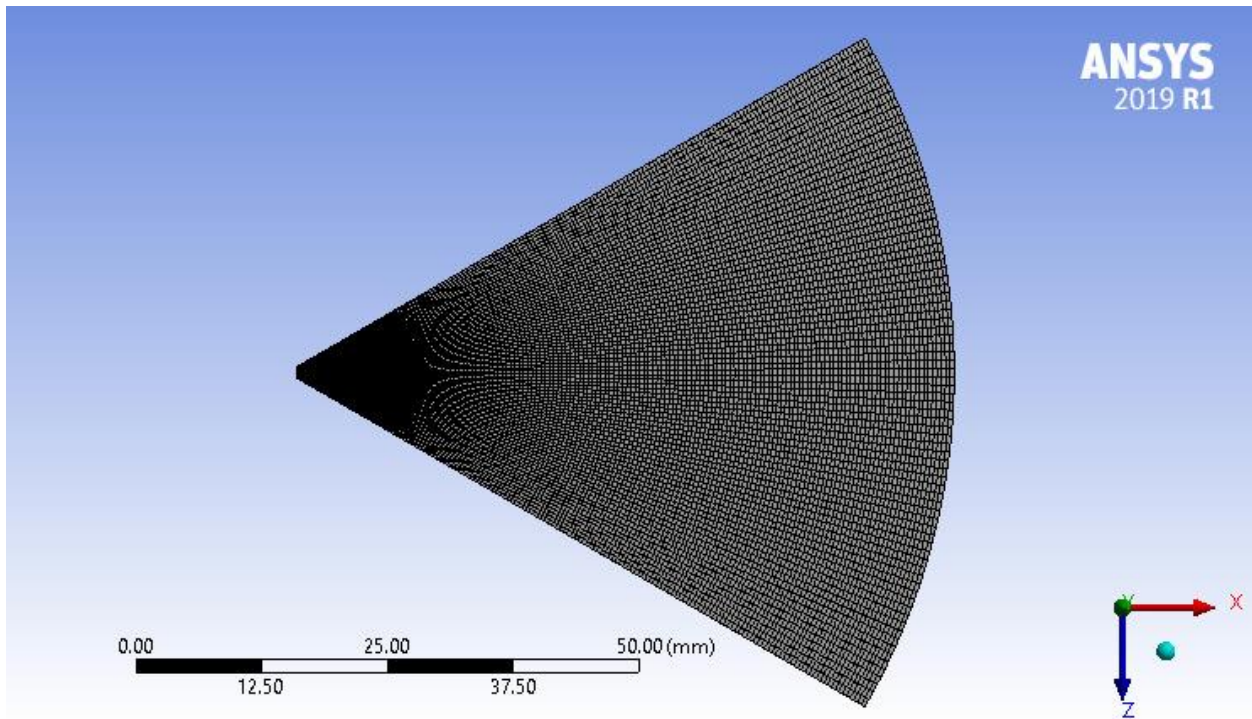
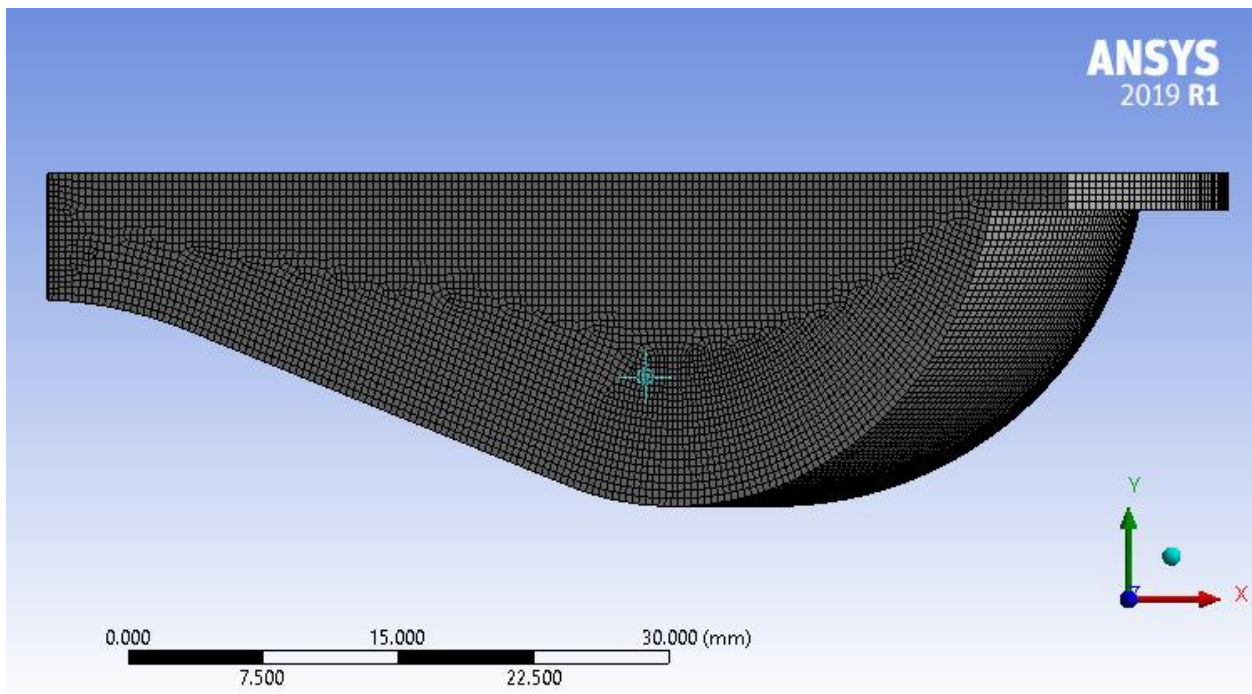*Figure 4.27: mesh of one sixth sector of engine cylinder*

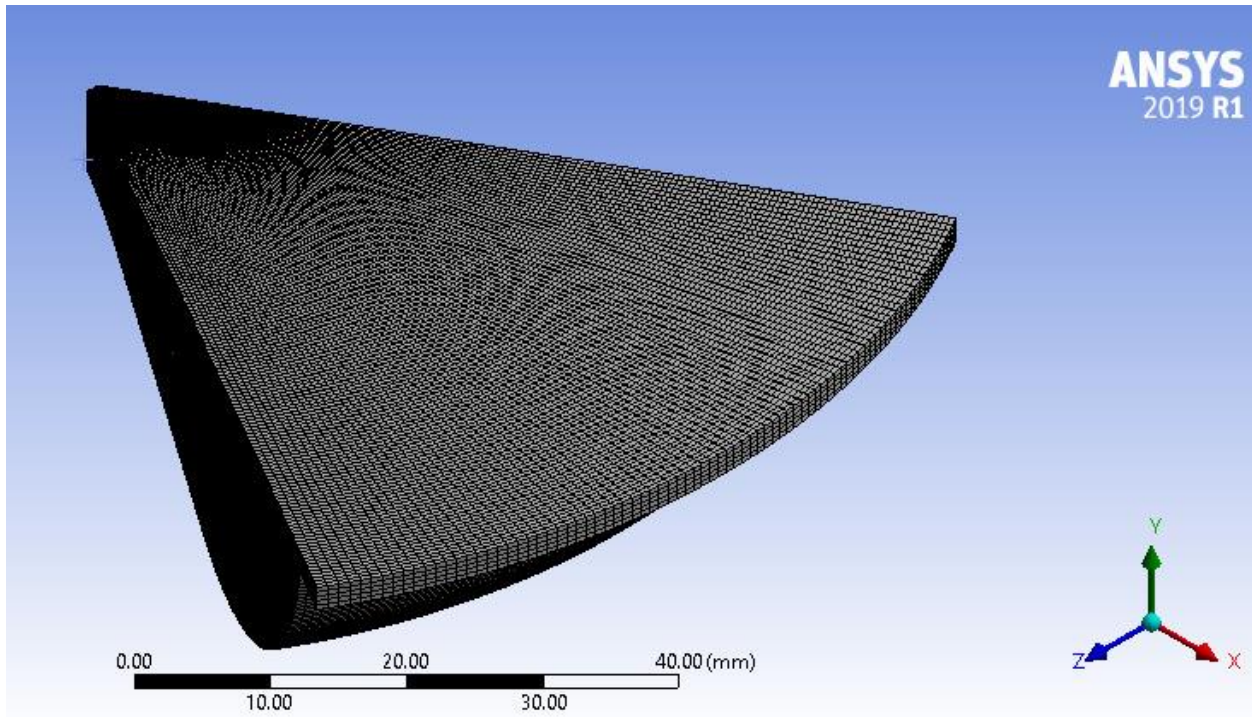*Figure 4.28: mesh of one sixth sector of engine cylinder*

Figure 4.29: mesh of one sixth sector of engine cylinder

Mesh of one sixth sector of engine cylinder is shown in above figures. Total elements taken for the mesh are 875201. These are the acceptable number of elements for the current calculations. Engine specification and injection parameters are given as follows.

Engine Specifications		Injection specifications	
Bore	150 mm	Injection type	Cone
Stroke	180 mm	Droplet velocity	35 m/s
Max Torque	295 kg-m	Droplet temperature	300 K
Ambient Pressure	4 MPa	Fuel type	n-decane
Nozzle Diameter	0.29 mm	Flow rate	0.003 kg/s

Injection pressure	20 MPa	Injection duration	4 ms

Table 4.1: injection specifications

Results and Discussions

Contours of mass fraction and temperature inside the one sixths sector of engine cylinder are shown here. Nozzle has six holes which ejects the 6 jets in six sectors of engine cylinder 60 degrees apart from each other. In the figures below mass fraction contours are shown at various planes and axis.

In figure 4.30 a top view of one sixth sector of engine cylinder is shown. In this view it is shown that when jet is evolved from the nozzle it splits approximately equally in the two sides of chamber sector. It is due to the fact that cone angle of 30 degrees is kept for the injection. This one sixth sector has total 60 degrees angle due to the fact that cylinder is divided into 6 sector and each has 60 degrees total angle. When jet is evolved from the nozzle hole it splits into two streams and equal amount of mass is distributed.

In figures 4.31 and 4.32 side views of one sixth sector are shown. Both the views are approximately same showing that at both sides almost same amount of mass is distributed. In figures 4.33 and 4.34 3D views of sector are shown. It shows how mass fraction is reduced in all sides of sector. It also shows the symmetry of injection streams at all sides.

In figures 4.35 and 4.36 Y-Z plane of sector is shown. In this plane mass fraction in two sides of sector is shown. Again it is evident that mass fraction is almost same in both sides. This implies that when jets are injected at a cone angle of 30 degrees a uniform mass distribution is achieved. Form figures 4.30 to 4.36 penetration length of jet is also of importance. It is seen that jet is not struck to the side wall of sector rather it is vanished before the half of the length from the center to the wall. Blue area in the contours show that there is zero mass fraction there. Yellow color in contours is dominant on both sides that shows the uniformity. Mass fraction contours show that all the mass injected in form of droplets is vaporized in the sector of engine cylinder.

Similarly from figures 4.36 to 4.40 temperature contours are shown in different planes and axes. It can be seen that where droplets are present the temperature is lower than the rest area. Initial ambient temperature of engine cylinder was 623K but after injection temperature at the place where injected particles travelled is lower down due to the evaporation of fuel droplets. In figure 4.37 plane contour is shown for temperature. It shows the temperature of sector in the presence of fuel mass fraction. Maximum temperature is 623K and minimum is 385K of the sector.

The present evaporation model works for the real engine applications. But certain things need to be addressed. Droplet diameter should be as small as possible to evaporate the mass quickly. In this work it is recommended that nozzle hole size should designed in a way so that after break up and other effects including the penetration length final size should reach up to 10 micron. In this study three different diameters are taken to see the evaporation time and droplet life time. It is obvious that droplets of small diameters evaporates more quickly. Nozzle taken in this study has a diameter of 290 micron. Average size of diameter of droplet after penetration length come out to be 25 micron for this nozzle. It is seen that 25 micron droplet take more time to evaporate than the 20 and 10 micron droplets. If nozzle hole is reduced it will also affect the size of droplet after penetration length and average diameter can be obtained smaller. Also there are large number of droplets are formed after injection and it is not necessary to evaporate each droplet. Some droplets strike to head wall before the complete evaporation. If diameter is as small that they do not strike the wall and evaporate completely before striking the wall it will produce more efficient combustion and hence increased efficiency can be achieved. Radiation effects are ignored in the present calculation because at the present engine conditions these effects are negligible.
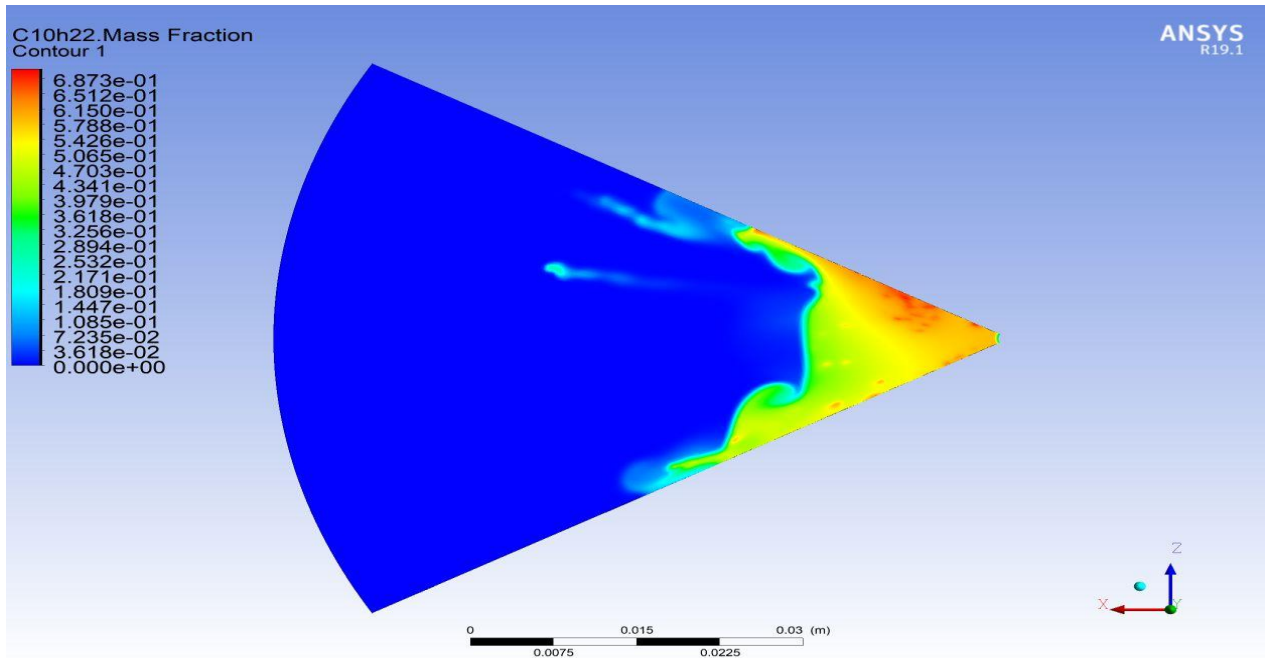
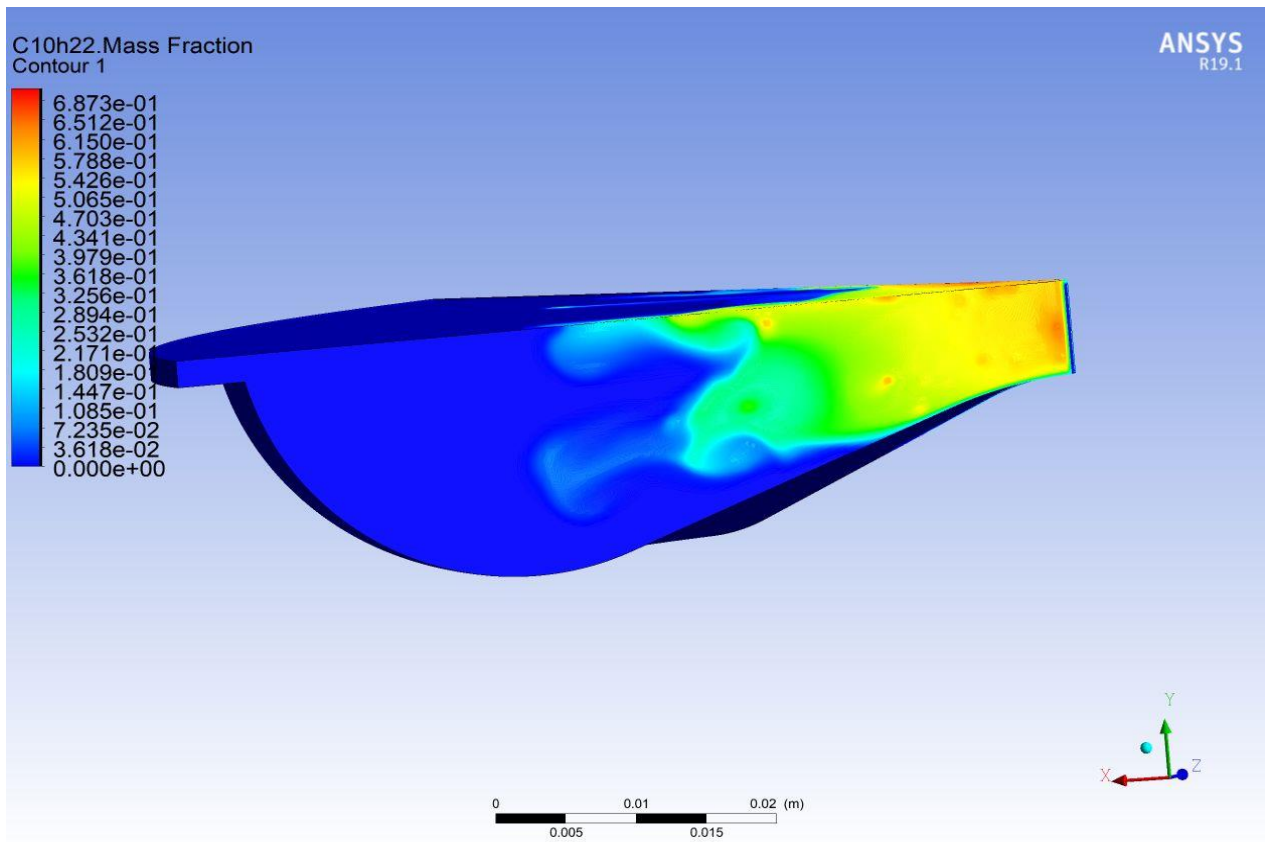*Figure 4.30: Contours of mass fraction of one sixth sector of engine cylinder*

Figure 4.31: Contours of mass fraction of one sixth sector of engine cylinder

50

Figure 4.32: Contours of mass fraction of one sixth sector of engine cylinder

Figure 4.33: Contours of mass fraction of one sixth sector of engine cylinder
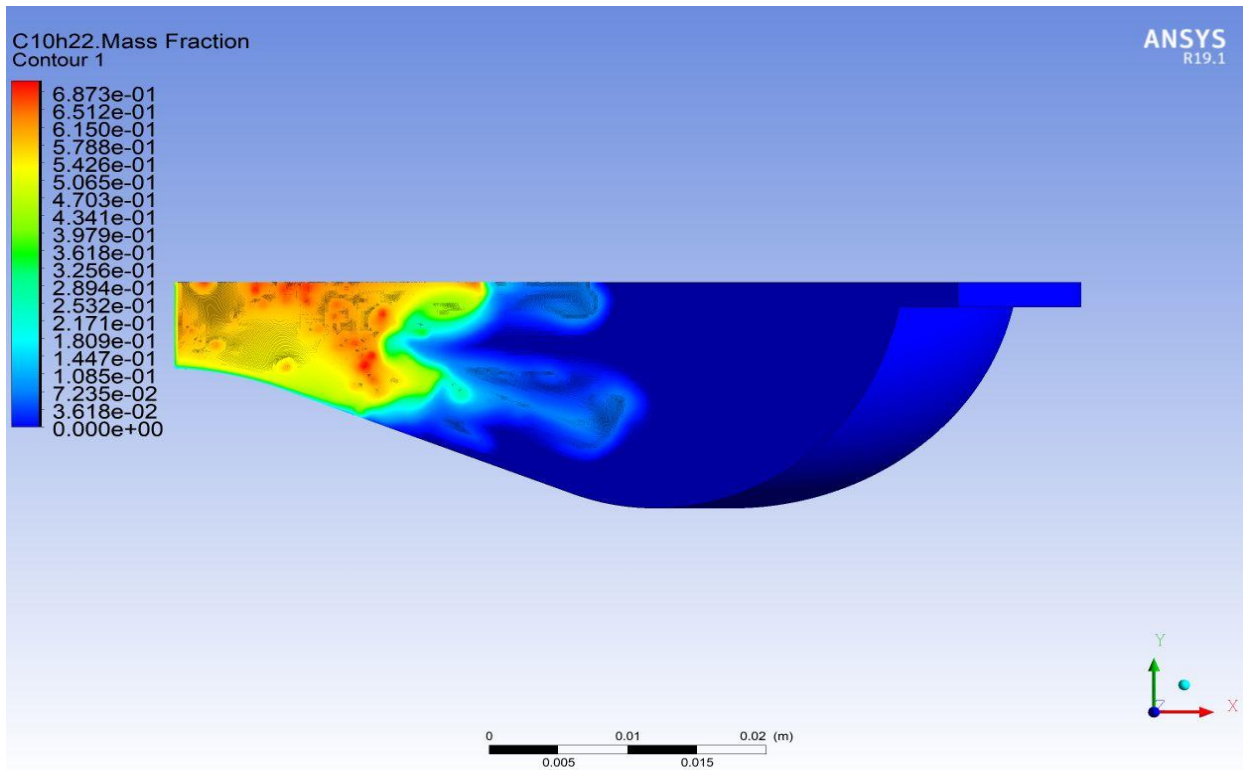
Figure 4.34: Contours of mass fraction of one sixth sector of engine cylinder

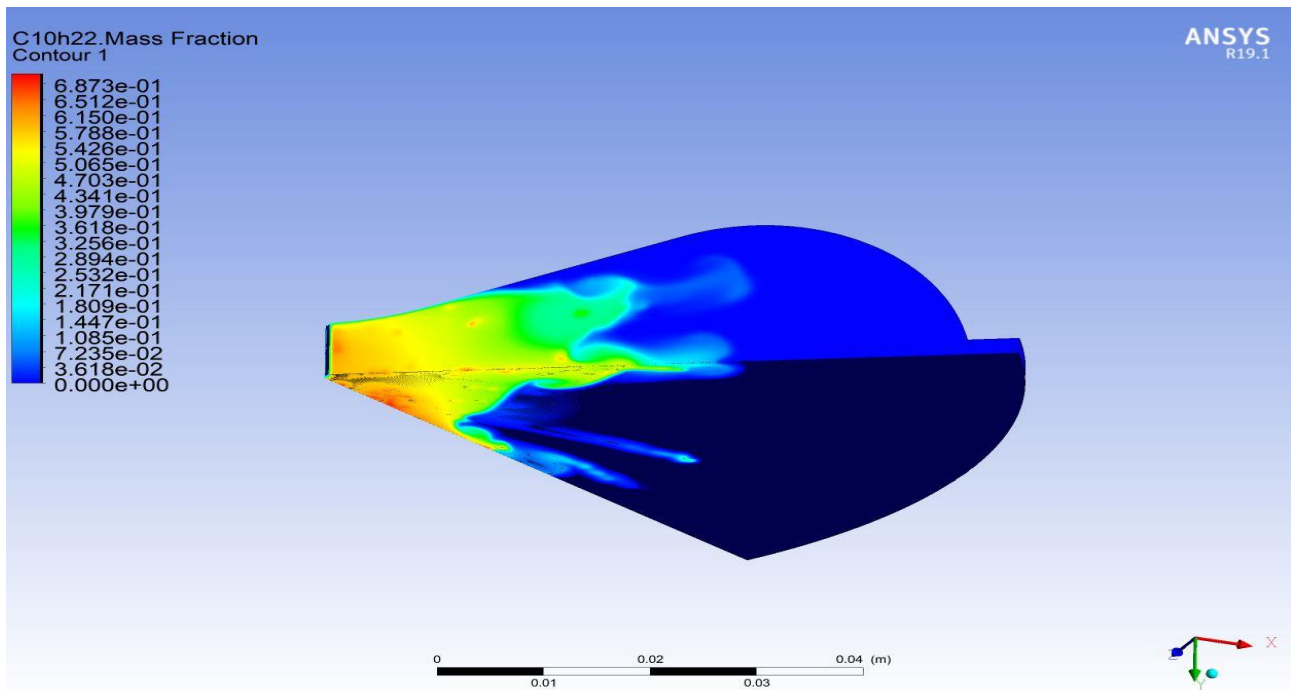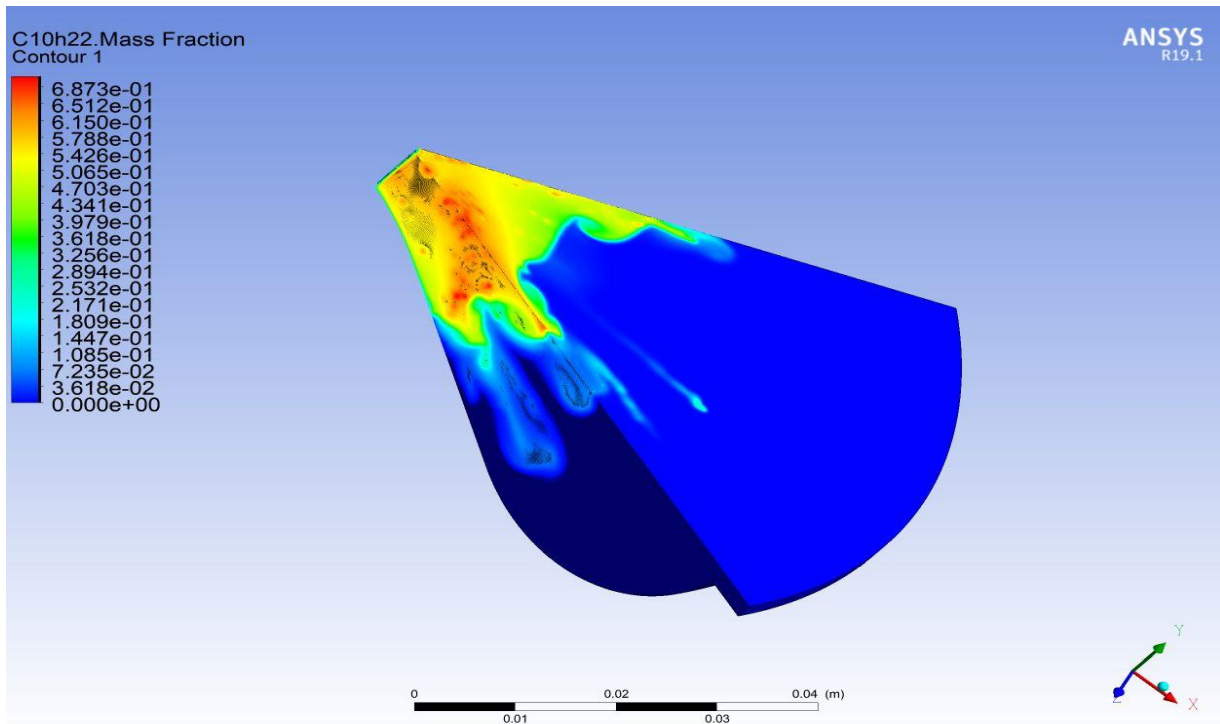

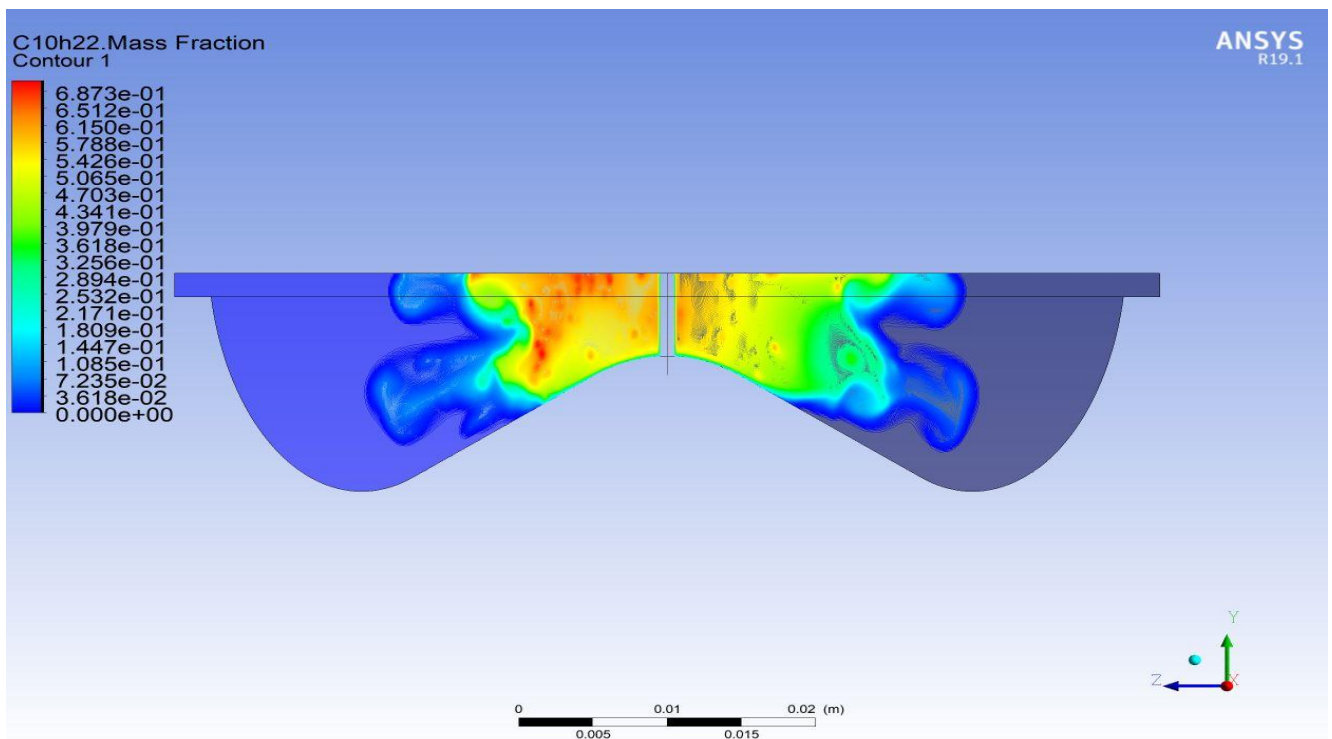*Figure 4.35: Contours of mass fraction of one sixth sector of engine cylinder*

Figure 4.36: Contours of mass fraction of one sixth sector of engine cylinder

Figure 4.37: Contours of Temperature of one sixth sector of engine cylinder

Figure 4.38: Contours of Temperature of one sixth sector of engine cylinder

Figure 4.39: Contours of Temperature of one sixth sector of engine cylinder

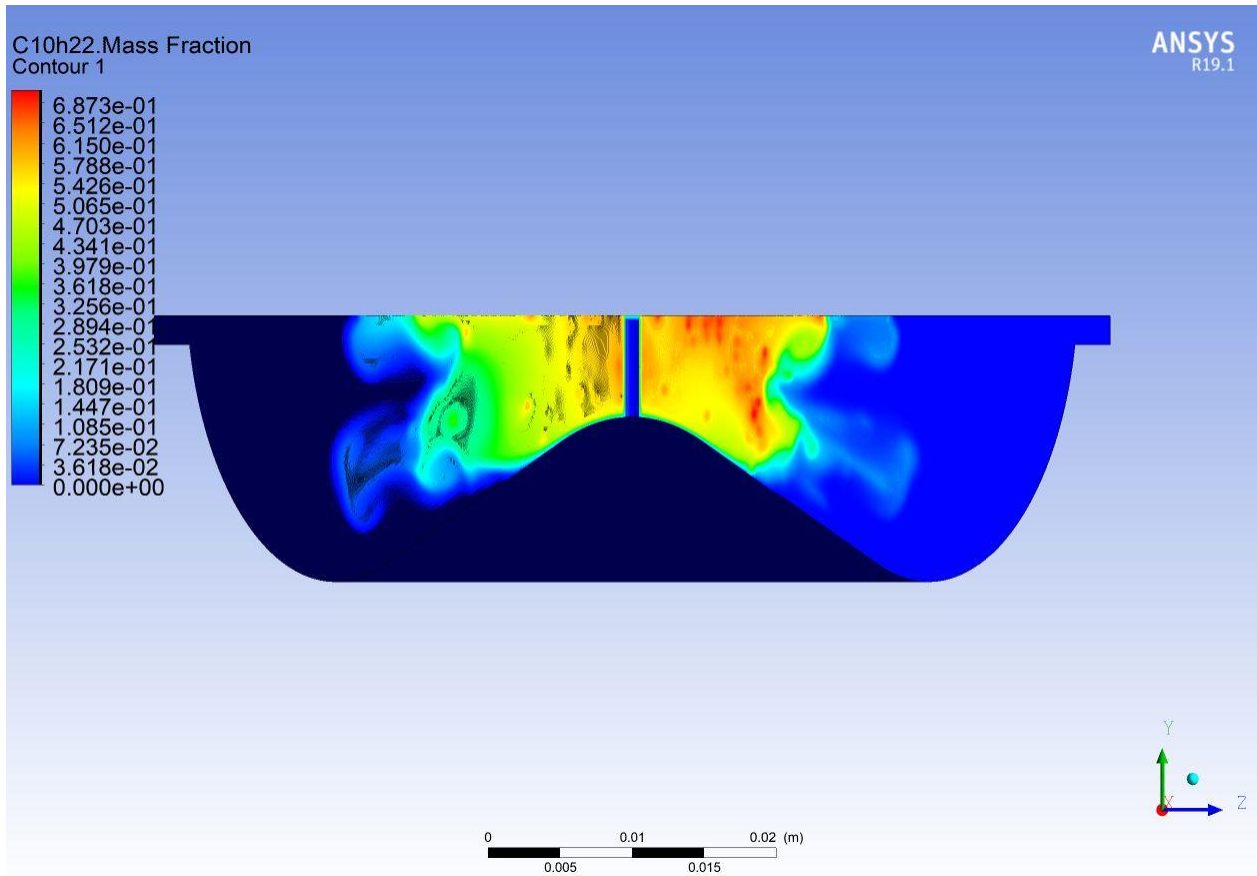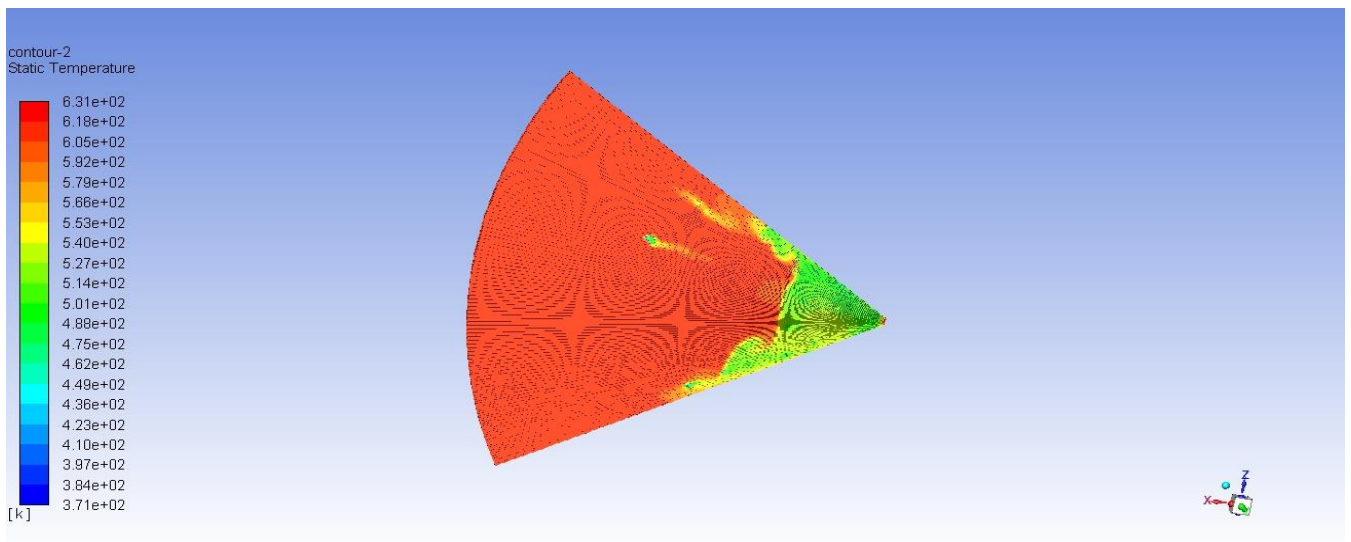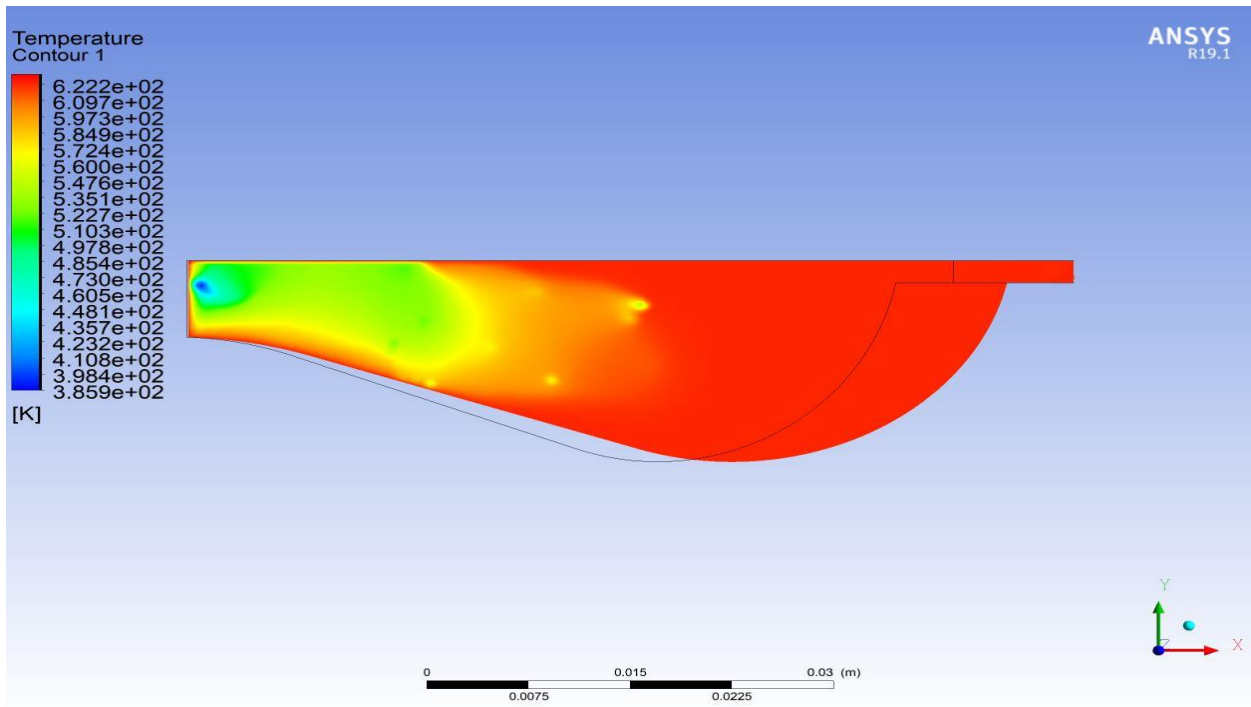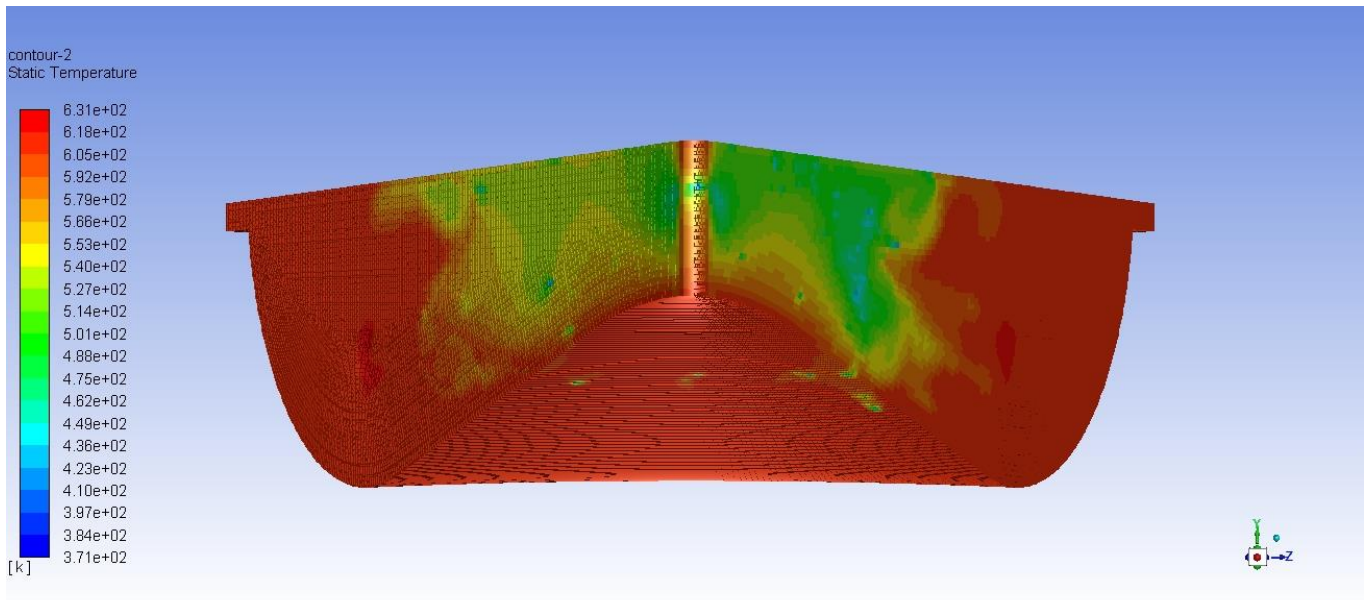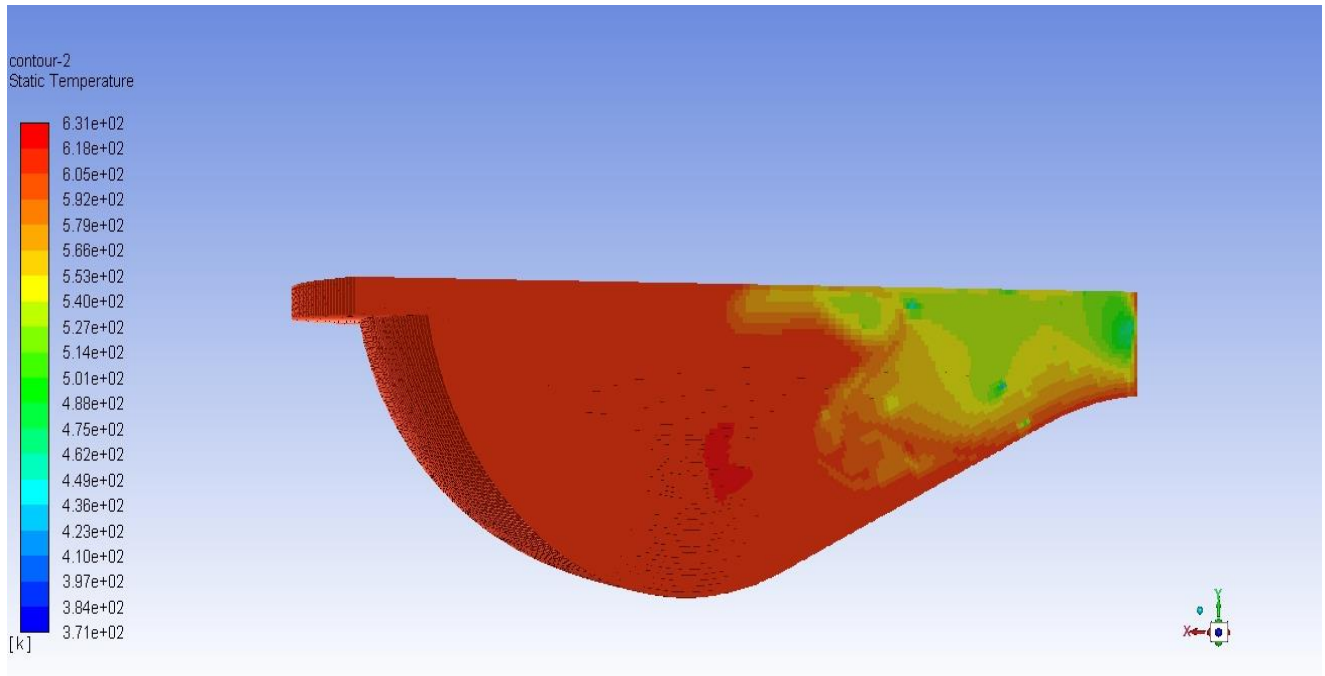*Figure 4.40: Contours of Temperature of one sixth sector of engine cylinder*
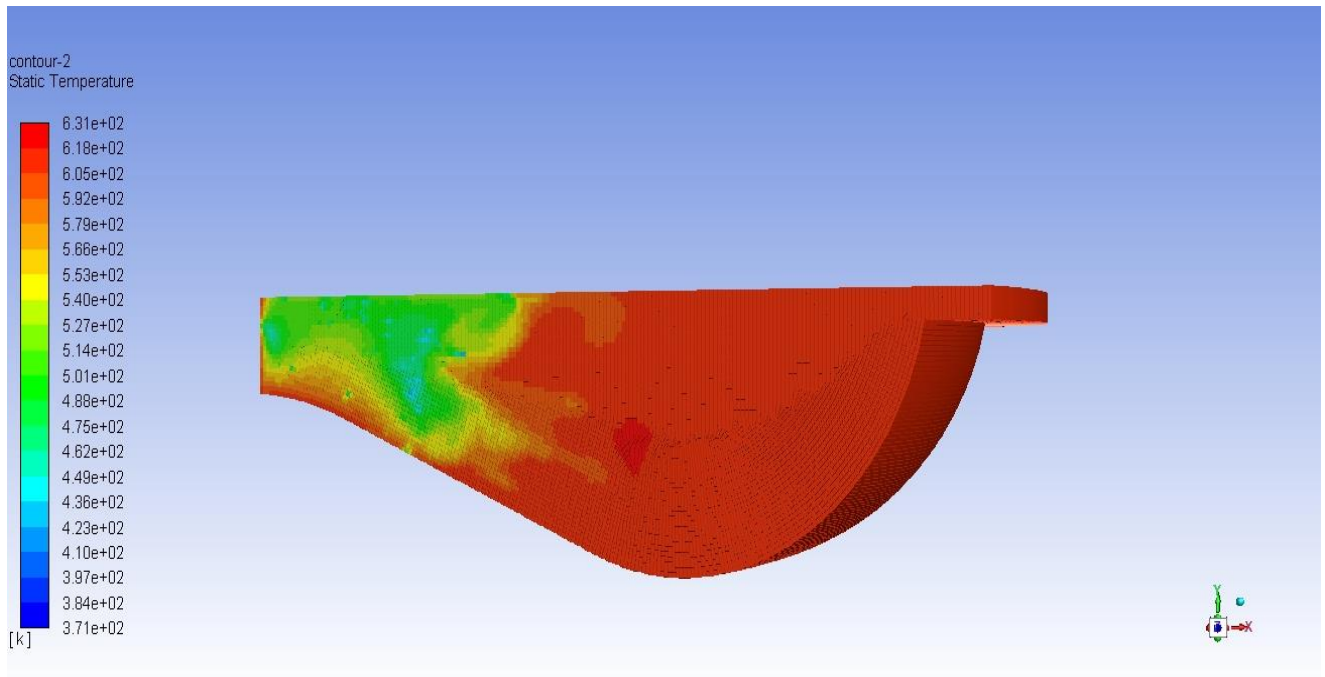
Figure 4.41: Contours of Temperature of one sixth sector of engine cylinder
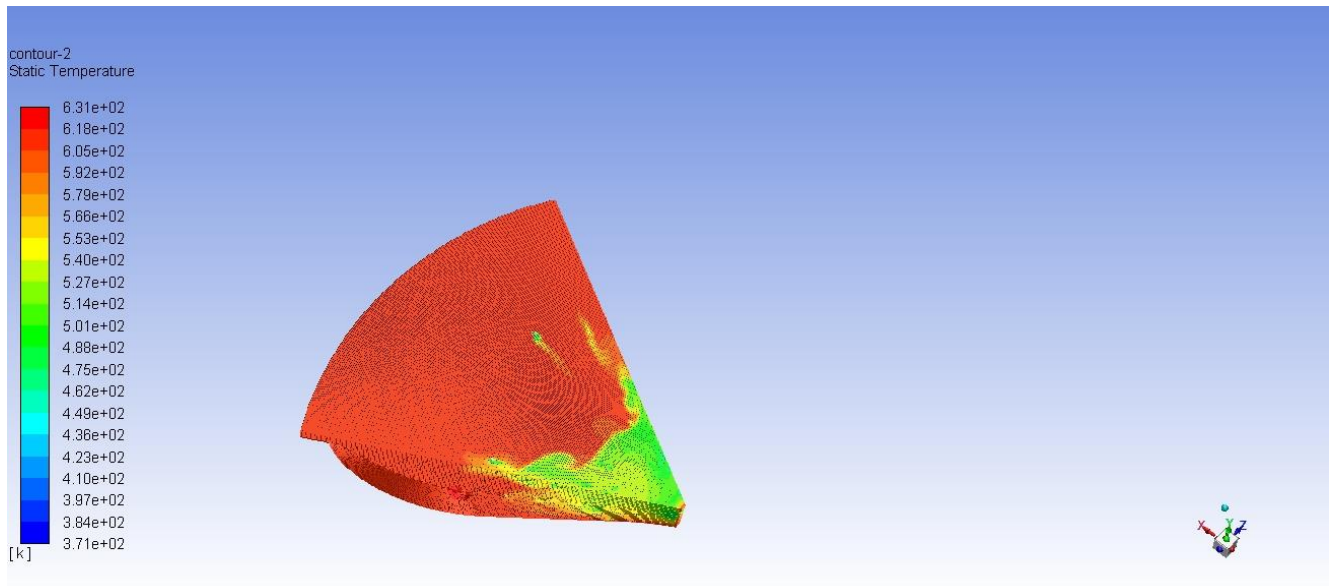
Figure 4.42: Contours of Temperature of one sixth sector of engine cylinder

DPM Summary

Fate	Number	Elapsed Time (s)			
		Min	Max	Avg	Std Dev
----	------	----------	----------	----------	----------
Evaporated	641	4.953e-04	2.268e-03	1.118e-03	2.840e-04

(*)- Mass Transfer Summary - (*)

Fate	Mass (kg)		
	Initial	Final	Change
----	----------	----------	----------
Evaporated	2.885e-06	0.000e+00	-2.885e-06

(*)- Energy Transfer Summary - (*)

Fate	Energy (J)		Change of Energy (J)		
	Initial	Final	Sensible	Latent	Total
----	----------	----------	----------	----------	----------
Evaporated	-8.721e-01	0.000e+00	-1.115e-02	8.833e-01	8.721e-01

56

Mesh Study

Mesh independence analysis is essential while performing numerical simulations. In the current work four different meshes are created and analyzed that are shown in figure 4-A. Finally a mesh of 0.89 million elements is selected for performing the numerical calculations. Total elements taken for the mesh are 893201. These are the acceptable number of elements for the current calculations.

Figure 4-A: Mesh sensitivity analysis

CHAPTER 5:

CONCLUSIONS

In this research evaporation of liquid fuel droplets of n-heptane and n-decane fuels is modelled numerically by considering the 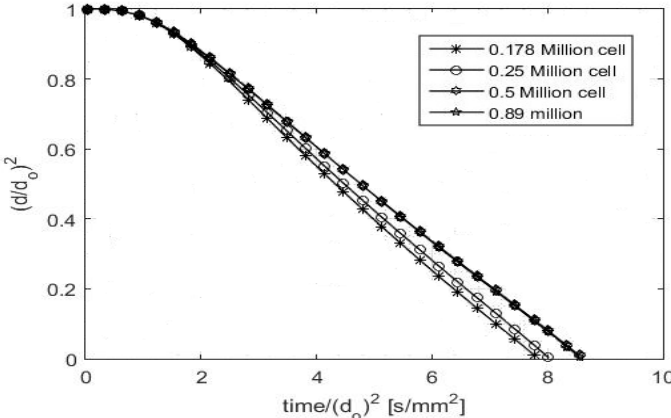turbulence effects present in the engine cylinder due to high temperature and pressure using the Realizable k-epsilon turbulence model. A realizable k-epsilon turbulence model is used in this research due the fact that it has low computation cost as compared to LES and DNS turbulence models. As far as accuracy is concerned DNS is the most accurate model but it computation cost is very high. LES is also an expensive model computationally. But in our problem the accuracy required is easily achieved by the k-epsilon turbulence model and results are in a good agreement with the experimental and numerical data available in literature. Evaporation of fuel droplets directly affects the engine efficiency and fuel economy for internal combustion engine. Incomplete combustion occurs due to incomplete evaporation of fuel droplets that causes the soot emissions and unburnt hydrocarbons in the atmosphere. In the present work it is shown that if droplet size is reduced to an optimal small diameter then it would completely evaporate in the combustion chamber before start of combustion. Moreover a parametric study is performed at different sizes and temperatures of droplets to achieve an optimal size of droplet and ambient temperature. Further it is shown that to model the evaporation process of diesel fuel droplets it is necessary to take into account the turbulence effects present in the cylinder otherwise deviation from the actual phenomenon would occur. Results show that droplet having the large diameter take more time to evaporate completely as compared to the smaller ones. Small droplets evaporate more quickly due to short heat up period than the larger ones. Droplets of same size behave differently at different ambient temperatures. Droplet evaporation time for high temperature is less than the low temperature. Further temperature profiles of droplets plotted against the injection time that shows that small droplets evaporates quickly by absorbing the temperature quickly. Droplets having larger diameters sustain for more time and their evaporation time is greater. Velocity of droplet is also plotted with the injection time and it is confirmed that at the same velocity droplets of small diameters have short heat up period and hence short evaporation time than the large size droplets. In the end comparison for both fuels is also given at same operating conditions and it is observed that n-heptane fuel droplets evaporate in a short time

than the droplets of n-decane fuel droplets. It is due to the fact that vaporization temperature of n-heptane is lower than the vaporization temperature of n-decane fuel. Also boiling temperature of n-heptane is lower than boiling temperature of n-decane fuel. Hence heat up period and evaporation time of n-heptane fuel droplets at high temperature and pressure conditions in a turbulent environment is lower than the n-decane fuel droplets. Finally evaporation model is applied to a heavy duty diesel engine to observe the evaporation of n-decane fuel droplets and acceptable results are obtained.

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CERTIFICATE OF COMPLETENESS

It is hereby certified that the dissertation submitted by **NS Ali Raza**, Reg No. **00000117618**,

Titled: ***Numerical Simulation of Evaporation in Fuel Spray Droplets in a Diesel Engine*** has

been checked/reviewed and its contents are complete in all respects.

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