Computational Fluid Dynamics Study on Droplet Size of Kerosene Fuel

S. Sapee

Faculty of Mechanical Engineering, Universiti Teknologi Malaysia, 81310 Johor, Malaysia.
syazwana.sapee@gmail.com

Abstract – *This article provides numerical simulation of Computational Fluid Dynamics study on droplet size for kerosene fuel. Fine spray with homogeneous mixture of fuel and air during the injection process is expected to be promising for optimisation of combustion processes in order to achieve high efficiencies and emissions as low as possible. Study on atomization and pressure swirl atomizer will be carried for droplet size affection factors. Numerical study of computational fluid dynamics applying Navier-Stokes equation will be conduct by using Gambit and FLUENT software to observe droplet size such as Sauter Mean Diameter (SMD) for kerosene fuel using 2D Discrete Phase Model with 2D axisymmetric and particle diameter for kerosene fuel using 3D Discrete Phase Model with 30° swirl dominated.* **Copyright © 2015 Penerbit Akademia Baru - All rights reserved.**

Keywords: Atomizer design, Computational Fluid Dynamics simulation, FLUENT software

1.0 INTRODUCTION

Nowadays fossil fuels have contributed energizing almost all sectors including industrial, transportation and agricultural sectors. The energy consumption by mainly fossil fuel because their adaptability, high combustion efficiency, handling facilities, availability and reliability [1]. However, it is estimated to be running out less than 50 years due to the limited storage under the stratum [2]. One of the most significant current discussions in optimization of combustion processes is important due to environmental pollution and limited fuel resources. Various combustion concepts have been developed in order to achieve high efficiencies and emissions as low as possible. To obtain the surface to mass high ratios in the liquid phase which lead to desired excessive evaporation rates, the liquid fuel must be fully atomized before being injected into the combustion zone in a compression ignition engine [3].

Atomization is typically accomplished by forcing the fuel through a nozzle into a thin sheet to induce instability thus emerged into ligaments which collapse into ultimately droplets. The discharging of the fuel through nozzle with specially shaped passages resulting droplets will be distributed through the combustion zone in a controlled pattern and direction.

Homogeneous mixture of kerosene fuel and air during the injection process is expected to be promising for optimization of combustion processes [4]. Therefore, characterization of the spatial and temporal droplet size distributions of the injected fuel is of great importance. Normal fuels are insufficient to produce vapor in combustion system, unless they are atomized into a large number of drops. The process of producing a large number of drops, droplets or also known as liquid particles by forcing fuel through a nozzle is called atomization. Fuel

transforms into sheet, next emerge into small ligaments then break up droplets due to surface tension action and potential energy. Collection of moving droplets results of turbulence jets in atomization known as spray.

There have few parameters in spray characteristic importance of gas combustor performance. Parameters involved mean drop size, drop size distribution, patternation are only dependent on the atomizer design however cone angle and penetration are partly depend by atomizer design and aerodynamic effect to which the spray is subjected after atomization is completed. According to an investigation by Ghaffarpour et al. [5] a swirl-stabilized combustor was required to determine characteristics of hollow-cone spray flames. Three years later Chehroudi et al. [6] presented a simplex atomizer with a nominal included cone angle of 30° to investigate hollow-cone spray and swirling air with a calculated nominal swirl number of 0.36 was produced with a swirl plate having an exit air velocity vector of 30° with respect to the chamber axis. The effect of atomizing gas pressure, spray distance and melt mass flow rate on the equilibrated droplet spray temperature has been examined by Underhill et al. [7]. He has summarized that spray temperatures at the substrate were consistently higher than the measured deposit temperatures, and in both cases increased with decreasing gas pressure; decreasing spray distance; and increasing mass flow rate. Choi et al. [8] observed that the droplet size in the core region is smaller than that in the outer region. Three years later, Kurihara et al. [9] noted that the particles with diameter smaller than 30 μm show fluid motion and the particles with diameter 50 μm or larger penetrate the turbulent air flow. The spray with droplets larger than 70 μm in diameter forms a hollow cone distribution, hence induces shear flow along the spray. Then the shear generates turbulence and the small droplets are drawn inside the hollow cone. By using Effervescent atomizer, Liu et al. [10] found that the spray cone angle decreases slightly at higher liquid mass flow rate and lower air/liquid mass flow rate ratio and with the increasing of air/liquid mass flow rate ratio, Sauter Mean Drop size reduces gradually at the same liquid mass flow rate.

Droplet size normally has been calculated to analyses evaporation rate. Measurement of the mean drop diameter was taken to compare atomization qualities of various sprays. Takei et al. [11] suggested implementing atomizer specific spray characteristics into a CFD code to improve the numerical simulation capabilities by. Phase Doppler Particle Analyze (PDPA) was used to characterize fuel spray formed by atomizer. In 2001, Palero and coworkers [12] demonstrated that using Multi-Intensity Layer is applied together with Stereoscopic PIV to obtain the measurement of the three velocity components for different droplet sizes in the spray. Most of studies used Sauter Mean Diameter (SMD) and Mass Mean Diameter (MMD) of droplet size as preferred characteristics of importance. The SMD is the diameter of a drop having the same volume-to surface area ratio as the total volume of all the drops to the total surface area of all the drops entirely whist the MMD is a value where 50% of the total volume (or mass) of liquid sprayed is made up of drops with diameters larger and smaller than the median value. Various dynamics and transport occurrences in droplet processes are highly dependent on the droplet size. In order to control and obtain the desired heat and mass transfer rate, the mean droplet size and drop size distribution are govern factors in fuel injection application. By reducing the mean droplet size higher heat release rate, easier light up, a wider burning range, and lower exhaust concentration of pollutant emission are possible to accomplish [13]. Subsequently very small droplets are necessary to provide high initial fuel evaporation rates for rapid ignition therefore the uniform distribution of droplet size in spray is required. Droplet size distribution can be represented both graphically and mathematically. Overall, the large droplets had sufficient momentum to penetrate through the atomizing air jet

and disperse widely. A lot of droplets appeared to burn individually, and several were quenched before burning out.

A device to convert a stream of liquid into a fine spray is known as atomizer. Fine droplets will increase area for evaporation hence faster the rate of evaporation. Performance of a liquid fuel atomizer has direct effects on combustion efficiency, pollutant emissions, and combustion stability. Three types of industrial used atomizer are pressure atomizer, rotary atomizer and twin fluid atomizer. For pressure swirl atomizer applications, mean droplet proportional to surface tension, liquid viscosity, and flow number or liquid flow rate. Allen et al. [15] investigated on five biodiesel fuels with various density and viscosity for atomization characteristics. Li [16] reported that to the dual pressure atomization nozzle, the flow rate range is wide and droplets size decreases with the increasing oil pressure also tends to stabilize. The flow structures inside nozzle and disintegration of liquid sheet define characteristics of the resultant spray. Mean drop size and droplet size distribution from the liquid sheet disintegration control the subsequent heat and mass transfer in a convection environment as in spray combustion. Liquid viscosity effects on mean drop size decrease with increase flow number or diminishes spray cone angle, whilst flow number effects mean droplet size decrease with increasing of liquid injection pressure. High pressure atomization produces high velocity spray and hence mean drop size is inversely proportional to liquid injection pressure. By reducing the length to diameter ratio of the final nozzle orifice, the mean droplet size also diminishes whereas mean drop size will increase if the length to diameter ratio for swirl chamber is increase [17, 18]. The variation of mean drop size and droplet distribution generated by pressure swirl atomizer with axial distance in a spray are depends to function of ambient air pressure and velocity, liquid injection pressure, and initial mean drop size and distribution. A study on effect of spray angle on emission characteristics with double swirl combustion system were carried out by Gao et al. [19]. It was reported that when the spray angle is 155°, the concentration of the particle is lower than that at 160° by 0.02~0.27 mg/m3, and the NOx concentration is higher.

Computational fluid dynamic (CFD) is a numerical method using fluid mechanics basis of solving and analyzing mathematical equations that represent physical laws problems correlated to fluid flows, heat transfer, mass transfer, chemical reactions, and other related occurrences. Problems such as conservation of mass, momentum, energy, and species are able to be solved using CFD whereas to predict internal flow and external flow [20]. Due to numerous advantages including experimental cost reduction (laboratory apparatus, duration of time and man power), large range of results and ability to simulate system in hazardous environment this simulation method extensively used in industrial and non-industrial sectors. Furthermore CFD application helps in enhancing the quality of the products before prototyping it. Zhou et al. [21] observed that turbulent flow of gas-phase was modeled by k-ε turbulent model. The main equation use by the CFD regularly is Navier-Stokes equation. The Navier-Stokes equation used includes continuity equation, momentum equation and energy equation for a compressible fluid. The continuity equation as below:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho u_j\right] = 0 \tag{1}$$

And the momentum and energy equation as describe follow:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}\left[\rho u_i u_j + \rho \delta_{ij} - \tau_{ij}\right] = 0 \; ; where \; i = 1,2,3 \tag{2}$$

$$\frac{\partial}{\partial t}(\rho e_0) + \frac{\partial}{\partial x_j}\left[\rho u_j e_0 + u_j p + q_i - u_i \tau_{ij}\right] = 0 \tag{3}$$

Assuming law for mono atomic gases for a Newtonian fluid, the viscous stress is written

as: $\tau_{ij} = 2\mu S_{ij}^*$ \hfill (4)

where the trace less viscous strain rate is given by:

$$S_{ij}^* = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{\frac{1}{3}\partial u_k}{\partial x_k}\delta_{ij} \tag{5}$$

Reichard et al. [22] presented droplet sizes ranging from 148 to 424 μm diameter and wind velocities ranging from 0.5 to 6.2 m/s agreed well with distances predicted by the computer program. In 1995, Zhu et al. [23] suggested a The simulations of drift distances up to 200 m (656ft) included temperatures (10° to 30° C; 50° to 86° F), discharge heights (0 to 2.0 m; 0 to 6.56 ft), initial downward droplet velocities (0 to 50 mis; 0 to 164 ft/s), relative humidities (10 to 100%), wind velocities (0 to 10.0 mis; 0 to 32.8 ftls), droplet sizes (10 to 2000 μm), and 20% turbulence intensity. Zhu et al. [23] later presented variable used in simulation were droplet diameter (10 to 600 μm), wind velocity (0.5 to 8.0 m/s), turbulence intensity (5 to 80%) and target width (6.35 to 50.8 mm) and reported Collection efficiency increased with increasing droplet size, wind velocity, and target width, but decreased with increasing turbulence intensity. Collection efficiencies calculated with FLUENT were very close to those determined experimentally in a wind tunnel. Bai et al. [25] investigated on three-dimensional flow field model of internal mixing nozzle was built to simulate the droplet size of mixing room and outlet by Fluent. The simulation suggested the droplet size decreases along with the increase of the air pressure and the air-liquid ratio. The droplet size increases in the mixing room, and then decrease sharply at the domain of the outlet.

2.0 METHODOLOGY

FLUENT software is one of the Computational Fluid Dynamic (CFD) simulation software or computational program, in modeling fluid flow and heat transfer for complex geometry, rotating reference frame meshing. It provides complete mesh flexibility by modeling flows in 2D or 3D geometries using unstructured solution-adaptive which support mesh type 2D triangular/quadrilateral, 3D tetrahedral/hexahedral, triangular/tetrahedral, quadrilateral/hexahedral, or mixed (hybrid) grid that includes prisms or pyramid where both conformal and hanging-nodes meshes are acceptable. It allows user to define grid size through fine or coarsen a grid based on the flow solution. This solution-adaptive grid capability is mainly useful for accurately calculating flow fields in regions with large gradients, such as free shear layers and boundary layers. Grid refining may results a good mesh to a level reduce computation effort. Mesh refinement similarly important to approaches the actual model. FLUENT program structure common process involves pre-processing, processing and post processing.

Started with Pre-processing; is the preliminary procedure in the CFD simulation possibly be done in Gambit or any CAD (Computer aided software) for instance Autocad and Solidworks. This paper chooses Gambit 2.2.30 software meshing software and pre-packaged in FLUENT

for pre-processing procedure consists of modeling the geometry, meshing, and selection of boundary condition. Physical domain of atomizer designed cases for rectangular axisymmetric 2D geometry domains as shown in Figure 1 meanwhile 3D geometry domains are made of a cylindrical shape of combustor attached with 45° swirl as presented in Figure 2.
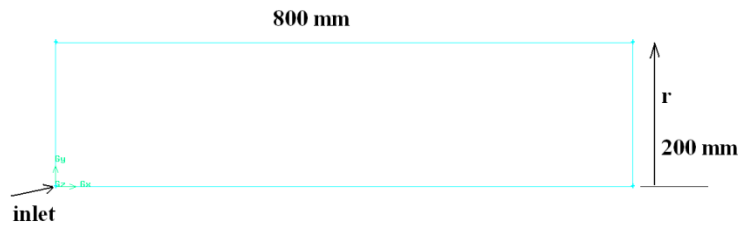
**Figure 1**: 2D geometry modeling of atomizer designed combustor
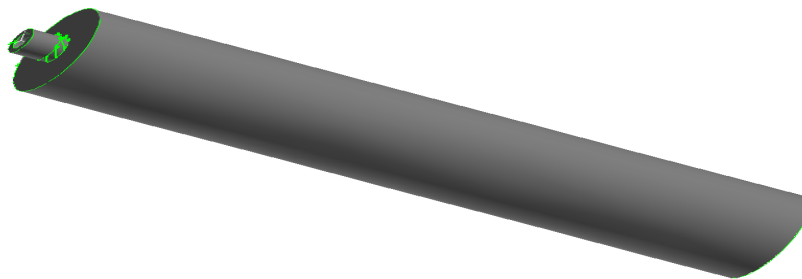
**Figure 2**: 3D geometry modeling of atomizer designed combustor

Followed by meshing, meshing is a process to generate grid and nodes to define the domain volume where increasing number of meshes or nodes will increase the accuracy of the model however finer the grid may need more time to simulate and sometimes cause instability. Both grid sizes are grid independent. As we focus on the spray flow at combustor inlet 2D axisymmetric modeling source of meshing started at origin (0,0,0) whereas for 3D modeling began with meshing edges; continue with faces meshing and finally is volume meshing and following size function. Size function of 2D model was determined with start size equal to 1, growth rate at 1.01 and maximum size of 8. In the other hand for 3D model, following parameters were chosen, size equal to 1, growth rate at 1.2 and maximum size of 5. Figure 3 shows meshing of 2D model and Figure 4 displays meshing of 3D model. The equisize skew of the grids generated from those size functions, need to be ensured that it is below 0.8 to be considers as good quality grids. Worst element of the grids for both 2D and 3D modeling were 0.262784 and 0.458791 relatively are acceptable to be used in further simulation.

Boundary conditions such as velocity inlet, wall, outflow, pressure inlet and outlet, mass flow inlet and other are selected after the meshing is done. Figure 5 and Figure 6 clarified the boundary condition of combustor for both cases. After the boundary conditions are selected, the mesh file in Gambit need to be saved and exports to FLUENT for processing procedure.
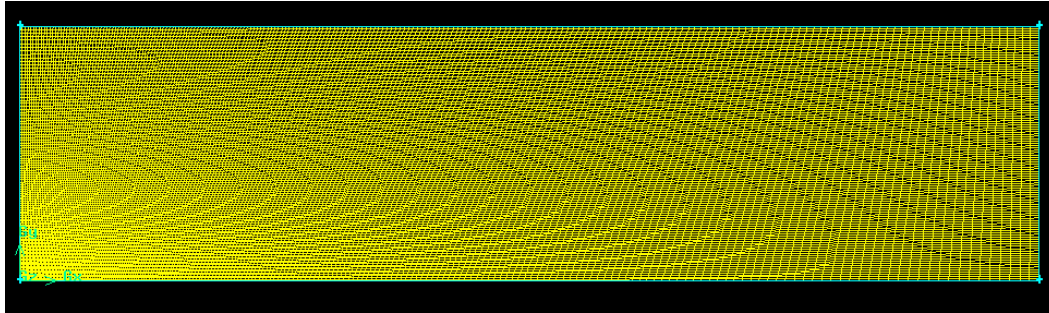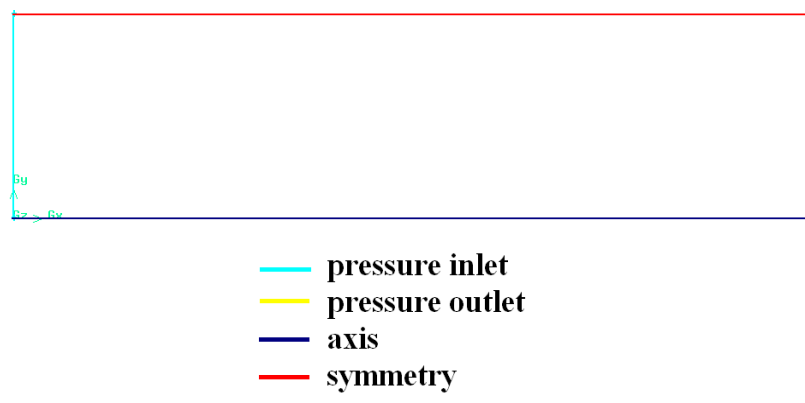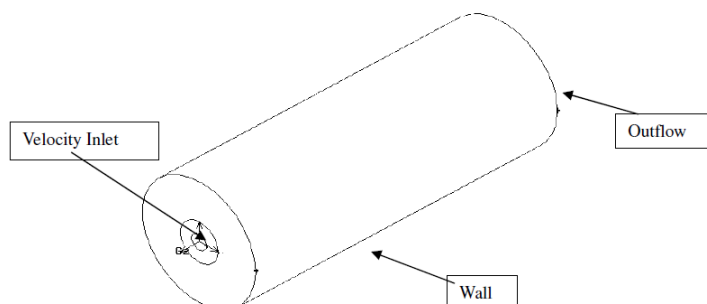
Figure 3: Meshing of 2D Model
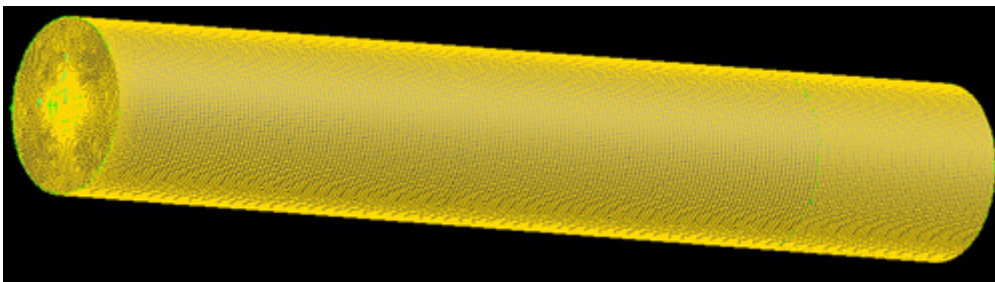
Figure 4: Meshing of 3D Model

pressure inlet
pressure outlet
axis
symmetry

Figure 5: Boundary condition selected for 2D Model

Figure 6: Boundary condition selected for 3D Model

Nest step, computational data obtained by calculation through iteration in processing procedure. The mesh file took from pre-processing procedure done in Gambit software is imported to FLUENT for further operation. For simulate fluid flow initially viscous model is selected to by choosing k-epsilon model to verify and validate the geometry of combustor model. Following defining boundary condition as summarized below:

Swirl-inlet
Velocity inlet : 15m/s
Tangential-Component of Flow Direction : 0.7071
Axial-Component of Flow Direction : 0.7071
Turbulent Intensity (%) : 0.099999994
Turbulent Viscosity Ratio : 10
Pressure, P : 1.01325 X 105 Pa

The initialization process plays major role which may affect data results. The simulation of combustor is performed through iteration. FLUENT will solve the Navier-Stokes equation for every node in the domain for solution. Once all the residual monitors show constant value, the simulation is considered to have converged and the iteration is terminated. Jet A-1 kerosene fuel properties were selected such as density, viscosity and surface tension refer as injection properties in for design input parameter in FLUENT simulation.

Table 1: Design Input Parameter

Parameters	Value
Liquid density, ρ_L	808kg.m^3
Liquid viscosity, μ_L	0.1kg/ms
Density of air, ρ_a	1kg.m^3
Spray half angle, Θ	20°
Liquid mass flow rate,	0.006kg/s
Pressure difference, ΔP_L	5 x 10^{5}Pa
Diameter of injector, D_0	0.001m

The final process of simulation described by post-processing, that displays the data obtained for the solution graphically. There are few ways to present the result graphically including x-y plot, line contour plots, shaded contour plots, vector plots and mesh plots. Further investigation on data analyzing as conducts in next chapter.
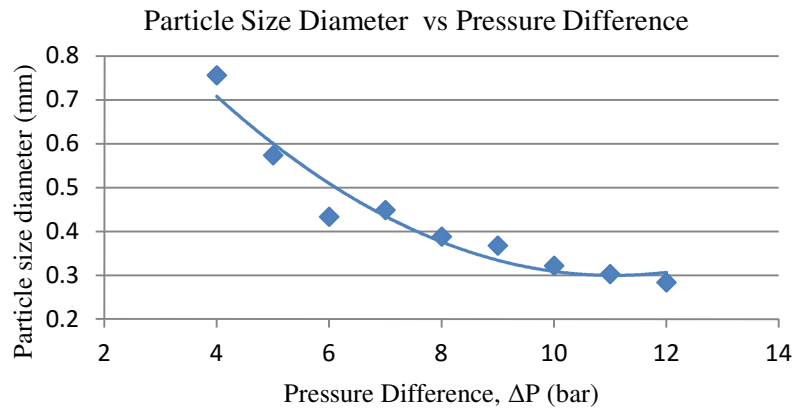

3.0 RESULT & DISCUSSION

3.1 Result of droplet size for 2D Discrete Phase Model

This section discuss on result of Jet A-1 kerosene fuel droplet size and spray characteristic for 2D Discrete Phase Model feature analysis of particle size diameter, particle traces colored, and sauter mean diameter conducted from data obtained in post-processing simulation.
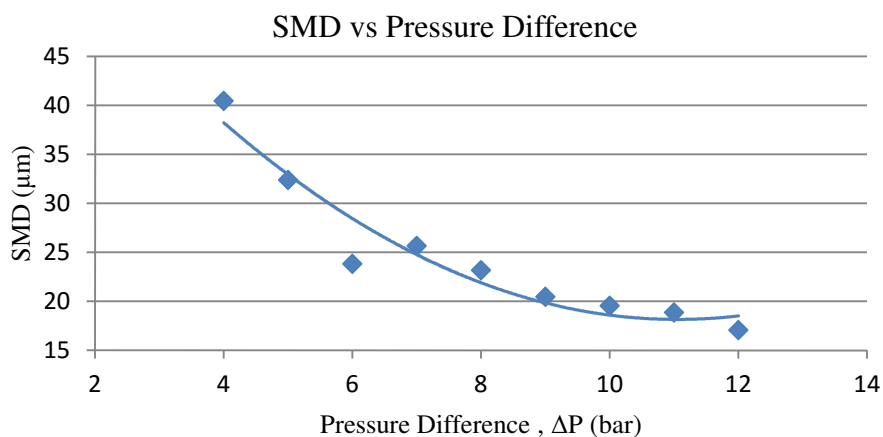
Figure 7 represents a graph of particle size diameter versus pressure differences. Data was collected from simulation of kerosene spray by FLUENT with considering maximum particle size from variable pressure difference. From above graph, particle size diameter gave highest value at pressure difference 4 bar and the smallest particle size diameter attempt at pressure difference 12 bar with 0.757 mm and 0.284 mm relatively. The graph evidently shows increasing pressure difference, particle size diameter is decreased. Increasing of pressure

difference could increase enough energy of spray fuel turbulence to overcome the preventive forces of the surface tension. Smaller turbulence structure distorts more quickly generated ligament and smaller size of droplets. Accordingly it can be concluded that, the increasing of pressure difference may decrease the particle size diameter of the spray.
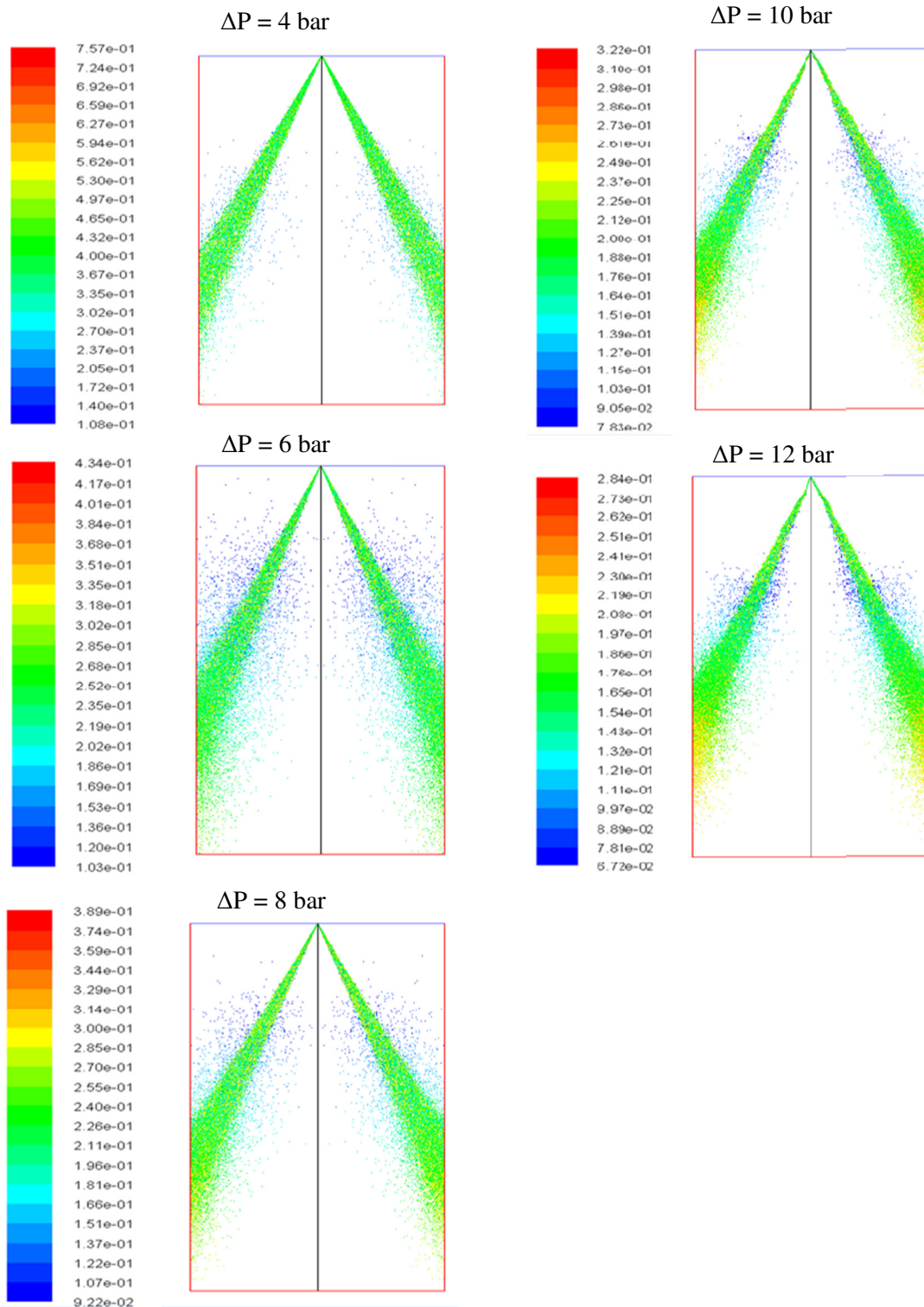

Figure 7: Graph of Particle Size Diameter versus Pressure Difference

Figure 7 represents a graph of particle size diameter versus pressure differences. Data was collected from simulation of kerosene spray by FLUENT with considering maximum particle size from variable pressure difference. From above graph, particle size diameter gave highest value at pressure difference 4 bar and the smallest particle size diameter attempt at pressure difference 12 bar with 0.757 mm and 0.284 mm relatively. The graph evidently shows increasing pressure difference, particle size diameter is decreased. Increasing of pressure difference could increase enough energy of spray fuel turbulence to overcome the preventive forces of the surface tension. Smaller turbulence structure distorts more quickly generated ligament and smaller size of droplets. Accordingly it can be concluded that, the increasing of pressure difference may decrease the particle size diameter of the spray.

**Figure 8:** Graph of Sauter Mean Diameter versus Pressure Difference

Figure 9: Diagrams of particle traces colored by particle diameter (mm)

Figure 8 showed the graph of Sauter Mean Diameter (SMD) versus pressure differences. The data collected from simulation of kerosene spray to investigate the effect of changing of pressure difference to SMD. From this graph, SMD gave highest value at pressure difference 4 bar and the smallest SMD exposed at pressure difference 12 bar with 40.43μm and 17.03μm

relatively. The graph indications plainly with increasing pressure differences, SMD is decreased. Increasing pressure caused increasing of sufficient energy of spray fuel turbulence to overcome the restraining forces of the surface tension. The smaller turbulence structures distort more rapidly generated ligament and smaller size of droplets. Thus it can be decided, the increasing of pressure difference will decrease the SMD of the droplets.
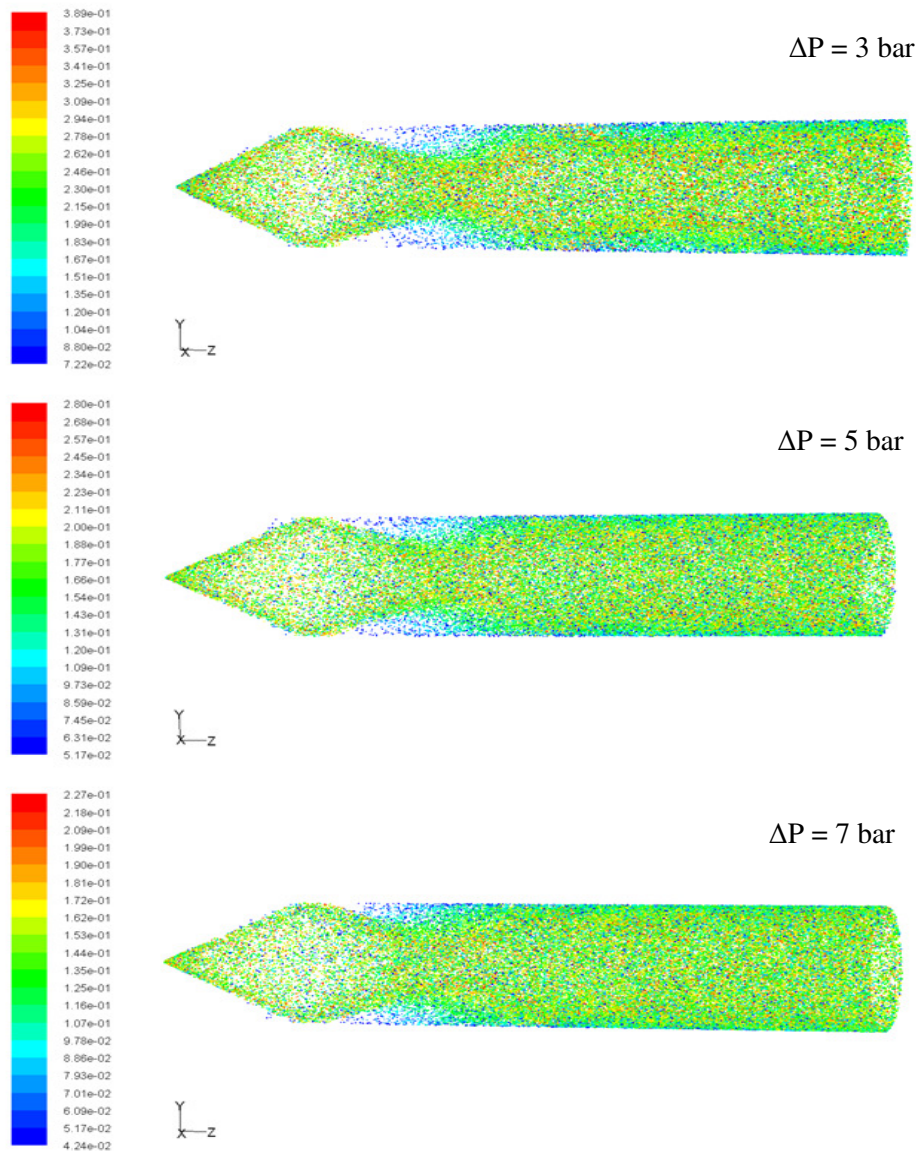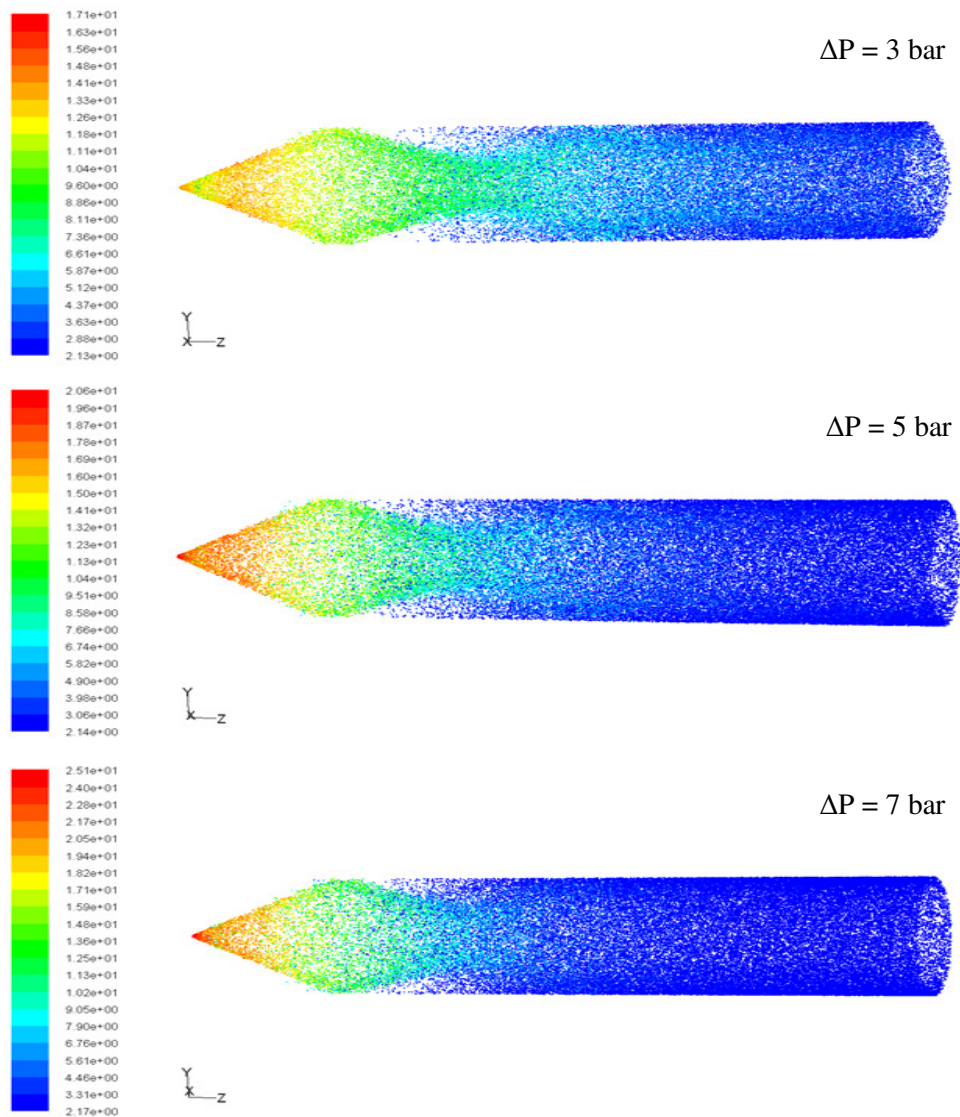
Figure 10: Particle Traces Colored by Particle Diameter

Figure 9 shows patterns of particle traces colored by particle diameter in millimeter that are obtained from simulation of FLUENT in several pressure differences. They are results from 2D Discrete Phase Model with 2D axisymmetric dominated pressure difference starting at 4 bar, increased 2 bar each until 12 bar. All diagrams gave same shape and pattern whilst particle diameter appears within the range of 0.0672 to 0.757. The smallest particle with diameter size of 0.0672 mm attempt at pressure difference 12 bar and the largest particle with diameter size of 0.757 mm occurred at pressure difference 4 bar. For each diagram revealed most of big droplet particles with large diameter are located at the inner part of the spray in the meantime

tiny ones are located at the outer part of the droplet spray distribution. Accordingly, particles travelling on the edge of the spray were more affected by shear between the air and the spray envelope, generating smaller droplets.

3.2 Result of droplet size for 3D Discrete Phase Model

This section discuss of result of Jet A-1 kerosene fuel spray characteristic for 3D Discrete Phase Model with 30° swirl dominated of combustor chamber from FLUENT simulation. Pressure was varied to investigate the effect to diameter and velocity of droplets deliberated as deliberated follow.

Figure 11: Particle Traces Colored by Particle Z Velocity

Figure 10 shows the particle traces colored by particle diameter in millimeter for various pressure differences. All of diagrams indicate most of largest droplet particle located at the inner part of the spray whilst the smallest particle is located at the outer part of the droplet distribution. The particle diameter that showed is within the range of 0.0424 mm - 0.389 mm. Droplets at pressure of 3 bar have maximum diameter of 0.389 mm and minimum diameter of

0.0722 mm whereas at 5 bar has a maximum diameter of 0.28 mm and minimum diameter of 0.0517 mm and at pressure 7 bar obtained 0.227 mm and 0.0424 mm relatively. The increasing of pressure may decrease the diameter size of particles in spray.

Figure 11 shows the particle traces colored by particle Z velocity for various pressures differences. All of diagrams have alike pattern where most of the highest velocity droplet particle located at the inlet part while the lowest velocity are located at outer part of droplet distribution. The particle Z velocity that showed are within range of 2.13 m/s to 25.1 m/s. Droplets at pressure difference of 3 bar has a maximum Z velocity of 17.1 m/s and minimum Z velocity of 2.13 m/s while at 5 bar 20.6 m/s and 2.14 m/s relatively whereas at 7 bar it shows 25.1 m/s and 2.17 m/s relatively.

4.0 CONCLUSION

As conclusion droplet size and spray characteristic of kerosene fuel are possible to obtain with k-epsilon model of CFD simulation using FLUENT particularly. The k-epsilon model was used to verify and validate the geometry of combustor model. Data result from simulation confirmed that changing of pressure difference may affect the spray and droplet characteristics such as diameter and velocity droplets. Increasing of pressure difference resulted decreasing of droplets diameter and increasing of droplets velocity. The droplets velocity and diameter profiles were presented to be dependent upon the location (axially and radials) in of spray distribution. Increments of injection pressure resulting high velocity droplets far from the nozzle were subject to aerodynamic break-up. The progression of the droplet sizes was concluded to be higher by the merging of droplets and the evaporation of small ones. These two CFD models are satisfied by using different design input parameters such as the diameter of atomizer, mass flow rate etc. Hence these models are qualified and will be used to simulate various parameters for kerosene spray further.

ACKNOWLEDGEMENTS

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