SIMULATION OF VARIANT AMBIENT CONDITION AND INJECTION PRESSURE ON MIXTURE FORMATION OF BIODIESEL SPRAY

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ABSTRACT

The global environmental change and global warming effects have been become a famous issue and also the major interest in the world. The search for higher energy efficiency of industrial scale of rapid compression machine (RCM) to obtain low emission especially Nitrogen Oxides (NOx) has demanded experimental studies that are complemented with Computational Fluid Dynamics (CFD) simulations. The purpose of this study is to simulate the physics flow pattern of mixture formation with tangential velocity between biodiesel and diesel fuel and air in the mixing chamber of RCM, to determine the nozzle flow and spray characteristics for different injection pressure of biodiesel spray to ambient variant conditions on mixture formation and comparing three types of Crude Palm Oil (CPO) biodiesel blends, B5, B10 and B15 with different ambient density on nozzle flow and spray characteristics by using CFD. To this end, an Eulerian-Lagrangian multiphase approach has been used to simulate the spray processes. CFD Fluent is utilized in this study to investigate the spray characteristics of biodiesel fuels. The simulation considered injection of biodiesel in the constant volume chamber of RCM. The boundary condition is set up at different ambient parameter while the other parameters are kept constant. The effect of fuel type, injection pressure and ambient parameter on the spray behaviour such as spray penetration has been studied under the presence of in-cylinder flow. The spray penetration variation with time for different ambient parameters and also various biodiesel types, shown the fact that all the fuels atomize faster in the presence of higher injection pressures and slightly slower in higher ambient densities. In particular, high injection pressures were predicted to be more necessary for the biodiesel fuels to develop their break-up. The high ambient temperature shorter the ignitions delay. The effects of these different parameters are analyzed into spray characteristics and compared with the experimental results.

ABSTRAK

Perubahan alam sekitar dan pemanasan global telah menjadi satu isu yang terkenal dan utama di dunia. Pencarian kecekapan tenaga yang lebih tinggi dari industri mesin mampatan pesat (RCM) untuk mendapatkan pelepasan rendah khususnya Nitrogen Oksida (NOx) telah menuntut kajian eksperimen yang dilengkapi dengan simulasi Computational Fluid Dynamics (CFD). Tujuan kajian ini adalah untuk mensimulasikan corak aliran fizik pembentukan campuran dengan halaju tangen antara biodiesel dan bahan api diesel dan udara di dalam kebuk campuran RCM, untuk menentukan aliran muncung dan ciri-ciri semburan bagi tekanan suntikan semburan biodiesel berbeza untuk pelbagai keadaan sekitaran ke atas pembentukan campuran dan membandingkan tiga jenis Minyak Sawit mentah campuran biodiesel, B5, B10 dan B15 dengan kepadatan sekitaran yang berbeza pada aliran muncung dan ciri-ciri semburan dengan menggunakan CFD. Untuk tujuan ini, pendekatan berbilang *Eulerian-Lagrangian* telah digunakan untuk mensimulasikan proses semburan. CFD *Fluent* digunakan dalam kajian ini untuk mengkaji ciri semburan bahan api biodiesel. Suntikan biodiesel dalam ruang isipadu malar RCM telah digunakan dalam simulasi ini. Keadaan sempadan ditubuhkan pada parameter sekitaran yang berbeza manakala parameter yang lain dimalarkan. Kesan jenis bahan api, tekanan suntikan dan parameter persekitaran ke atas tingkah laku semburan seperti penembusan semburan telah dikaji pada aliran dalam silinder. Perubahan penembusan semburan dengan masa bagi parameter persekitaran yang berbeza dan pelbagai jenis biodiesel menunjukkan semua bahan api menyembur lebih cepat pada tekanan suntikan yang lebih tinggi dan lebih perlahan pada ketumpatan sekitaran yang lebih tinggi. Khususnya, tekanan suntikan yang tinggi diramalkan untuk menjadi lebih perlu bagi bahan api biodiesel untuk meningkatkan perpecahan mereka. Suhu sekitaran yang tinggi melambatkan pencucuhan. Kesan parameter yang

berbeza dianalisis pada ciri-ciri semburan dan dibandingkan dengan keputusan eksperimen.

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ABBREVIATION

ASOI	After start of injection
ASTM	American Society for Testing and Materials
BTM	Bubble Tracking Method
B5	Biodiesel CPO5
B10	Biodiesel CPO10
B15	Biodiesel CPO15
CFD	Computational fluid dynamics
CPO	Crude Palm Oil
IC	Internal combustion
LES	Large-Eddy Simulation
NMOG	Non-methane organic gas
NOx	Nitric oxide
PM	Particulate matter
RBDPO	Refined Bleached Deodorized Palm Oil
RCM	Rapid compression machine
RP	Rayleigh–Plesset
SAE	Society of Automotive Engineers
STD	Conventional diesel
TDC	Top-Dead Center
UHC	Unburned hydrocarbons
VOF	Volume of fluid

CHAPTER 1

INTRODUCTION

1.1 Research background

As one of the alternative energy sources, biodiesel is considered as a feasible candidate to substitute petroleum diesel fuel for its advantages in power delivery, regulated emissions and closed carbon cycle[1]. There were many studies on the fuel-air premixing that responsible to the ignition of diesel spray which linked to the improvement of exhaust emission [2-7]. The diesel engine is considered as a thermodynamically efficient engine marketed for automotive use. Years of development has made the diesel engine well-regulated and effective, resulting in better fuel consumption and a cleaner engine. Nonetheless, due to the potential impact on the automotive industry, developing a clean diesel engine has been in the head of research for the past decade[8].

A new emission standard has recently been proposed by the State of California to reduce the combined emissions of non-methane organic gas (NMOG) and nitric oxide (NOx) by 20% and particulate matter (PM) by 52% from the current standard (LEV II), active from 2014 through 2022 [9]. The California emission standard is one of the strictest in the world and has been widely accepted in many other states in the USA. Automotive manufacturers will have to meet this regulation for all new vehicles sold in the coming era. To achieve this requirement, the industry must investigate a range of factors that can potentially reduce engine emissions, including fuels, combustion process, chemical-kinetics, in-cylinder flow, fuel-air mixture formation, sprays, engine geometries, etc. [8].

There are many efforts to overcome this problems and development of the diesel engines and new method technologies with the objective to reduce these harmful emissions. One of the solutions advanced in diesel engine applications is better fuel droplet atomization and air-fuel mixture. The evolution of high-pressure-injection technology will result in fine atomization and will provide for better air-fuel mixture [10]. In recent times, the pressure of the injection systems has reached 100 MPa or more, and a number of researchers are showing interest in the performance of the high pressure injectors. This is necessary for biodiesel as biodiesel fuels are more reluctant to break up compared to conventional diesel fuels. This is due to their higher surface tension and viscosity. The surface tension force of the liquid fuel resists the aerodynamic drag forces, which are responsible for liquid jet disintegration. Conversely, the role of viscosity is to overwhelm the instabilities formed on the liquid surface from growing and disintegrating the liquid [11].

Spray penetration and fuel distribution should be carefully investigated in order to study the effect of the high injection pressure spray. For these times, these investigations are more focused on engine management, combustion control and fuel injections and alternative fuel usage. The research shows that the injector nozzle geometries play a significant role in spray characteristics and formation of fuel-air mixture in order to improve spray performance, and decrease some pollutant products from internal combustion engine system by using Computational Fluid Dynamic (CFD) software.

The wide range of applications and the integral multiphase phenomena taking place in sprays have made them remarkable and significant flows for both industrial and academic studies. Optimization of the sprays contributes significantly to high efficiency and low emission combustion in direct injection diesel engines. Ambient flow conditions such as pressure [12] and temperature [13], and combustion chamber flow field structure [14] effect the spray formation and development subsequently the mixture formation in the chamber. Increasing the spray angle indicates to a reduction in droplet velocities. Alternatively, impingement distance does not have a major influence on the droplet velocities since it is related to the travelling distance of the droplets [15].

In order to achieve higher levels of atomization to enhance the mixture formation, ultra-high injection of the sprays has been implemented, taking into account fuel type, [11] and chamber geometry effects [16] The effect of different classical and hybrid break-up models on the spray formation and break-up has also been investigated [17]. These days, computational simulations have been applied as a key analysis tool in engine research to establish correspondence with experimental studies and provide new information for designers.

A major advantage of using Computational Fluid Dynamics (CFD) is the flexibility of simulation setups and the time and cost efficiencies to compare with experiments. The present research is being carried out to investigate the physical phenomena associated with diesel engine combustion. Major CFD commercial codes that are available in the market currently include ANSYS CFX, ANSYS FLUENT, AVL FIRE and CD-adapco STAR-CD and STAR-CCM+, while KIVA and OpenFOAM are becoming popular as open source codes [8]. In this study, FLUENT has been chosen for taking advantage of its ability to simulate general flow problems. It offers different kinds of models to evaluate engine characteristics.

For this research, there will be simulations on fuel spray during ignition delay will be observed and analyzed. The simulation is done by following the experiment results in Rapid Compression Machine (RCM). Eventually, ignition delay happen as time interval from start of injection to ignition accompanying with truly heat recovery. Analysis on the fuel spray and the effect on mixture formation under variant ambient and injection pressure of biodiesel spray by using simulations and modeling will be retrieved as well as the effects on combustion system indirectly.

1.2 Problem statement

In the diesel engines system, biodiesel stands out as an alternative to substitute the diesel as the fuel production, transportation and storage technology, the availability of the fuel source, the compatibility of the fuel to current engine hardware, the performance of engine using new fuel, and the most important, the emission of engines. More or less, utilization of biodiesels significantly increased the production of nitrogen oxide (NOx) emissions and particulate matter (PM) in which rose a critical issue for the current users and environmental pollutant. Many researchers have contributed a lot of significant ideas to overcome the hazardous gases coming from biodiesel engines specifically in controlling the parameters. Fuel characteristics of biodiesel still an unsolved problem due to its oxidation stability, stoichiometric point, biofuel composition, antioxidants on the degradation which can cause more emission of NOx and PM.

Other than that, biodiesel spray gives effect to high viscosity in which help in controlling the combustion process indirectly during early stage of combustion process. This early stage is called an ignition delay in which happened within the premixing of fuel and air, thus allowing formation of mixtures. Fundamentally, experimental was conducted using RCM in order to observe and analyzed the ignition delay, spray formation and mixture formation. However, this technique subsequently increased the cost as well as time consumption compared to the simulation method.

Moreover, higher cost is one of the important constrain need to be optimized for conducting experimental due to various parameters need to be tested and the significant changes of the spray characteristics are complicated to observe. Besides, the critical behaviour inside the experimental instrument is invisible through the experiment work. Therefore, the aim of this research was employed CFD simulation to obtain the effects of variant ambient condition and injection pressure of biodiesel spray. In addition, the influence spray of the nozzle was studied. The behaviour of fluid flow inside orifice, spray characteristics regarding nozzle flow and spray penetration are analysed from the simulation results. The CFD simulation is one of the alternative approaches in determining the uncertainties that were unable to be achieved by experimental works in terms of reduction of cost as well as time constrain.

1.3 Objective

The objectives of this research are:

(i) Simulate the physics flow pattern of mixture formation with tangential velocity between biodiesel and diesel fuel and air in the mixing chamber of rapid compression machine.
(ii) Determine the nozzle flow and spray characteristics for different injection pressure of biodiesel spray to ambient variant conditions on mixture formation by using CFD.
(iii) Comparing three types of CPO biodiesel blends, B5, B10 and B15 with different ambient density on nozzle flow and spray characteristics by using CFD.

1.4 Scope

In this project, the behaviours of mixture formation between biodiesel fuel and air inside the mixing chamber are studied by using rapid compression machine concept. The nozzle parameter was held fixed at 0.129 mm hole diameter with 6 holes, respectively. Also, this study involves a geometry that use cylindrical hole. The nozzle orifice injector angle used is fixed at 60° with an equivalent ratio fixed at 0.37. The working fluids were air, and the alternative fuel blends of crude palm oil (CPO) B5, B10 and B15. The working fluids are compromised with the other variant parameters as such ambient temperatures with 750 K, 850 K, 950 K and 1050 K; ambient densities of 16.6 kg/m^3 for 4 MPa, 25.0 kg/m^3 for 6 MPa and 33.3 kg/m^3 for 8 MPa and also for variant injection pressures of 100 MPa, 130 MPa, 160 MPa and 190 MPa. The spray chamber consists of disc type with a diameter of 60 mm and a width of 20 mm. The time consumed for ignition delay period based on the boundary condition is from 0.5 ms to 1.5 ms has been considered. Besides, the variant conditions of injector's orifice are study in terms of behaviour of nozzle flow and spray characteristics to predict the combustion and production of emission. The mixture formation results are analysis base on physics flow pattern inside the mixing chamber at different positions along y-axis. Last but not least, all the simulations were completed by software of ANSYS FLUENT.

1.5 Significance of study

Development of new application, innovation and modification on an existing design tool will enhance to the improvement of quality production. Therefore, the study on fuel injection system can decrease the air pollutant and benefit to the environment. However, nozzle injector with six holes shape can give impact to the spray characteristics and indirectly affect the mixture formation at variant ambient and injection pressure of the system. The simulations of high injection pressures up to 190 MPa being done as these results can be used for further research in air entrainment of spray due to spray had over the wall chamber.

A specific modification on the injector nozzle geometry can improve the spray performance significantly. CFD analysis complements testing and experimentation reduces the total effort required in the laboratory. CFD simulation is another popular approach to study the injection of fuel spray [8]. By itself, CFD is not the answer to all questions regarding complex thermal-fluid phenomena, but it has recognised decisively as crucial tool, together with traditional theoretical and experimental methods, in the analysis design, optimization and trouble-shooting of thermal-fluid system.

On the other hand, by using CFD simulation giving a good visualise result compared to the experimental observations. Additionally, simulation helps in determining the study for extreme condition prediction as experimental gives high cost and maintenance. Besides, CFD simulation was validated with the experimental results in order to obtain a medium for further simulation in which also provides advantages in respect of saving energy, time and cost.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

In modern high injection system with a systematic control of mixture formation empower in achieving the considerable improvements in terms of fuel consumption reduction and engine out-raw emissions. Fuel injection system is widely used in the field of constant volume chamber system nowadays. However, the prediction of spray and mixture formation becomes gradually complex because of growing numbers of parameters due to more flexible injection systems. Previous researches e.g., [18-21] have shown that spray injection parameters have a strong effect on the processes of evaporation, mixture formation, ignition, combustion and pollutant formation in diesel engines also showed that the nozzle geometry influenced the spray characteristics and mixture formation. The mechanisms of turbulent flow, fuel atomization, and the interaction between fuel and air in a diesel engine are yet to be fully understood. A number of researchers are currently studying the characteristics of flow and fuel properties by using presently available techniques and technologies. This study implements the interactions between fuel and air in diesel engine by simulating in the constant volume chamber for rapid compression machine (RCM). The reviews are followed by the discussion of simulation sub models which are applied in CFD software. This chapter describes the relevant information from previous literature like biodiesel, mixture formation, spray characteristics, and Computational Fluid Dynamics (CFD).

2.2 Previous Studies

It has been reported on experiments in the ultra-high injection system at the primal stage of its technology by Kato et al. [22] and Yokota et al. [23] where they examined the effects of the injection pressure ranging from 55 to 250 MPa and also the variations of nozzle orifice and injection duration. They concluded that the Sauter mean diameter is interrelated with the average injection pressure and also the change of the injection pressure in time from their studies. Additionally, by utilizing the ultra-high injection pressure and smaller orifice diameter, a shorter combustion process and reduced soot formation are recognised.

There is an experimental and numerical investigation of free sprays at ultra-high injection pressure in the range of 150 to 355 MPa by Lee et al. [24]. There is no significant change in the Sauter mean diameter on attaining an injection pressure of 300 MPa. , and a reduced growth rate of the penetration length were reported from the investigation. Besides that, Tao and Bergstrand [25] studied the effect of ultra-high injection pressures on engine ignition and combustion using three-dimensional numerical simulations. Fast flame propagation and short combustion phase were reported as the advantage of high pressure injection in producing reduced ignition delay. Also, three different rates of injection profiles were examined. At the early stage of combustion, there is a rate falling injection in which the injection rate is decreasing during the injection process, was found to shorten fuel burn duration and expand at the later stage, and rate rising injection performed inversely [11].

On the other hand, rate rising injection expected a wider flame area at high temperature and reduced the nitrogen oxide (NOx) formation due to faster cooling after combustion. Compared to the case of injection in a constant volume chamber, flame lift-off lengths were observed to be constant at different injection pressures. To study the characteristics of ultra-high injection pressure sprays numerically, it is also important to understand the role of different types of spray models [11].

From the University of Hiroshima, Nishida's research group has conducted many experiments utilizing a number of ultra-high injection pressures, micro-hole nozzles, spray wall-impingement setup, and diesel and alternative diesel fuels [24-

30]. The combination of 300 MPa injection pressure and 0.08 mm nozzle-hole diameter reportedly gave the best performance in terms of turbulent mixture rate and droplet size reduction to decrease the mixture process and lean mixture formation, which also agrees with the findings of Kato et al. [22] and Yokota et al. [23].

Choi et al. [39] found that the flow pattern around the spray is similar at different injection pressures. Nevertheless, strong flow recirculation was observed at higher injection pressure. Desantes et al. [26], McCracken and Abraham [27] and Park et al. [28] have studied the spray characteristics in cross-flow to observe the effect on particle size and mixing process. Moreover, correlation of penetration and dispersion of a gas jet and sprays was examined by Iyer and Abraham [29]. The effects of gas density and vaporization on penetration, injection condition and dispersion of spray have been discussed by Naber and Siebers [30], Kennaird et al. [31] and Post et al. [32]. Jagus et al. [33] assessed injection and mixing using LES turbulence modeling.

Lin and Reitz [34] and Jiang et al. [35] have presenting about comprehensive reviews of droplet phenomena. The differences between popular breakup models have been discussed by Djavareshkian and Ghasemi [36] and Hossainpour and Binesh [37]. They described on the application of WAVE (or Kelvin-Helmholtz) and KH-RT (Kelvin-Helmholtz Rayleigh-Taylor) models, and found better agreement with experimental data using KH-RT. Karrholm and Nordin [38] have studied on the interaction of the mesh, turbulence model and spray in a constant volume chamber. The effect of spray-in-cylinder-flow interaction is realized in the combustion process has been studied by a number of researchers [39].

2.3 Cavitation

Cavitation is one of the important methods in order to reduce the emissions from combustion at source is improves the spray breakup and introduce smaller droplets size inside the combustion chamber [40]. The physical flow inside the injector nozzle gives major influence on the spray formation. There is sudden drop of the high pressure when across the injector nozzle in which liquid within the small nozzle to accelerate, while cavitation created by the extreme high velocity and low pressure regions as shown in Figure 2.1[40]. However, cavitation inside the nozzle has been resulted as one of the essential parameters which can affect fuel spray atomization.

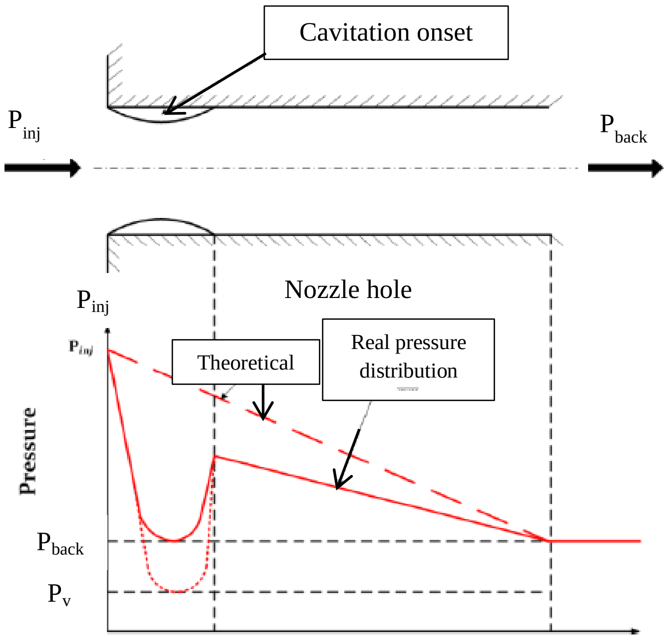

Figure 2.1: Cavitation formation inside nozzle [40]

Nevertheless, there are positive effects to the fuel spray breakup development by cavitation. Gavaises determined that the cavitation will damage the bubble collapse areas, while the engine exhaust emissions improved by the association of string cavitation structure inside nozzle [41]. Akira Sou *et al.* had investigated the cavitation flow in an injector nozzle numerically. They purposed the combination equations used such as Eulerian–Lagrangian Bubble Tracking Method (BTM), Large Eddy Simulation (LES), and the Rayleigh–Plesset (RP) to simulate an incipient cavitation, in which only cavitation bubble clouds appear. In this case, they found a good agreement with the prediction of cavitation using the combination equations [42]. Meanwhile, Payri *et al.* had conducted an experimental study on the effects of geometric parameters on cavitation phenomena within a visual closed vessel by using laser technologies. The outcomes of their study showed that the jet angle has noticeable affected by the cavitation behaviours [43]. J.M. Desantes *et al.* had conducted an experimental study on the influences of cavitation phenomena at near-nozzle field through visualization technique in order to detect cavitation bubbles injected in a chamber pressurized with liquid fuel. The visible increment of spray cone angle and spray contour irregularities has been found in which related with the presence of cavitation bubbles at the orifice outlet. They assumed that this fact was an improvement of atomization induced by the collapse of cavitation bubbles at the nozzle exit [44]. Payri *et al.* had studied the effect of cavitation phenomenon to the spray cone angle and found a significant rise involved the cavitation appearance [45]. In the meantime, there is a similar result obtained by Hiroyasu by visualizing separately internal flow and macroscopic spray from different large-scaled nozzles [46].

2.4 Nozzle Orifice

Nozzle hole gives a significant impact to the flow inside the nozzle orifice, spray characteristics, cavitation and turbulence levels and influences to the combustion indirectly [47-50]. By comparing the spray characteristics of two different nozzle diameter injectors, Li-jun Yang *et al.* found that the atomization behaviour was affected by the nozzle diameter. The spray angles of injector with the nozzle diameter of 1.5 mm are smaller than the injector with nozzle diameter of 2 mm by comparing two injectors under the same pressure drop. The size of swirl chamber and the tangential inlets are the same for the two injectors. A rotating fluid jet is produced from the swirl injector (nozzle diameter = 1.5 mm) under the same pressure drop, In contrast, the 2 mm nozzle diameter of injector is swing to form a twisted ribbon-like structure under the larger swirl strength [51].

2.4.1 Cylindrical nozzle

Cylindrical nozzle is the standard nozzle shape as it has the same diameter of nozzle inlet and outlet. Cylindrical nozzle is a type of nozzle with cylindrical shaped head of nozzle exit. Besides, cylindrical nozzle is much more likely to cavitate compared to conical nozzle as it has a small conicity and low values of the rounding radii [52]. Figure 2.2 below shows the geometry of cylindrical nozzle head and its output.

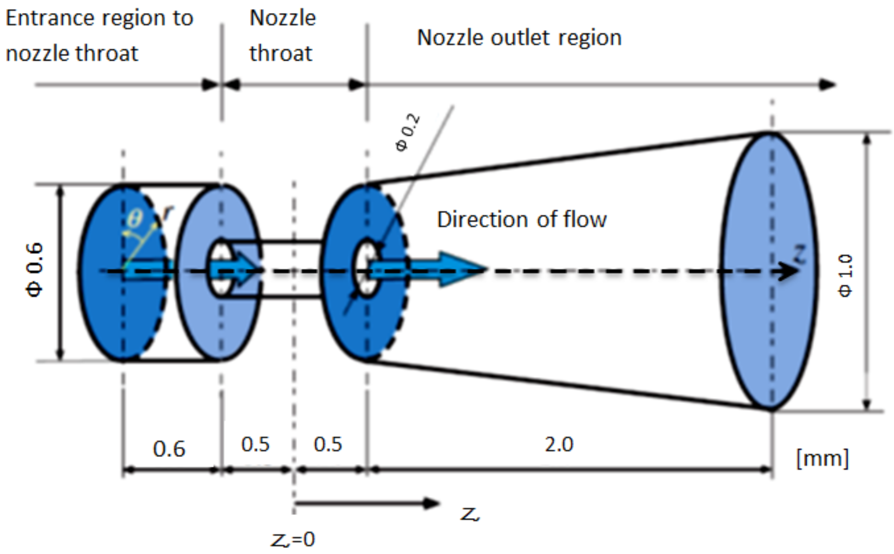

Figure 2.2: Schematic diagram of the cylindrical nozzle head and exit [53].

The mass flow rate of cylindrical nozzle rises proportionally with the root of the pressure differential to the point where it achieved its stability. This situation happened because of the appearance of the cavitation phenomenon. Since cylindrical nozzle is a cavitating nozzle, thus its critical cavitation number is defined as K_{crit}, which corresponding of cavitation starts in the injector orifice to the pressure drop. The critical cavitation number could be associated the point which the mass flow rate starts to stabilize [45]. This phenomenon occurs when detected by the stabilization of the mass flow rate across the orifice at a given value of the injection pressure. Besides, this phenomenon causes the further decline in discharge pressure which is known as choking. Hence, cavitation occurs if the cavitation number that corresponds to these pressure conditions is lower than the critical value of K_{critT} [45]. The values of the critical cavitation number can be calculated using the equation:

$$K = \frac{P_i - P_v}{P_i - P_b} \qquad (2.1)$$

Where P_v represent the vapour pressure.

Masatoshi Daikoku and Hitoshi Furudate studied the disintegration of liquid jet by cavitation inside a cylindrical nozzle with different ratio nozzle's length per diameter. The result showed the breakup of the dispensing jet is promoted when the length-diameter ratio L/D of a nozzle is low as the cavitation bubbles are formed inside the nozzle to promote spray breakup [54].

2.5 Spray and breakup models

Sprays are generally studied due to their vast range of scientific and industrial applications. Since the spray influence the consequent processes of mixture formation, ignition, and combustion also pollutant formation, the characteristics of fuel sprays injected into the combustion chamber of an internal combustion (IC) engine are important. Well-atomized fuel evaporates faster due to a longer contact time with the ambient air as well as increased interaction surface. [19,54,55]. This enhances the fuel-air mixing and increasing oxygen availability. Accordingly, the properly prepared mixture can spontaneously ignite. The combustion process of an efficient mixture leads to a maximum burning of the injected fuel. The series of events mentioned above can be very important in reducing the unburned hydrocarbons (UHC) [8].

All the above mentioned processes take place in a very short time. An efficient break-up of the fuel jet and the droplets acts to be even more critical in this fleeting time interval. Sprays under high injection pressures up to 200 MPa have been widely studied both experimentally and numerically, whereas for more effective atomization recommends the application of ultra-high injection sprays. This is even more necessary for biodiesel fuels as biodiesel fuels are more hesitant to break-up compared to conventional diesel fuels as mentioned in the research background. The complication of the multiphase phenomena taking place in the spray flows requires a profound understanding of the relevant processes [57]. It is not easy to thoroughly analyze all the details of the sprays with one set of experiments due to the complexity of the flow field. There are numerous experimental studies on different features of fuel sprays. Likewise, different experimental techniques are necessary to gain information about different parameters. On the other hand, a well-established and validated numerical model delivers the chance to investigate a variety of spray characteristics. A parametric study can be implemented in a simulated environment with minimal cost and time

In CFD, spray mechanisms are represented by mathematical models. There are two approaches which are used in multiphase flows; Euler-Lagrange and Euler-Euler. The fluid phase is considered as a continuum and modeled by the Navier-Stokes equations for both of these approaches. For the Euler-Lagrangian approach, the Lagrangian discrete phase model is introduced in general CFD codes to calculate the disperse phase by tracking particles, droplets or parcels [58]. The trajectories of particles in a turbulent flow field are predicted by the turbulent dispersion models. To reduce the computational time of the particle collision calculation, the O'Rourke algorithm is employed [59]. The outcomes of collisions are also determined by this algorithm, i.e., whether the droplets coalesce or reflect apart [60].

The mathematical model of the droplet evaporation is mostly concerned about the phase of fuel vapor diffusion from the surface of the droplet into the ambient gas. Two models are frequently utilized by researchers. The hydrodynamic model focuses on the diffusion of droplet for controlling its vaporization and the kinetic model is concerned with the molecules' detachment from the surface of a droplet [60]. The disintegration of existing droplets is modeled to numerically simulate different kinds of breakup modes.

2.5.1 Solid Cone Fuel Spray Structure

Full solid cone sprays are formed at high pressures in direct injection diesel engines. The pertinent processes are shown in Figure 2.3 [61]. Existence of the break-up process is influenced by the flow characteristics inside the nozzle. It is significant for the role of the nozzle geometry on the turbulence level at the nozzle exit, and the possible occurrence of cavitation. Higher level of turbulence at the exit can enhance the instabilities at the near exit region of the fuel jet. Eventually, the growth of these instabilities at the interface of the liquid and gas phases leads to the disintegration of the liquid jet into liquid ligaments.

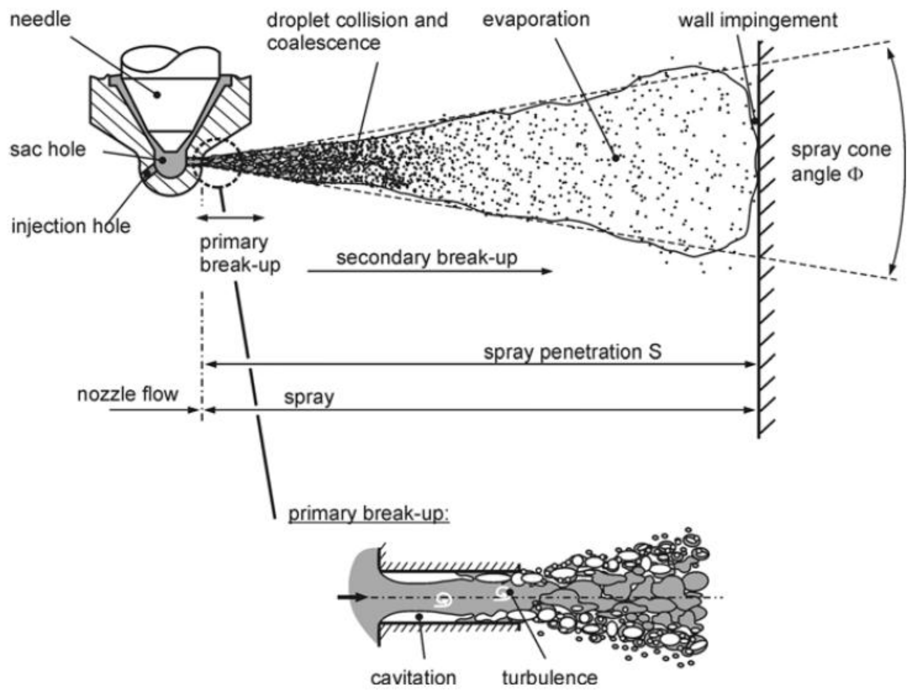

Figure 2.3: Relevant processes of a fuel spray [61].

Besides, there is also a probability for the local static pressure drops below the vapor pressure of the fuel. This pressure drop commonly occurs in nozzles with sharp corners. Liquid flow is locally accelerated as a result of flow separation at the sharp corners of the nozzle. This pressure drop can lead to the nucleation of the cavitation bubbles. The bubbles are transported to the nozzle exit and as according to the local flow conditions; the bubbles may shrink, expand, or collapse. Imploded bubbles will increase the turbulence level at the exit region. The collapse of the bubbles gives to the disintegration of the fuel jet into liquid ligaments and large droplets. Therefore, this is called the primary phase of break-up. This primary phase of the break-up is known as turbulence-induced break-up [8].

It is accompanied with some drawbacks even though the influence of the cavitation bubbles to the fuel jet break-up is beneficial to the atomization purpose. As explained in the above of Figure 2.3, the cavitation region can extend towards the downstream. This extension of the vapor zone decreases the liquid effective area. The minimum cross-sectional area of the liquid is called the “vena contracta”. In the worst case scenario the vapor zone evolves downstream up to the nozzle exit. In this case the nozzle is said to be flipped [62, 63]. Apparently the reduction of the liquid effective area is the negative effect of the cavitation. Accordingly, the effective injection mass flow rate drops. This may result in lower accumulated heat release and power generation of the internal combustion engines.

A result of the dominance of the aerodynamic forces over the surface tension force after a primary breakup is a farther downstream, as the larger droplets break up into smaller ones in the secondary break-up phase. The secondary phase is generally called the aerodynamic-induced break-up [61, 64, 65]. The gas-liquid interface becomes unstable as a result of the velocity difference at the shear layer of the liquid jet. The amplitude and frequency of these instabilities are dependent on the gas and liquid properties and the flow conditions. Ultimately, they control the surface tension forces and disintegrate the liquid if the instabilities are not dampened by the viscous forces.

In line for the roll-up of the liquid shear layer, ambient air is engulfed into the spray and the mixing process starts. This is called the entrainment process. A significant part of the air entrainment occurs at the tip of the spray. The entrainment process sets the stagnant air into motion in the form of secondary vortex field if the spray is injected into an initially quiescent chamber [66]. Entrainment of ambient air and the radial movement of the low kinetic energy droplets towards the outside region expand the spray in the spanwise direction. This results in a conical shape of the spray.

Larger and faster droplets are located in the dense region near the spray axis, while the droplets become smaller and slower as a result of aerodynamic interaction with the continuous phase near the outside area. [15, 67]. Droplets are located in the near-field and around the spray axis are subjected to a higher number of collisions in the dense region. Higher number of collision can result in the combination of the droplets [68, 69]. The droplets have appropriately atomized in the downstream zone in which depending on the ambient temperature, the evaporation of the droplets can be the dominant process in the mixture formation.

2.5.2 Spray Penetration

Spray penetration is define as the maximum distance reached when liquid-fuel or liquid injected into the stagnant air from the nozzle head and is dominated by two opposing forces which are the aerodynamic resistance of the surrounding gas and kinetic energy of initial fuel jet. High penetration detected by a narrow and compact spray while low penetration usually endure more air resistance and have high cone angle of atomized spray. The droplet size along with the easiness of liquid stream atomized after being injected by different biofuel blends are influenced by the properties of density, surface tension and viscosity. Figure 2.4 shows the particle penetration is affected by different biofuel blends. This figure also shows comparison between the various biofuel blends and the maximum lengths from the injector [70].

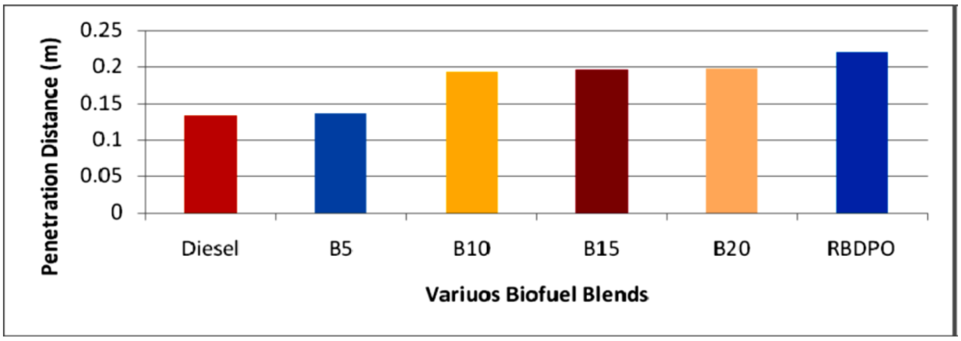

Figure 2.4: The graph of penetration distance (m) against various biofuel blends [70].

M. Battistoni *et al.* had done a simulation regarding with biodiesel and diesel as the comparison. The simulation results show that Diesel produced a faster and denser spray which remains compact for a long time with conical hole, meanwhile diesel enhances spray breakup at cavitating hole [71].

Penetration for both diesel and biodiesel for both different hole shapes can also be compared and shown in Figure 2.5. Diesel spray injected from the conical hole with a higher liquid penetration, while diesel spray injected from the cylindrical hole and both biodiesel sprays shows lower and similar penetration trends versus time [71].

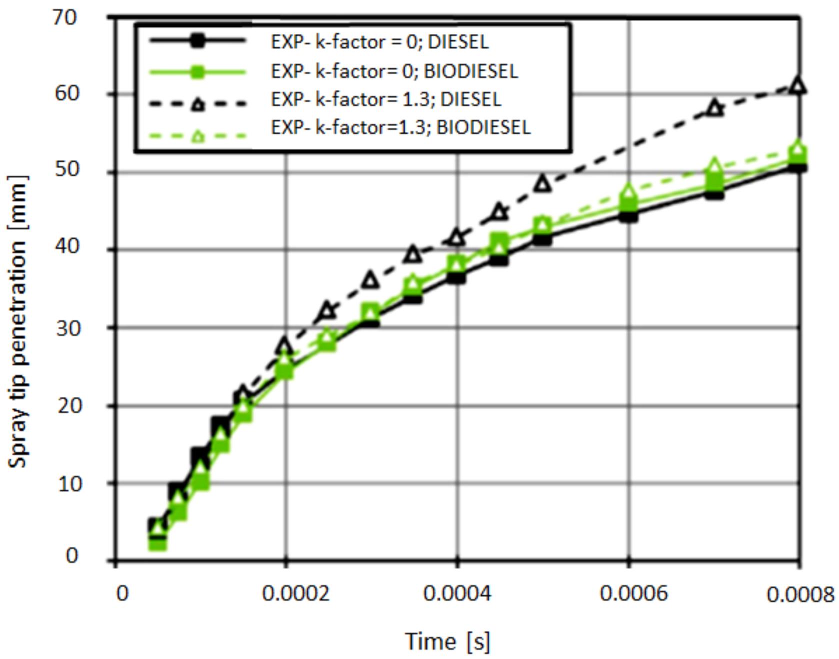

Figure 2.5: The graph of spray tip penetration against time [71].

2.5.3 Spray droplets

A droplet is a small particle of liquid which is generally in a spherical shape and people also called it as particles. For instance, potential energy is produced as liquid mix with air pressure for two-fluid nozzles or liquid pressure for hydraulic nozzles along the nozzle geometry. The potential energy will cause the liquid to spread into small ligaments in which those ligaments then break up into very small spherical pieces, which are usually called droplets, drops or liquid particles. The surface tension of a liquid causes droplets and soap bubbles to undergo interattraction in a spherical form and then resist spreading out and this is also the reason why particles is in round shape. Sprays are formed when the interface between a liquid and a gas becomes deformed and droplets of liquid are generated [70]. Figure 2.6 demonstrates the spray pattern from spray nozzle.

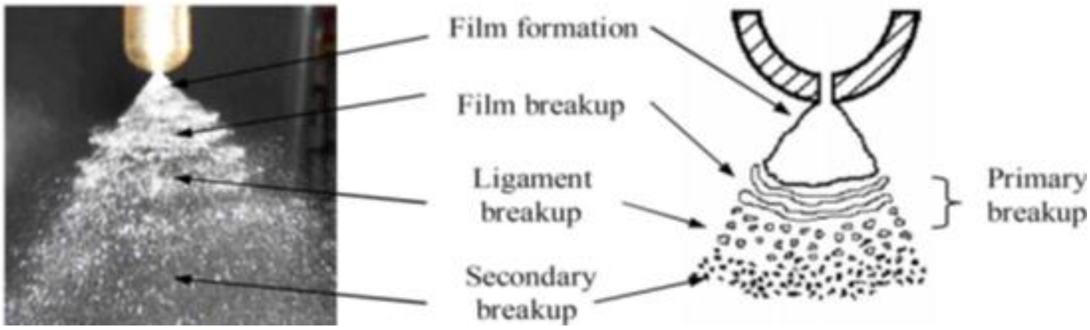

Figure 2.6: A typical spray pattern from spray nozzle [72].

2.6 Eulerian-Langragian multiphase approach

The Eulerian–Lagrangian framework denotes a natural dispersed phase flows approach. Eulerian-Lagragian multiphase approach is well known and established in the previous researches of spray simulation. Formulation of coupled Eulerian (gas-phase flow) and Lagrangian (liquid-phase flow) is generally used to stand for the spray dynamics and interaction between the gas and liquid multiphase flow [73-77]. Besides, this approach also used for direct modeling of the individual droplets undergo, such as droplet dispersion, spray break-up, and wall interactions. On the other hand, the indirect modeling depends on the volume fraction of the droplets and the density distribution required using the method of alternative Euler–Euler approaches [74]. Nevertheless, the restriction of these adopted approaches is the needs of computationally efficient algorithms specifically when large number of droplets is obtained [73]. S. Som *et al.* conducted a simulation analysis on injector flow and spray characteristics between petrodiesel and biodiesel using the Eulerian-Lagrarian appoarch in CFD software [50]. Besides, W.P. Jones *et al.* performed large-eddy simulation of spray combustion in a gas turbine combustor. They working on the Eulerian description for the continuous phase and it were coupled with Lagrangian approach for the dispersed phase [73]. Furthermore, Jakub Broukal and Jirí Hájek studied the validation of an effervescent spray model with secondary atomization and its application to modeling of a large-scale furnace. Still, they also applied the Eulerian-Lagrangian approach of two-phase flow on spray simulations based on the latest industrially relevant model [78].

2.7 Ignition Delay

Ignition delay is defined as time interval from start of injection to ignition accompanying with truly heat recovery. In this definition, the pressure difference between the pressure in firing condition, p_f, and the pressure after compression without fuel injection, p_a, is taken into account. The pressure difference, p_f -p_a, indicates the net pressure excluding the effect of the heat loss to the chamber wall [79].

Figure 2.7 shows the history of pressures during ignition delay period. The figure explained on the pressure can affect the period of ignition delay which the ignition delay period will be longer in higher pressure as well as temperature.

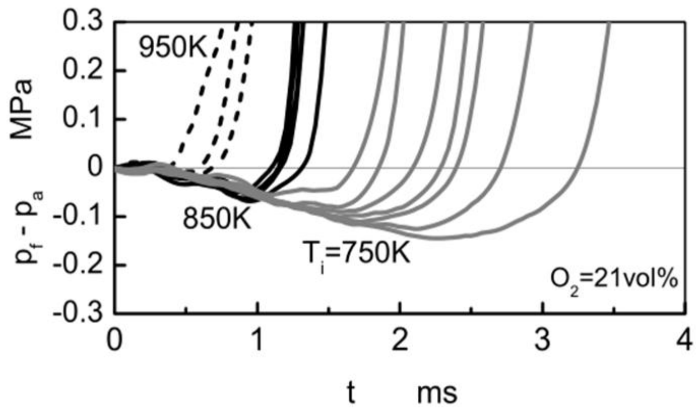

Figure 2.7: Histories of pressures during ignition delay period [79].

Figure 2.8 shows the relation between ignition delay and combustion characteristics and NOx concentration after combustion at different ambient temperature Ti and oxygen concentration. The Q t is total heat release, Δ_{tb} the combustion duration and (dQ/dt) max the maximum heat release rate. It can be said that NOx is remarkable as lengthens the ignition delay period. Thus, this can lead to combustion process where the longer of ignition delay will contribute to the better mixture formation and combustion process.

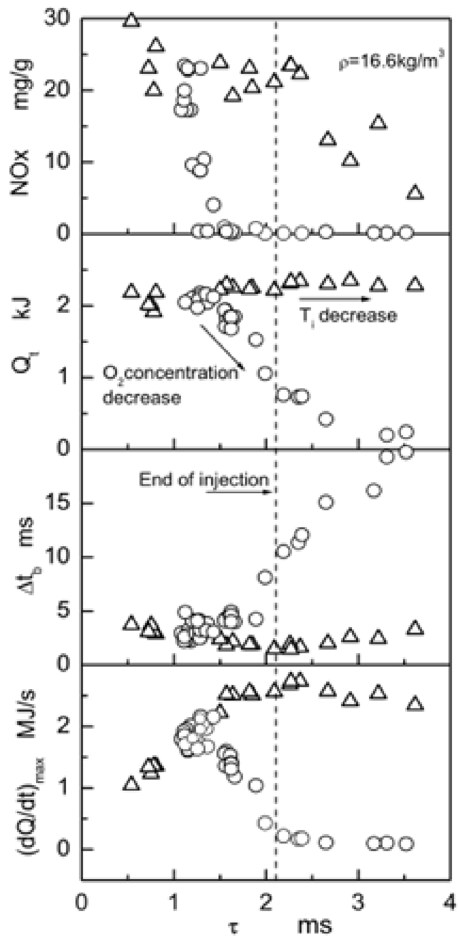

Figure 2.8: Relation between ignition delay and combustion characteristics [79].

2.8 Crude Palm Oil

Crude palm oil (CPO) is the oil that is made from the palm oil which extracted from the palm nut kernel. The composition of CPO consists some beneficial constituents with high concentrations as such phospholipids, serols, carotenoids, tocopherols, tocotrienols, aliphatic hydrocarbons, triterpene alcohols, squalene and aliphatic alcohols before it can become clear oil selling on grocery shelves [80, 81]. It is a type of natural oil with high amounts of saturated fat when compared to others high in unsaturated fat natural oils such as vegetable and olive oil. CPO plays a significant role in economical as its value is fit for human consumption ingredient for refined palm oil. Demands of CPO are increasing in global market due to the limited annual production [80].

Amir Khalid *et al.* performed an experimental research about the effect of preheated fuel on mixture formation of biodiesel spray by using CPO biodiesel by transesterification which was taken from Universiti Tun Hussein Onn Malaysia (UTHM) biodiesel pilot plant [82]. Table 2.1 and Table 2.2 show the comparison fuel properties characteristics of the standard fuel diesel (STD) and blending ratio biodiesel with the value of B5, B10, and B15 which referred to the ratio of the mixture. Additionally, Mohammad Nazri Mohd Jaafar *et al.* conducted a spray analysis using RBDPO and its blends compared to diesel fuel [83] in which the physical properties of the biodiesel blends were based on the ASTM standard which tabulated in the Table 2.3.

Table 2.1: The properties of STD and blending ratio of biodiesel at ambient temperature [82]

Fuel type	Properties			
	Density (g/cm^3)	Kinematic viscosity (cP)	Flashpoint (°C)	Water content (ppm)
STD	0.833736	3	80	79.6
B5	0.837048	3	91.5	120.1
B10	0.837664	2.9	92	158.6
B15	0.840428	3	93.5	219
B20	0.841172	3.1	94.5	294.7
B25	0.841716	3	97	363.3
B30	0.845852	3.2	97.5	397.1
B35	0.844816	3.4	99.5	426.9
B40	0.848236	3.2	100	558

Table 2.2: Properties of blending ratio biodiesel at various temperature [82].

Blending of Biodiesel	Density (g/cm^3)			Viscosity (cP)			Acid Value (mgKOH/g)			Flashpoint (^{o}C)		
	30^{o}C	25^{o}C	6^{o}C	30^{o}C	25^{o}C	6^{o}C	30^{o}C	25^{o}C	6^{o}C	30^{o}C	25^{o}C	6^{o}C
B5	0.8553	0.8530	0.8538	3.6000	3.6000	3.5000	0.2805	0.2591	0.2943	86.1667	85.3333	85.3333
B10	0.8555	0.8550	0.8563	3.5000	3.8000	3.7000	0.3084	0.2662	0.3013	84.0000	85.0000	86.1667
B15	0.8562	0.8564	0.8568	3.6000	3.6000	3.5000	0.3224	0.3221	0.3853	87.5000	87.1667	85.5000
B20	0.8575	0.8578	0.8575	3.5000	3.5000	3.8000	0.3506	0.3644	0.3783	87.3333	89.0000	86.0000
B25	0.8583	0.8568	0.8589	3.6000	3.7000	3.7000	0.5184	0.4201	0.5044	89.1667	92.0000	93.1667
B30	0.8599	0.8584	0.8599	3.8000	3.6000	3.6000	0.5055	0.4903	0.4626	87.8333	91.6667	88.1667
B35	0.8671	0.8613	0.8605	3.5000	3.6000	3.6000	0.5323	0.5329	0.5600	91.1667	92.0000	93.1667
B40	0.8691	0.8656	0.8650	3,7000	3.7000	3.7000	0.5464	0.6163	0.5741	98.0000	102.0000	99.3333
B45	0.8651	0.8680	0.8655	3.8000	3.8000	3.9000	-	-	-	102.8333	104.3333	100.1667

Table 2.3: Fuel properties of RBDPO blends and Diesel fuel [83].

Sample	Specific gravity (ASTM D1298)	Density (kg/m^3) (ASTM D1298)	Kinematics viscosity (Cst) (ASTM D445)	Surface tension (N/m)
B0	0.8321	831.6	3.472	0.0300
B5	0.8371	836.6	4.083	0.0305
B10	0.8412	840.6	4.65	0.0305
B15	0.8452	844.6	5.442	0.0305
B20	0.8502	849.6	5.809	0.0305
B25	0.8542	853.5	6.422	0.0305
B100	0.915	905.5	35.14	0.0345

Furthermore, Amir Khalid *et al.* performed an experimental investigation to determine the effect of preheated biodiesel on fuel properties, spray characteristics and mixture formation using the direct photography system. Meanwhile, preheated fuel is found an increment in such a way to enhance the spray penetration, resulted the spray area is increased and enhanced fuel-air premixing [82]. Figure 2.9 indicates their result from the experiment, the graph of projected spray area versus the spray tip penetration for all types of blending ratio fuel.

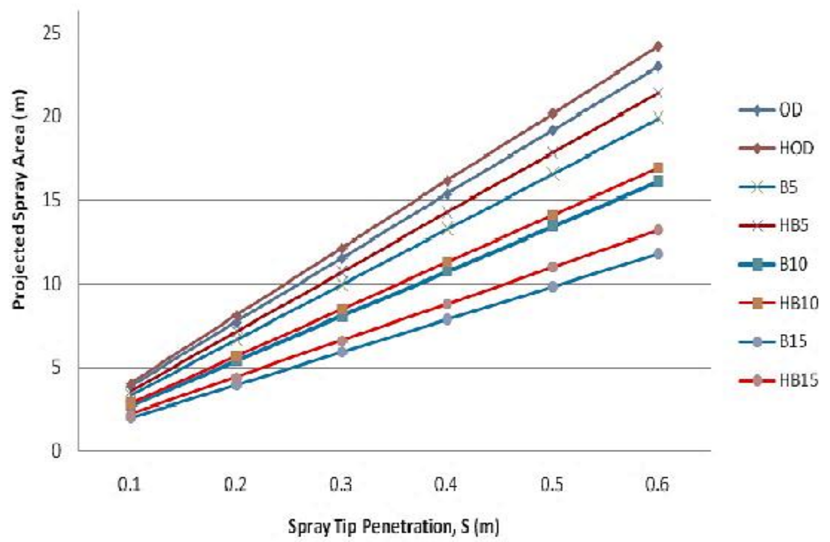

Figure 2.9: Projected Area comparison [82].

2.9 Pre-Processing

Computational Fluid Dynamics (CFD) is a type of fluid mechanics that used numerical methods and algorithms to analyse problems which involving fluid flows. In the case of engine applications, due to its complex geometry, the flow domain is meshed by several different approaches. An engine model to be simulated in ANSYS FLUENT 13.0 [84] is meshed with a hybrid topology. Pre-processing method is considered in doing the meshing. Mesh density generally have three levels, they are coarse, medium and fine which represents as the fineness of grid produced in the mesh generation [85]. A multi-block methodology is exploited to split the calculation domain into four major zones which are chamber, piston layer, ports and valve layer, as seen in Figure 2.10. The zones adjacent to reciprocating boundaries such as the piston and valves are meshed with quadrilateral cells (structured mesh) and layered. Tetrahedral cells (unstructured mesh) are used in the chamber zone because the valves move into this zone and its cells deform and must be remesh. Interfaces must be created between the chamber and valve layer zones in order to

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