Numerical Simulation of a Liquid Jet Atomization and Break-Up Using ANSYS-CFX 12.0

Yash Akhil Bhatt
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Numerical Simulation of a Liquid Jet Atomization and Break-Up using ANSYS-CFX 12.0

by

YASH AKHIL BHATT

Thesis Submitted in Partial Fulfillment of the Requirements for the Degree of Master of Science in Aerospace Engineering

Embry-Riddle Aeronautical University
Daytona Beach, Florida
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Numerical Simulation of Liquid Jet Atomization and Break-Up using ANSYS-CFX

by

Yash Akhil Bhatt

This Thesis was prepared under the supervision of the Candidate’s Thesis Advisor, Dr. Vladimir Golubev, Department of Aerospace Engineering, and has been approved by the members of his Thesis Committee. This Thesis was submitted to the Department of Aerospace Engineering and was accepted in partial fulfillment of the requirements for the Degree of Master of Science in Aerospace Engineering.

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ABSTRACT

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Break-up and atomization characteristics of JetA liquid fuel were investigated numerically. The results have been compared to various experimental results to evaluate the accuracy of the numerical model. The CFD code ANSYS-CFX 12.0 was used to carry out the steady state analysis at different time scales. A comparison between the atomization characteristics of a pressure jet atomizer and an air-blast atomizer is shown. By employing a Lagrangian particle tracking method to track the path of the liquid particles, the liquid jet/spray phenomena was studied in light of low and high back pressure environments. The ‘BLOB’ primary atomization model and the Cascade Atomization and Breakup model ‘CAB’ which is an extension of the Enhanced Taylor Analogy Breakup model ‘ETAB’ was incorporated for analyzing the secondary breakup. Parameters taken into consideration were the JetA liquid particle traveling time and distance, Sauter Mean Diameter, Weber number, JetA Liquid Average Velocity and the turbulence kinetic energy.
ACKNOWLEDGEMENTS

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LIST OF SYMBOLS

\(D_{lg}\) = Diameter of Liquid, Gas Jet

\(U_{lg}\) = Velocity of Injected Liquid, Gas

\(\nu_{lg}\) = Viscosity of Injected Liquid, Gas

\(Re_{lg}\) = Reynolds Number of Liquid, Gas

\(We\) = Weber Number

\(Oh\) = Ohnesorge Number

\(Re_{\text{eff}}\) = Effective Reynolds Number

\(M\) = Momentum Ratio

\(V_{\text{slip}}\) = Slip velocity between the gas and liquid

\(\rho_{lg}\) = Density of liquid and gas

\(\sigma\) = Surface Tension

\(d_{32}\) = Sauter Mean Diameter

\(\alpha_f\) = Volume fraction of fluid/surrounding gas

\(\frac{\partial}{\partial t}, \frac{\partial}{\partial (x,y,z)}\) = Partial derivative w.r.t. time, spatial

\(\dot{n}\) = Mass flow rate

\(r_p\) = Radius of particle

\(K_{br}\) = Break-up constant

\(C_D\) = Drag Constant
1.0 INTRODUCTION

1.1 Thesis Objective

To obtain an understanding and investigate the atomization and break-up process of a liquid. Due to the many challenges the current research demands, Computational Fluid Dynamics (CFD) is being used on a wide basis to get to the crux of the matter.

CFD, now used as a third leg, along with experiment and theory, has the potential to provide valuable insight to the process of atomization and the nature of the flow field. The Florida Centre of Advanced Aero Propulsion (FCAAP) is a tie up between Embry-Riddle Aeronautical University, University of Florida, University of Central Florida and Florida State University has come up with the task of studying the atomization and vaporization characteristics of pure and blended biofuel droplets. The commercial CFD code ANSYS-CFX is capable of predicting the phenomena of fuel jet atomization and break-up with the help of various mathematical models that it possesses. The process of atomization is one in which liquid is disintegrated into droplets by the action of internal and/or external forces. In the absence of such forces, surface tension tends to pull the liquid molecules together to form liquid jets or sheets.

ANSYS-CFX is a pressure-based solver that incorporates various finite-volume schemes. The commercial code supports equation sets governing turbulent and chemically reacting flows. The flow solution is computed iteratively on a computational grid, which can be generated using the classical grid generation software called GridGen.
Previous experiments such as that of Lasheras et al [12, 13] have dealt with the atomization and break-up studies of a high-speed water jet by an annular high-speed annular air jet. The results obtained from these studies were used to validate numerical results for a CFD methodology developed by Brinckman et al [2] for compressible flows. Lin et al [16] studied various break-up regimes and break-up mechanisms involved in atomization. A detailed review article, regarding the secondary atomization process containing abundant literature on experimental methods, break-up morphology and break-up times, are studied by Guildenbecher et al [6]. As far as the numerical simulation of primary and secondary atomization is concerned, there has been a comprehensive study carried out by Jiang et al [8] who present various physical models and advanced methods used in computational studies of two-phase jet flows. Jiang et al [8] throw light on the DNS (Direct Numerical Simulation) and LES (Large Eddy Simulation) approach in multiphase modeling. In traditional CFD based on Reynolds-averaged Navier Stokes (RANS) approach, physical modeling of atomization and sprays is an essential part of the two-phase flow computation [8]. In advanced CFD numerical techniques like direct numerical simulation (DNS) and large-eddy simulation (LES) are used for modeling of atomization and sprays [8]. A similar approach using DNS has been adopted by Lebas et al [14] by incorporating the so-called (Eulerian-Lagrangian Spray Atomization model) ELSA to model multiphase flows. Shi et al [21] came up with a study of the simulation of high-speed droplet spray dynamics of diesel fuel in light of different environments, fuel velocity, jet penetration depth, droplet diameters and number density function. There has been considerable amount of literature on the phenomenon of liquid jet atomization and break-up since the past few decades. There has been significant amount of work on atomization and break-up characteristics of biofuel, however, these
studies have been limited to using the blends of biofuel with diesel fuel which, is more commonly known as, biodiesel. The parameters of study i.e. the weber number, sauter mean diameter (SMD), liquid penetration depth and the turbulence kinetic energy have been the key issues that have received prime focus in this area of research and have been found to repeat themselves in every research paper in the field, irrespective of the fluid under consideration.

This thesis focused on simulating the atomization and break-up characteristics of a JetA fuel at different conditions using ANSYS-CFX 12.0. Steady state simulations were run to predict the results. Experimental results from Wu et al. [22], Hiroyasu et al. [7] and Lasheras et al. [12, 13] were obtained to validate the numerical results. A comparison between the atomization characteristics of a pressure jet atomizer and an air-blast atomizer is discussed.

Figure 1 gives a brief outline of the steps taken in undertaking this research and provides a guide for this document. Further light shall be thrown on every step in the later chapters.
Chapter 1: Introduction

The coordinate systems used in this thesis will be discussed in more detail in later chapters.

It has been well known for many years that the Earth has an inherent magnetic field. All the details of the generation of Earth’s magnetic field are not completely understood, but it is currently described by dynamo theory. At low altitudes the Earth’s magnetic field can be approximated as a tilted dipole. As the altitude increases Earth’s magnetic field becomes compressed on the dayside, stretched on the nightside, and generally deformed away from being a dipole field through its interaction with the IMF. The area contained within Earth’s magnetic field is referred to as the magnetosphere. The major components of the magnetosphere are all shown in Figure 1.2. The first boundary the solar wind plasma encounters is the bow shock.

Figure 1.1: Solar Corona - Solar Wind [Walker, 2001]
1.2. Relevant Theory & Specific Issues

Understanding of fuel jet break-up and atomization is of prime importance to multiphase flow and combustion problems and has widespread applications ranging from fuel injectors in gas turbines and jet engines to spray painting and drying applications.

1.2.1. The Atomization Process

In gas turbine combustion chambers, atomization is normally accomplished by spreading the fuel into a thin sheet to induce instability and promote disintegration of the sheet into drops. Thin sheets may be obtained by discharging the fuel through orifices with specially shaped approach passages, by forcing it through narrow slots, by spreading it over a metal surface, or by feeding it to the centre of a rotating disk or a cup. Hence, the fuel breaks up from a thin jet or a thin sheet into ligaments, which eventually breaks down into drops that are distributed throughout the combustion zone in a controlled pattern and direction [15].

1.2.1.1 Break-up Regimes

There are four main break-up regimes that have been identified corresponding to different combinations of liquid inertia, surface tension and aerodynamic forces acting on a liquid jet. These are named as Rayleigh regime, the first wind-induced regime, the second wind induced regime, and the atomization regime [12]. When a liquid jet of diameter $D_j$ and velocity $U_j$ is discharged into a stagnant gas, Rayleigh instability arises when the jet diameter is small and the jet Reynolds number $Re_j = U_j D_j / \nu_j$ is not too large i.e. of the order of $10^2$. At larger Reynolds numbers, the jet becomes wavy because of aerodynamics effects and the first-wind induced regime is developed. When the Reynolds number is further
increased, the wind stress at the gas/liquid interface strips off droplets, and at larger Reynolds numbers, i.e. $10^5$, atomization due to short-wavelength shear instability takes place that leads to second-wind induced regime and eventually the atomization regime.

In order to get an idea about the instabilities and the wavelengths the reader can refer to figure 2 for details. This thesis does not focus on the stability analysis of atomization. In order to further delve into the topic of stability analysis the reader can refer to [4, 12, and 15].

The liquid break-up and atomization can be divided into two regions of interest i.e. a near field primary break-up region and a far field secondary break-up region. Primary break-up is characterized by the formation of ligaments and other irregular liquid elements. The irregular liquid elements are unstable because they are subjected to relatively large drag forces exerted by the surrounding gas, which leads to droplet deformation. Droplet deformation eventually leads to secondary break-up.

![Figure 2. Schematic of different lengths in the break-up process [12]](image)
1.2.1.2. Primary Atomization

According to Lefebvre [15], “Atomization can be considered as a disruption of the consolidating influence of surface tension by the action of internal and external forces”. Primary break-up takes place in the region close to the nozzle exit. The primary breakup, which is dominant in the first few jet diameters, is essentially related to the non-miscible shear instability, and results in the stripping of the liquid jet by the high shear forces at the gas/liquid interface. The process of atomization itself can be characterized by a number of factors among which the length of the intact core of the liquid jet, which is also known as “break-up length”. The length of intact liquid jet core determines the primary atomization region and is very important for the performance of atomizing nozzles and for the development of computational models of the atomization process. The destabilization of the liquid jet close to the nozzle exit is a Kelvin-Helmholtz type instability where surface tension acts as a stabilizing force and imposes a lower cut-off for the waves that can grow [13].

1.2.1.3. Secondary Atomization

The liquid sheet is broken up into different kinds of parent droplets, due to its relative motion through the gas, which in turn are broken down into child droplets. This phenomenon is known as secondary atomization. Based on the value of the Weber number, the Pitch and Erdman correlations are given by [6, 18]:

1. Vibrational break-up ($We \leq 12$): Large fragments are produced and the time taken for the break-up as opposed to other break-up mechanisms is longer. Hence, this mechanism is not given much importance.
2. Bag break-up (12<\textit{We} \leq 50): The liquid bulk or large droplet deforms into a thin disk normal to the flow direction, followed by a severe deformation at the centre of the disk into a thin balloon-like structure, which will finally lead to break-up. In short, a thin bag forms behind the droplet rim.

3. Bag and Stamen (50<\textit{We} \leq 100): This break-up also known as multi-mode break-up is similar to bag break-up. A thin bag is blown downstream while being anchored to a massive toroidal rim. A column of liquid (stamen) is formed along the droplet axis parallel to the approaching flow. The bag bursts first and the disintegration of rim and stamen follows.

4. Sheet Stripping (100<\textit{We} \leq 350): It involves deflection of the periphery of the disk in the downstream direction instead of the deflection of the center of the disk. For sprays, most droplet breakups occur in the stripping break-up regime. Shear forces strip droplets from liquid ligaments. Part of this break-up takes place due to Kelvin-Helmholtz (K-H) instabilities.

5. Catastrophic break-up (\textit{We}>350): Catastrophic break-up has a similar mechanism as stripping break-up, but it involves more explosion type break-up i.e. the droplet immediately disintegrates. Waves with large amplitude and long wavelength related with Rayleigh-Taylor (R-T) instabilities ultimately penetrate the droplet creating several large fragments. This is referred to as catastrophic breakup.

Hence, a larger Weber number indicates a higher tendency towards fragmentation. Figure 3 shows a description of all the break-up mechanisms.
1.2.2. Parameters

Two of the most important parameters that contribute towards atomization are the Reynolds number and the Weber number. For the near field development, the Reynolds number has to be large ($Re \geq 10^3$) in order for the jet to become turbulent near the nozzle. For a coaxial jet the liquid jet Reynolds number can be defined as, $Re_l = U_l D_l / \nu_l$ and for the gas, $Re_g = U_g D_g / \nu_g$. Hence, the effective Reynolds number to characterize the total flow (gas plus liquid) is given by,
The Weber number and the Ohnesorge number are two important dimensionless parameters that are used in correlations for various break-up regimes. The former is a ratio between the aerodynamic deformation pressure force exerted on the liquid (estimated with the initial velocity difference) and the restoring surface tension forces, where $\sigma$ is the interfacial surface tension force. The latter represents the ratio of the viscous forces to the surface tension forces where $\mu_l$ is the liquid molecular viscosity and $d$ is the droplet diameter.

\[
Re_{eff} = \left( \frac{U_g D_g}{v_g} \right) \left[ 1 - \frac{D_2^2}{D_1^2} + \frac{D_1^2}{MD_g^2} \right]
\]  

The Weber number connects the gas induced drag force, which leads to deformation to the liquid surface tension which tends to maintain a spherical droplet shape, i.e. resists deformation. When a droplet is exposed to gas flow, significant deformation occurs at a Weber number of unity.

Thus, the Weber number connects the gas induced drag force, which leads to deformation to the liquid surface tension which tends to maintain a spherical droplet shape, i.e. resists deformation. When a droplet is exposed to gas flow, significant deformation occurs at a Weber number of unity.

The other parameter that plays an equally important role in atomization studies is the droplet size, especially downstream of the flow. The droplet size is found to vary and is a function of the flow parameters. The droplet size distribution (DSD) in sprays is the crucial parameter needed for the fundamental analysis of the transport of mass, momentum and heat in engineering systems. Moreover, the DSD determines the quality of the spray and consequently influences to a significant extent the processes of fouling and undesired
emissions in oil combustion. The droplet size is typically characterized by the Sauter Mean Diameter (SMD) i.e. the diameter of the sphere that has the same volume to surface area ratio as that of the particle of interest. If the actual surface area \( A_p = \sum N_i d_i^2 \) where \( d_i \) is the diameter of each droplet and \( N_i \) is the number of droplets per unit volume in each size group) and the volume \( V_p = \sum N_i d_i^3 \) of the particle are known the SMD is given by,

\[
d_{32} = 6 \frac{V_p}{A_p}
\]  

(4)

The dependence of the droplet size on the gas velocity has been found to be approximated by the power law \( d_{32} \sim U_g^{-n} \) with \( n \) ranging usually from 0.8 to 1.3 and possible reaching a value as large as 2 in exceptional cases [13].

The unbroken length of the spray is known as the liquid intact length \( L_b \) where the break-up begins, whereas the length needed for the liquid jet to be completely broken into drops and ligaments is known as the liquid core length \( L \) as shown in figure 2 [12]. According to Villermaux, Rehab and Hopfinger [12, 13] along with the break-up length or the liquid intact length, the other parameter that plays an equally important role to better describe the break-up process is the momentum flux ratio per unit volume, which is given by,

\[
M = \frac{\rho_g U_g^2}{\rho_l U_l^2}
\]  

(5)
2.0. NOZZLE AND CHAMBER CONFIGURATION

There were two types of nozzle geometries that were incorporated to analyze the process of primary and secondary atomization. The first configuration involved an air-blast atomizer and the other type of configuration was a pressure jet atomizer. An alternative low-speed atomizer is the pressure swirl atomizer.

2.1. Pressure Jet Atomizer

A pressure jet atomizer is somewhat similar to a pressure swirl atomizer where the liquid is injected into a stationary gas stream at an extremely high velocity. The important parameters to take note of in all the atomizers, is the spray angle, injection velocity, nozzle design, back pressure, droplet size distribution and the spray penetration depth [21]. While incorporating the pressure jet atomizer, the outlet diameter of the nozzle was specified as opposed to incorporating the entire nozzle geometry as in the case of the air blast atomizer.

2.2. Air-blast Atomizer

When surrounded by a gas with a momentum flux greater than that of the liquid, the transfer of kinetic energy from the high-speed gas to the liquid causes the break-up of the jet, a process known as air-blast atomization [13, 15]. An air-blast atomizer is similar to an air assist atomizer where the air is supplied from a compressor or a high-pressure cylinder, it is important to keep the airflow rate down to a minimum. However, in the case of an air assist atomizer there is no restriction on air pressure, the atomizing air velocity can be made very large. Thus, air assist atomizers are recognized by relatively small quantity of air with a very high velocity air. The air velocity in an air-blast atomizer is limited to a maximum value of 120 m/s corresponding to the pressure differential across the liner wall, a larger amount of air
is required to achieve good atomization. This air is not wasted since, after atomizing the fuel, it flows into the primary combustion zone where it provides the part of air required for primary combustion [15]. Air-blast atomizers have many advantages over pressure atomizers, especially in their applications to gas turbine engines of high-pressure ratio. They require lower fuel pressures and produce a finer spray [15].

The nozzle/injector geometry used in the analysis for an air-blast atomizer is shown in Figure 4. The geometry was adopted from the experimental observations of Lasheras et al [13]. Brinckman et al [2] implemented a concise version of the geometry in their research. The inner jet is a liquid core surrounded by a high-speed air jet.

![Figure 4(a). Coaxial jet nozzle configuration from Lasheras et al. [12]](image)

![Figure 4(b). Co-annular Jet from Brinckman et al. [2]](image)
As shown, the nozzle has an inner fuel diameter of $d_f = 2.9\text{mm}$, which is expanded through a 6-degree half cone angle to an outlet diameter of $D_f = 3.8\text{mm}$. The diffuser at the outlet modifies the pipe flow velocity but does not lead to flow separation. The nozzle diameter of the annular air jet is $D_g = 5.6\text{mm}$. 
3.0. GRID GENERATION

The geometrical model was constructed using GridGen V15.10 [19]. GridGen is a meshing software used to apply a three-dimensional, structured, hexahedral grid and an unstructured grid to the nozzle geometry. For the pressure jet atomizer, an entire 360 degrees of the model/cylinder was used for meshing and CFD computation. In the case of the air-blast atomizer, 1/8th or a 45 degree cut/section of the cylindrical model was used to model the liquid jet. One of the problems that hindered the grid independence study was the fact that the ANSYS-CFX license at Embry-Riddle Aeronautical University could not handle a grid size of more than 512000 nodes. Hence, the computational grid had less than 512000 nodes, which compromised on the accuracy and resolution of the numerical results.

3.1. Pressure Jet Atomizer
A cylindrical structured hexahedral grid to model the atomization of a liquid jet/spray in a pressure jet atomizer as shown in Figure 5 was used. It consists of a cylindrical domain and in order to capture the atomization and break-up the numerical accuracy was enhanced by a highly refined and clustered mesh near the axis of the cylinder. The cylinder had a radius of 5cm and a length of 100cm. Grid quality was partially ensured by Jacobian and aspect ratio analyses. The mesh had 444080 nodes and 438450 elements.
3.2. Air-blast Atomizer

1/8\textsuperscript{th} of the cylindrical model was used to model the atomization process of a liquid jet/spray in an air-blast atomizer. The nozzle dimensions were obtained from the experiments carried out by Lasheras et al \cite{12,13} as shown in Figure 4b. An unstructured, tetrahedral grid as shown in Figure 5.1 was used.

\textbf{Figure 5.1. Cylindrical grid for computational flow domain of pressure jet atomizer}
Figure 5.2. Unstructured 45 degree grid used for the air-blast atomizer
4.0. SIMULATION METHODOLOGY

4.1. Flow Conditions

There have been various experiments carried out to study the atomization and break-up process two of which have been focused on in this thesis. There were two experimental cases that were used to carry out the numerical simulation. Considering the pressure jet atomizer, the cases discussed in this thesis are a slight variation of the experimental data produced by Hiroyasu et al. [7], Wu et al. [22].

<table>
<thead>
<tr>
<th>Cases</th>
<th>Injected Liquid</th>
<th>Spray Parameters</th>
<th>Gas (Nitrogen)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1a</td>
<td>Material: Diesel Fuel Oil</td>
<td>Nozzle Diameter: 0.3mm</td>
<td>Pressure: 1atm</td>
</tr>
<tr>
<td></td>
<td>Density: 840 kg/m$^3$</td>
<td>Mass flow rate: 0.007 kg/s</td>
<td>Temp: 25 deg</td>
</tr>
<tr>
<td></td>
<td>Surface Tension: 0.0295 N/m</td>
<td>Spray angle (estimated): 1.68 deg</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Velocity: 122.2 m/s</td>
<td></td>
</tr>
<tr>
<td>Case 1b</td>
<td>Material: n-hexane</td>
<td>Nozzle Diameter: 0.3mm</td>
<td>Pressure: 30atm</td>
</tr>
<tr>
<td></td>
<td>Density: 665 kg/m$^3$</td>
<td>Mass flow rate: 0.005 kg/s</td>
<td>Temp: 25 deg</td>
</tr>
<tr>
<td></td>
<td>Surface Tension: 0.0184 N/m</td>
<td>Spray angle (estimated): 9.14 deg</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Velocity: 102.5 m/s</td>
<td></td>
</tr>
<tr>
<td>Case 2</td>
<td>Material: n-hexane</td>
<td>Nozzle Diameter: 0.127mm</td>
<td>Pressure: 14.8atm</td>
</tr>
<tr>
<td></td>
<td>Density: 665 kg/m$^3$</td>
<td>Mass flow rate: 0.001 kg/s</td>
<td>Temp: 25 deg</td>
</tr>
<tr>
<td></td>
<td>Surface Tension: 0.0184 N/m</td>
<td>Spray angle (estimated): 3.56 deg</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Velocity: 127 m/s</td>
<td></td>
</tr>
</tbody>
</table>

Table 1. Experimental conditions for the pressure jet atomizer

Cases 1a & 1b were performed by Hiroyasu and Kadota [7] and case 2 was performed by Wu et al [22]. The numerical conditions listed in Table 2 use JetA liquid fuel instead of diesel fuel oil and n-hexane. Also, the operating pressure in case 1b is 10atm in the numerical conditions instead of 30atm in the experimental conditions. It was observed that in spite of changing the material, the mass flow rate and the spray angle remained the same.
### Table 2. Numerical conditions for the pressure jet atomizer

The spray angle for cases 1a, 1b and 3 was estimated based on the empirical formula given by Duckowicz [21],

$$\tan \frac{\theta}{2} = A \left(\frac{\rho_a}{\rho_d}\right)^{0.5}$$  \hspace{1cm} (6)

The constant $A$ is a function of the nozzle internal geometry. In the present study, $A$ was taken to be 0.4 [21], which is a good choice for jet sprays in the parameter range of interest.

As far as the air-blast atomizer is concerned the flow conditions are shown in Table 3. The flow conditions were adopted from one of the cases studied by Lasheras et al. [12, 13]. The pressure was varied while all the other quantities like the velocity, mass flow rate, temperature and material were kept constant. Table 4 displays the flow conditions that emulate the flow conditions in a gas turbine chamber. The pressure in this case is 10MPa, is similar to that in a gas turbine chamber.
### Table 3. Flow conditions for the air-blast atomizer

<table>
<thead>
<tr>
<th>Cases</th>
<th>Injected Liquid</th>
<th>Spray Parameters</th>
<th>Gas (Air)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cases 3a, 3b, 3c</td>
<td>Material: JetA Liquid Fuel ($C_{12}H_{23}$)</td>
<td>Nozzle Diameter: 3.6 mm</td>
<td>Pressure: 1 atm, 10 atm, 14.8 atm</td>
</tr>
<tr>
<td></td>
<td>Density: 780 kg/m$^3$</td>
<td>Mass flow rate: 0.004 kg/s</td>
<td>Temp: 1150K</td>
</tr>
<tr>
<td></td>
<td>Surface Tension: 0.0255 N/m</td>
<td>Spray angle (estimated): 6 deg</td>
<td>Velocity: 84.1 m/s</td>
</tr>
<tr>
<td></td>
<td>Velocity: 0.51 m/s</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 4. Flow conditions (Gas Turbine Case) for the air-blast atomizer

<table>
<thead>
<tr>
<th>Cases</th>
<th>Injected Liquid</th>
<th>Spray Parameters</th>
<th>Gas (Air)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 4</td>
<td>Material: JetA Liquid Fuel ($C_{12}H_{23}$)</td>
<td>Nozzle Diameter: 3.6 mm</td>
<td>Pressure: 10 MPa</td>
</tr>
<tr>
<td></td>
<td>Density: 780 kg/m$^3$</td>
<td>Mass flow rate: 0.004 kg/s</td>
<td>Temp: 1150K</td>
</tr>
<tr>
<td></td>
<td>Surface Tension: 0.0255 N/m</td>
<td>Spray angle (estimated): 6 deg</td>
<td>Velocity: 84.1 m/s</td>
</tr>
<tr>
<td></td>
<td>Velocity: 0.51 m/s</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 4.2. Modeling Multiphase Flow and Primary and Secondary Break-up Models

There are two options available for modeling multiphase flow in ANSYS-CFX. One of them is the Eulerian-Eulerian multiphase model and the other is the Lagrangian Particle Tracking multiphase model. Based on the literature survey carried out by the author it has been observed that the Lagrangian droplet model has been the most popular method to simulate sprays. In this kind of approach, the droplets, which are formed through the atomization process of the liquid jet, are tracked in a Lagrangian frame of reference through Monte Carlo methods, whereas the gas phase is described in a Eulerian frame of reference. Unlike the Eulerian-Eulerian model the Lagrangian particle-tracking model does not treat the liquid and gas as two separate phases. The liquid particles/droplets are modeled using the Lagrangian
method while the surrounding gas is modeled as a phase using the Eulerian model. Within
the particle transport model in ANSYS CFX 12.0, the total flow of the particle phase is
modeled by tracking a small number of particles through the continuum fluid. The particles
could be solid particles, drops or bubbles.

The application of Lagrangian tracking in CFX involves the integration of particle paths
through the discretized domain. Individual particles are tracked from their injection point
until they escape the domain or some integration limit criterion is met. Each particle is
injected, in turn, to obtain an average of all particle tracks and to generate source terms to the
fluid mass, momentum and energy equations. Because each particle is tracked from its
injection point to final destination, the tracking procedure is applicable to steady state flow
analysis [1]. The governing continuity and momentum equations are given by:

\[ \frac{\partial \alpha_f}{\partial t} + \frac{\partial \alpha_f u_f}{\partial x} = 0 \]  

(7)

\[ \frac{\partial \alpha_f u_f}{\partial t} + u_f \frac{\partial \alpha_f u_f}{\partial x} = -\alpha_f \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[ \alpha_f (v + v_T) \left( \frac{\partial u_f}{\partial x} + \frac{\partial u}{\partial x} \right) \right] + \frac{1}{\alpha_f \rho_f} M_f \]  

(8)

Where, \( \alpha_f \) is the fluid (gas) volume fraction which, as an approximation was set to a value of
one. \( v_T \) is the eddy viscosity and \( v \) is the kinematic viscosity.

\( M_f \) is the momentum exchange between the gas and the particles.

The main task of an atomizer (or primary break-up models) is to determine starting
conditions for the droplets that leave the injection nozzle.
These conditions are:

- Initial particle radius
- Initial particle velocity components
- Initial spray angle

These parameters are mainly influenced by the nozzle internal flow (cavitation and turbulence induced disturbances), as well as by the instabilities on the liquid-gas interface. There are a large variety of approaches of different complexities documented in literature. In this thesis the primary break-up model ‘Blob Method’ was implemented to define the injection conditions of the droplets [1].

In this approach, it is assumed that a detailed description of the atomization and breakup processes within the primary breakup zone of the spray is not required. Spherical droplets with uniform size, $D_p = D_{\text{nozzle}}$, are injected that are subject to aerodynamic induced secondary breakup.

Assuming non-cavitating flow inside the nozzle, it is possible to compute the droplet injection velocity by conservation of mass as follows:

$$U_{\text{p,initial}}(t) = \frac{\dot{m}_{\text{nozzle}}(t)}{A_{\text{nozzle}} \rho_p}$$  \hspace{1cm} (9)

$A_{\text{nozzle}}$ is the nozzle cross-section and $\dot{m}_{\text{nozzle}}(t)$ is the mass flow injected through the nozzle.

The spray angle is either known or can be determined from empirical correlations. The blob method does not require any special settings and it is the default injection approach in CFX.
For the numerical simulation of droplet breakup, a so-called statistical breakup approach is used in CFX. In this framework, it is assumed that if a droplet breaks up into child droplets, the particle diameter is decreased accordingly to the predictions of the used breakup model. The particle number rate is adjusted so that the total particle mass remains constant (mass of parent droplet = $\Sigma$ mass of child droplets). Using this assumption, it is not required to generate and track new droplets after breakup, but to continue to track a single representative particle.

To model the secondary breakup the ‘Cascade Atomization and Break-Up’ model (CAB) is used. The CAB model is a further development of the ETAB (Enhanced Taylor Analogy Break-Up) model. The enhanced TAB model uses the same droplet deformation mechanism as the standard TAB model. O'Rourke and Amsden proposed the so-called TAB model that is based on the Taylor analogy. Within the Taylor analogy, it is assumed that the droplet distortion can be described as a one-dimensional, forced, damped, harmonic oscillation similar to the one of a spring-mass system. In the TAB model, the droplet deformation is expressed by the dimensionless deformation $y = 2(x/r)$, where $x$ describes the deviation of the droplet equator from its original shape and position. The droplet deformation using the TAB model is shown in Figure 7.
However, the ETAB model uses a different relation for the description of the breakup process. It is assumed that the rate of child droplet generation, \( \frac{dn(t)}{dt} \), is proportional to the number of child droplets:

\[
\frac{dn(t)}{dt} = 3K_{br}n(t)
\]  

(10)

The constant \( K_{br} \), depends on the break-up regime and is given by,

\[
K_{br} = \begin{cases} 
   k_1\omega & \text{We} \leq We_t \\
   k_1\omega\sqrt{We} & \text{We} > We_t 
\end{cases}
\]  

(11)

\( We_t \) being the Weber number that divides the bag breakup regime from the stripping break-up regime. \( We_t \) is set to a default value of 80. Assuming a uniform droplet size distribution, the following ratio of child to parent droplet radii can be derived:

\[
\frac{r_{P,\text{child}}}{r_{P,\text{parent}}} = e^{-K_{br}t}
\]  

(12)

However, unlike the CAB model, the TAB and ETAB model do not take into account the catastrophic break-up i.e. for \( We > 350 \). Thus, the CAB model takes into consideration the bag, stripping and the catastrophic break-up. Hence, the break-up constant, \( K_{br} \), for different regimes, for the CAB break-up is given by,
\[ K_{br} = \begin{cases} 
 k_1 \omega & 5 < We < 80 \\
 k_1 \omega \sqrt{We} & 80 < We < 350 \\
 k_3 \omega We^{3/4} & 350 < We 
\end{cases} \] (13)

4.3. Turbulence Model

To account for the turbulence, the widely used two-equation models were used since they provide a good compromise between the numerical effort and computational accuracy. The \(k-\epsilon\) and the shear stress transport (SST) models were used to account for the turbulence effects. Using the \(k-\epsilon\) model occasionally led to convergence problems, which is when the SST model was implemented. The difference between the results obtained for both the models was negligible. Considering the \(k-\epsilon\) model in ANSYS-CFX 12.0, \(k\) is the turbulence kinetic energy and is defined as the variance of the fluctuations in velocity. It has dimensions of \((L^2,T^{-2})\); for example, \(m^2/s^2\). \(\epsilon\) is the turbulence eddy dissipation (the rate at which the velocity fluctuations dissipate), and has dimensions of \(k\) per unit time \((L^2,T^{-3})\); for example, \(m^2/s^3\) [1]. The \(k-\omega\) based SST model accounts for the transport of the turbulent shear stress and gives highly accurate predictions of the onset and the amount of flow separation under adverse pressure gradients [1]. The turbulence kinetic energy and dissipation transport equations for the \(k\)-epsilon model are given by,

\[ \frac{\partial k}{\partial t} + u_j \frac{\partial k}{\partial x_j} = \tau_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial}{\partial x_j} \left[ (\nu + \sigma_r) \frac{\partial k}{\partial x_j} \right] \] (14)

\[ \frac{\partial \epsilon}{\partial t} + u_j \frac{\partial \epsilon}{\partial x_j} = \alpha \frac{\epsilon}{k} \frac{\partial u_i}{\partial x_i} - \beta \frac{\epsilon^3}{k} + \frac{\partial}{\partial x_j} \left[ (\nu + \sigma_r) \frac{\partial \epsilon}{\partial x_j} \right] \] (15)

Where, \(\tau_{ij}\) is the stress tensor, \(\epsilon\) is the turbulence dissipation rate, \(k\) the turbulence kinetic energy and \(\nu_r = \frac{c_p k^2}{\epsilon}\) is the eddy viscosity.

The constants are \(c_p = 0.09, \alpha = 1.44, \beta = 1.92, \sigma_k = 1.0, \sigma_r = 1.3\).
To account for the effect of turbulence dispersion the turbulence structure of the gas flow is modeled by a random process along the droplet trajectories [21]. In turbulent tracking, the instantaneous fluid velocity is decomposed into mean and fluctuating components,

$$ U_f = u_f + u'_f $$

(16)

Now particle trajectories are not deterministic and two identical particles, injected from a single point, at different times, may follow separate trajectories due to the random nature of the instantaneous fluid velocity. It is the fluctuating component of the fluid velocity, which causes the dispersion of particles in a turbulent flow [1]. The model of turbulent dispersion in particles that is used in ANSYS CFX 12.0 assumes that the particle is always within one single turbulent eddy. Each eddy has a characteristic fluctuating velocity $u'_f$, lifetime, $\tau_e$, and length, $l_e$. When a particle enters the eddy, the fluctuating velocity for that eddy is added to the local mean fluid velocity to obtain the instantaneous fluid velocity. The turbulent fluid velocity, $v_f$, is assumed to prevail as long as the particle/eddy interaction time is less than the eddy lifetime and the displacement of the particle relative to the eddy is less than the eddy length. If either of these conditions is exceeded, the particle is assumed to be entering a new eddy with new characteristic $u'_f$, $\tau_e$, and $l_e$.

The turbulent velocity, eddy and length and lifetime are calculated based on the local turbulence properties of the flow:

$$ u'_f = \Gamma \left( \frac{2k}{3} \right)^{0.5} $$

(17)

$$ l_e = C_k^{0.35} k^{1.5} $$

(18)

$$ \tau_e = \left( \frac{l_e}{2k/3} \right)^{0.5} $$

(19)

where, $k$ and $\varepsilon$ are the local kinetic energy and dissipation, respectively, and $C_k$ is the
turbulence constant and \( \Gamma \) represents random numbers with zero-mean, variance of one and normal distribution.

4.4. Wall Boundary Conditions

The Wall Boundary Conditions were assigned using GridGen. The boundary conditions for the pressure jet atomizer are depicted in Figure 8.1, and are as follows:

1. The top and bottom of the cylinder were assigned an opening boundary condition allowing for gas flow entrainment. An opening boundary condition allows the fluid to cross the boundary surface in either direction. For example, all of the fluid might flow into the domain at the opening, or all of the fluid might flow out of the domain, or a mixture of the two might occur. An opening boundary condition might be used where it is known that the fluid flows in both directions across the boundary [1].

2. The cylinder wall was assigned as a no slip and smooth boundary condition.

The particle injection region or the nozzle exit centre was located axially at 1cm from the top of the cylinder. This was done to eliminate the possible influence of the opening at the top of the cylinder. The initial droplet size in this case is equal to the nozzle diameter (blob method for primary atomization). The initial droplet injection velocity, spray angle and the spray mass flow rate were specified [21].
The wall boundary conditions for the air-blast atomizer model as shown in Figure 8.2. are as follows:

1. The air inlet allows the flow of air at a velocity of 84 m/s.

2. The fuel inlet and the outflow was an opening boundary condition with no pressure gradient. The fuel particles were injected at the centerline at 19mm from the nozzle opening.

3. Along with the nozzle axis that is assigned the symmetry boundary condition, there are two symmetry planes assigned on each side of the nozzle axis.

4. The atmosphere, wind and nozzle walls were assigned as a no-slip adiabatic wall.
4.5. Numerics

The first order upwind-based scheme was used for steady state results. It was observed that, the simulation results when compared to available second order high-resolution scheme results had negligible differences. The first order upwind scheme was used to accelerate convergence. The solutions at steady state or at each time scale for transient simulations of the flow field were assumed to be converged when the dimensionless mass and momentum residuals ratios were less than 0.0001. Running the simulations for convergence criteria of 0.00001 had negligible effects on the results.
4.6. Assumptions and Discrepancies

The simulation results obtained were somewhat close to the experimental results. Some of the factors that contributed towards the discrepancies stem from the following factors:

1. The conditions at which the numerical simulations were carried out for case studies 1a, 1b and 2 were conducted at different pressures and room temperature. The realistic conditions can be different from the conditions at which the simulations were carried out. For example, the spray velocity is very sensitive to the surrounding conditions and other uncertain experimental factors that cannot be included in the simulations.

2. The computations were not performed on a cluster or on high performance computers. The simulations took a long time to reach convergence because of the slow processor speed.

3. Empirically calculated spray angles and mass flow rates can be different from the realistic values.
5. RESULTS AND DISCUSSIONS OF THE STEADY STATE SPRAY DYNAMICS

The following presents and discusses the results of the numerical simulations for the cases 1a, 1b and 2 (refer to Table 2 section 4.1), cases 3a, 3b, 3c (refer to Table 3 section 4.1) and finally, case 4 i.e. the gas turbine combustion case. For cases 1a, 1b and 2, nitrogen (N$_2$) was used as the surrounding stationary, quiescent gas medium and JetA liquid fuel as the injected liquid. The gas chosen was in accordance with the gas phase combustion material available in the ANSYS-CFX 12.0 library. Grid independence was verified by comparing the results obtained with the medium and fine grid levels.

The results shown in this case are for the fine grid level. For cases 3a, 3b and 3c, air was used as the surrounding high speed gas medium and JetA liquid was injected at a low velocity. An unstructured tetrahedral grid was used in this case. The three cases had different operating pressures (case 3a – 1atm, case 3b – 10atm, case 3c – 14.8atm) however, the rest of the variables were kept constant as shown in Table 3. For the gas turbine chamber case (refer to Table 4 section 4.1) the operating pressure was 10MPa.

Two variants for the simulation of case 1 were performed, viz., ‘Case 1a’ and ‘Case 1b’ (refer to Table 2 section 4.1). All three cases have similar operating temperatures i.e. a spatially averaged temperature of 25 degrees. However, the operating pressure for case 1a is 1atm, case 1b is 10atm and case 2 is 14.8atm. After the liquid is injected from the nozzle, taking into account the high injection velocities, it takes a short time to reach steady state. For example, Wu et al [22] reported that the characteristic time for steady state in their tests is about 30ms.

While running steady state simulations for case study 1a, there were various convergence
problems encountered when the time scale was reduced below 0.25 seconds. Hence, the results presented for case 1a were obtained by running the simulations for a time scale of 0.5 and 0.25 seconds. However, while running simulations for case 1b the time scale was varied from 0.5 to 0.005 seconds. The physical time scale used for case 1b was 0.5s, 0.25s, 0.1s, 0.03s, 0.01s and 0.005s. The physical time scale used for case 2 was 0.25s, 0.1s, 0.03s, and 0.01s. For cases 3a, 3b, 3c and 4 the simulations were performed at a timescale of 2 seconds.

5.1. Particle Traveling Time and Distance

One of the important correlations that lead to interesting conclusions about the liquid jet/spray penetration depth is the particle traveling time and distance. The distance traveled by the jet depends on the drag force acting on the particles. Greater the drag force, higher the particle injection velocities required to overcome the drag force. Each particle representing a group of particles possessing the same characteristics, individually labeled by subscript 'p' is assumed to obey the following set of equations:

\[
\frac{dx_p}{dt} = u_p
\]  

\[
m_p \frac{du_p}{dt} = \frac{1}{8} \pi \rho_g d_p^2 C_D (U_g - u_p) |U_g - u_p|
\]

where \( x_p \) is the particle position, \( u_p \) is the particle velocity, \( m_p \) is the particle mass, \( \rho_g \) is the gas density and \( C_D \) is the drag coefficient. The droplet drag coefficient can be written as,

\[
C_D = \begin{cases} 
24(1 + 0.15 \Re_p^{0.687})/\Re_p & \text{for } 0.0 < \Re_p \leq 1000 \\
0.44 & \text{for } 1000 < \Re_p 
\end{cases}
\]

where \( \Re_p \) is defined as,

\[
\Re_p = \frac{\rho_g |U_g - u_p| d_p}{v_g}
\]
Thus, the drag force is proportional to the gas density $\rho_g$ and $\rho_g \sim p$ according to the ideal gas law. Hence, a larger drag force will decrease the liquid jet depth or the distance traveled by the particles. Figure 9a shows the comparison between JetA particle traveling time and JetA particle traveling distance for cases 1a and 1b at a physical time scale of 0.25s. As shown, for the same time scale, the liquid jet for case 1a penetrates or travels the same distance faster (0.001s) compared to case 1b (0.0052s). Excellent agreement was obtained between the simulation results and the experimental results for case 1a. However, the difference is that diesel fuel oil was used as the injected liquid in the experimental results as opposed to JetA liquid in the numerical simulations.

![Graph showing comparison between JetA particle traveling distance and time for cases 1a and 1b at a physical time scale of 0.25s.](image)

**Figure 9a. JetA Particle Traveling Distance Vs JetA Particle Traveling Time for cases 1a & 1b at a physical time scale of 0.25s**

Figure 9b shows the comparison between JetA particle traveling time and JetA particle traveling distance for cases 1b and 2 at a physical time scale of 0.1s. Similar to the results in
Figure 9a, for Figure 9b, for the same time scale, the spray in case 1b travels approximately the same distance in less time (0.0025s) compared to case 2 (0.00825s). At time scales of 0.25s and 0.1s, the time taken by the particles in case 1b to travel the same distance is 0.0052s and 0.0025s.

![JetA Particle Traveling Distance Vs JetA Particle Traveling Time](image)

**Figure 9b. JetA Particle Traveling Distance Vs JetA Particle Traveling Time for cases 1b & 2 at a physical time scale of 0.1s**

Since, the results for the particle traveling time and distance for case 1a at time scales of 0.5s and 0.25s are qualitatively similar and therefore, only results for case 1b at different time scale are presented.

5.2. Sauter Mean Diameter (SMD)

Figures 10a, 10b and 10c compare the SMD particle tracks for case 1a, case 1b and case 2 at a physical time scale of 0.25s. These figures clearly indicate the influence of back pressure on the liquid penetration depth. The two cases 1a and 1b have the same nozzle diameters.
(0.3mm), different injection velocities (122.2m/s & 102.5m/s respectively) and different back pressures (1atm and 10atm respectively). Case 3 has a nozzle diameter of 0.127mm, back pressure of 14.8atm and an injection velocity of 127m/s. While considering the same case, there was not much difference between the SMD particle tracks for time scales of 0.5s and 0.25s. The SMD particle tracks for cases 1a, 1b and 2 at time scales of 0.5s and 0.25s are qualitatively similar, and therefore only those at a time scale of 0.25s are shown. However, when the three cases (1a, 1b and 2) are compared to each other there is a significant amount of difference between the SMD particle tracks. This is attributed due to the difference in the back pressure (the pressure inside the chamber) between the two cases. The particles in case 1a travel a significant amount of distance downstream of the spray till they are broken down into fine droplets of extremely small diameters. As opposed to case 1a the particles in case 1b are broken down into fine droplets earlier downstream once they exit the nozzle. Also, due to the high back pressure compared to cases 1a and 1b the particles in case 2 are broken down into droplets almost immediately once they exit the nozzle. Hence, the back pressure plays an important role in predicting the distance traveled by the particles.

![Figure 10(a). SMD Particle Tracks for case 1a at a time scale of 0.25s](image-url)
According to Kleinstreuer et al. [21] the droplets with the smallest size lie in the peripheral region of the liquid jet cone. This is because the droplets at the periphery have larger gas-droplet slip velocities when compared to the droplets in the liquid jet or spray core where entrainment velocities exist. Thus, peripheral particles/droplets experience larger drag forces and higher Weber numbers. A new small droplet inherits a small amount of momentum of the parent droplet and thus are surpassed by the droplets in the core and left behind by the liquid jet/spray front [21]. In this thesis, the particle/droplet diameters could not be compared against the radial distance due to numerical errors.

Figure 10(b). SMD Particle Tracks for case 1b at a time scale of 0.25s

Figure 10(c). SMD Particle Tracks for case 2 at a time scale of 0.25s
Another observation was the dispersion of the particles along the radial distance. As opposed to case 1a, where the particles travel a considerable distance downstream of the nozzle and then spread out in the radial direction, in case 1b, the particles disperse along the radial distance prematurely, once injected from the nozzle. In case 2, since the diameter of the nozzle is less than half of the nozzle diameter in case 1a and 1b, the cone of the jet is smaller and narrower. A jet with low back pressure (1atm) such as that in case 1a, shows a long and thin cone compared to a jet with high back pressure (10atm & 14.8atm) in case 1b and case 2. Figure 10 compares the SMD against the axial distance for cases 1a and 1b at a time scale of 0.25s. As shown in Figure 11, in case 1a, the SMD remains constant (at a value i.e. equal to the nozzle diameter 0.3mm) till the jet reaches a distance of 0.018m from the nozzle and then starts reducing in size till it reaches a distance of 0.055m from the nozzle and eventually fluctuates around the value 5e-05 further downstream.

In case 1b, as shown in figure 11, the SMD does not fluctuate as significantly as it does in case 1a once the particles exit the nozzle. There is a steep drop in the SMD after a distance 0.02m from the nozzle and the values downstream are much smaller than that of case 1a. In both the cases, the primary break-up region, modeled by the blob method, is evident since the value of the SMD is equal to the exit diameter of the nozzle.
In addition to the comparison between two different cases, the SMD for the same case was compared at different time scales. For case 1a, the SMD was compared at time scales of 0.5s and 0.25s. Since, there were convergence problems encountered for case 1a at time scales below 0.25s, the results available for case 1a are limited to the above mentioned time scales. However, for case 1b the SMD was compared at time scales of 0.5s, 0.25s, 0.1s, 0.03s, 0.01s and 0.005s. Figures 12a and 12b show the variation of SMD for cases 1a and 1b respectively at different time scales.

**Figure 11. SMD along the axial distance for case 1a & 1b for a time scale of 0.25s**
For both the time scales (0.5s & 0.25s) the SMD in case 1a follows a similar trend after an axial distance of 0.018m from the nozzle exit. However, once the jet reaches a distance of 0.05m from the nozzle the SMD for a time scale of 0.25s decreases to a lower value than that at 0.5s. The SMD at a time scale of 0.5s fluctuates around a value of 0.0001m further downstream whereas, that at 0.25s fluctuates around a value of 5e-05. Considering case 1b, for all the time scales ranging from 0.5s to 0.005s the SMD follows a similar trend along the axial distance and fluctuates around a value of 2.5e-05.
Figure 12(b). SMD along the axial distance for case 1b at different time scales

Contour plots for cases 1a, 1b and 2 at time scales of 0.5s and 0.25s are qualitatively similar therefore only those at 0.25s for both the cases are shown. Figures 13a, 13b and 13c show the SMD contours on the symmetry (XY) plane of the cylinder for all three cases 1a, 1b and 2 respectively, at a time scale of 0.25s. All the figures show that the core flow, near the exit of the nozzle is predominantly associated with primary break-up followed by secondary break-up downstream of the spray. The residuals for cases 1a and 2 required less number of iterations to reach convergence compared to case 1b. The reason for this is unclear.
Figure 13(a). SMD contours (m) for Case 1a at a time scale of 0.25s

Figure 13(b). SMD contours (m) for Case 1b at a time scale of 0.25s

Figure 13(c). SMD contours (m) for Case 2 at a time scale of 0.25s
In the case of the air-blast atomizer, slower and incomplete atomization takes place in case 3a as shown in Figure 14a. As pressures increase, the secondary atomization takes place closer to the nozzle and at an increased rate. Additionally, the atomization effect dramatically increases as well. For lower pressures, the spray angle is higher compared to the spray angle for higher pressures.

Figure 14(a). Contour plot for JetA Liquid Fuel SMD for case 3a (1atm) using the air-blast atomizer

Figure 14(b). Contour plot for JetA Liquid Fuel SMD for case 3b (10atm) using the air-blast atomizer
5.3. Weber Number (We)

The following presents and discusses the results of the Weber number (We) for all three cases (refer to Table 2, Section 4.1). The sensitivity of different operating conditions or different cases on the Weber number is demonstrated. Figure 15a and 15b display a time scale variation for the Weber number measured along the axial distance for cases 1a and 1b.

In case 1a, the Weber numbers of the particles injected out of the nozzle is 150 for a time scale of 0.5s and 130 for a time scale of 0.25s. Since, $100 < \text{We} \leq 350$ the particles undergo a sheet stripping kind of break-up once injected out of the nozzle.
Figure 15(a). Time scale variation for Weber number measured along the axial distance for Case 1a

Further downstream at a distance of 0.02m from the nozzle the Weber number goes on decreasing and lies between the value of 55 and 90. Since, $50 < We \leq 100$, the particles lie in the bag and stamen regime of break-up. The bag break-up ($12 \leq We \leq 50$) is observed from 0.04m to 0.06m downstream of the nozzle. Eventually, the Weber reduces to a value of 0 to 15 at the exit of the cylinder, which is the vibrational break-up regime.
As opposed to case 1a, the Weber numbers encountered for case 1b had higher values once they were injected out of the nozzle. The Weber numbers range from 1100 for a time scale of 0.1s to 1550 for 0.005s at the nozzle exit. Since $\text{We} > 350$, the particles lie in the catastrophic break-up regime, i.e., the droplet/particle disintegrates immediately. The secondary break-up regime or catastrophic regime exists till an axial distance of 0.025m from the exit of the nozzle. The trends show that the Weber number for all the time scales vary from an average value of 1300 at the exit of the nozzle to 0 at a distance of 0.03m from the exit of the nozzle. Thus in terms of the Weber number, the life of the particle along the axial distance is short-lived. The other break-up regimes are not visible. The high values obtained for case 1b can be attributed due to the high back pressure. Liquid jets or sprays with high back pressure exhibit much higher Weber numbers. In Eq (2) the gas density is more dominating than the
slip velocity to produce a larger Weber number [21]. Thus, the particles/droplets in the liquid jet/spray break up into tiny particles/droplets very easily.

5.4. JetA Liquid Averaged Velocity

Larger drag forces decrease the liquid jet velocity. Hence, in a high back pressure environment, a larger velocity is needed to overcome the drag forces. Figures 16a, 16b and 16c display contours of JetA liquid Averaged Velocity for cases 1a, 1b and 2 respectively at a time scale of 0.25s. Comparing Figures 16a and 16b, it can be seen that, although the injection velocities for the two cases, i.e. cases 1a & 1b are approximately the same, the particles/droplets in case 1a disintegrate and break-up much slower than those in case 1b. As mentioned before, this is due to the different drag forces, which are proportional to the gas density $p$. Also, according to Kleinstreuer et al [21], the particles with lower velocities always lie in the outer or peripheral region surrounding the core.

In case 2 due to a high back pressure of 14.8atm the particles travel a very short distance and are almost negligible in size at the end/outlet of the cylinder.

Figure 16(a). JetA liquid averaged velocity for case 1a at a time scale of 0.25s
Wu et al [22] and Kleinstreuer et al [21] have experimentally and numerically resp., studied the behavior of the droplet/particle velocity along the radial distance. However, these studies do not discuss the behavior of the particle velocity along the axial distance.
Figure 17(a). JetA Liquid Average Velocity Vs Axial Distance for Cases 1a & 1b at a time scale of 0.25s

Figure 17a shows the variation of the particle-averaged velocity against the axial distance for cases 1a and 1b at a time scale of 0.25s. For Case 1a, the velocity gradually reduces from a value of 122.2 m/s at the nozzle exit to 60 m/s at the outlet of the cylinder. However, the trend repeats itself for cases of high back pressure where there is a steep drop in the velocity from 102 m/s at the nozzle exit to 12 m/s at the cylinder outlet for case 1b.

Figure 17b shows the variation of the particle averaged velocity against the axial distance for cases 1b and 2 for a time scale of 0.1s. In case 2, as opposed to case 1b, the drop in velocity is almost vertical because of the high back pressure.
Figure 17(b). JetA Liquid Average Velocity Vs Axial Distance for Cases 1b & 2 at a time scale of 0.1s

5.5. Turbulence Kinetic Energy

Figures 18a, 18b and 18c are contour plots for turbulence kinetic energy. During the interaction between droplets and gas, both the phases gain momentum from each other. In this case, a high speed liquid jet is injected into a quiescent gas atmosphere. Turbulence kinetic energy is mainly produced and transported by the shear stress on the gas caused by the momentum exchange. As shown in Figure 18a, case 1a produces much larger turbulent effects because of smaller gas densities. The gas densities, aforementioned, are directly proportional to the back pressure. Therefore, as shown in Figure 18b and 18c, for cases 1b and 2 respectively, the turbulence kinetic energy has a lower value compared to case 1a. This is because of the higher gas-phase density, i.e. by a factor of 10 and 14.8 in case 1b and case 2 respectively. The turbulence kinetic energy is more intense near the nozzle exit. Roughly
speaking, the turbulence kinetic energy is also intense closer to the axial centerline except that the kinetic energy along the centerline is smaller than the nearby side areas [21].

Figure 18(a). Turbulence Kinetic Energy for Case 1a at a time scale of 0.25s

Figure 18(b). Turbulence Kinetic Energy for Case 1b at a time scale of 0.005s

Figure 18(c). Turbulence Kinetic Energy for Case 2 at a time scale of 0.01s
Contradictory to the pressure jet atomizer, the turbulence kinetic energy in an air-blast atomizer had higher values downstream of the liquid jet as shown in Figures 19a, 19b and 19c. This is because the momentum exchange between the air and the fuel particles takes place downstream of the liquid jet. The fluid particles are accelerated during the secondary atomization regime resulting in a higher particle velocity downstream. The increase in particle number paired along with higher velocity downstream results in a higher turbulent energy. The magnitude of the turbulence kinetic energy is significantly lower (30-40 m$^2$/s$^2$) compared to the pressure jet atomizer (190-565 m$^2$/s$^2$). This is because the velocity of the jet injected from the nozzle in the pressure jet atomizer is higher (100-120 m/s) compared to the velocity at which the momentum exchange takes place for an air-blast atomizer.

![Contour plot for Turbulence Kinetic Energy for Case 3a (1atm) using the Air-blast atomizer](image)

**Figure 19(a).** Contour plot for Turbulence Kinetic Energy for Case 3a (1atm) using the Air-blast atomizer

As in the case of the pressure jet atomizer, the value of the turbulence kinetic energy increases with higher back pressure (see Figure 19b, 19c). Again, this is because the density of air increases with the increase in back pressure.
Figure 19(b). Contour plot for Turbulence Kinetic Energy for Case 3b (10atm) using the Air-blast atomizer

Figure 19(c). Contour plot for Turbulence Kinetic Energy for Case 3c (14.8atm) using the Air-blast atomizer

5.6. Gas Turbine Combustion Chamber Case

Figures 20a and 20b display the contours for the SMD and turbulence kinetic energy for the gas turbine combustion chamber case (refer Table 4 section 4.1). The back/chamber pressure in this case was 10MPa i.e. approximately 100atm. As observed, the region near the exit of the nozzle has a diameter equal to the exit diameter of the nozzle. The nozzle diameter goes
on decreasing further downstream. However, the length of the jet is relatively short and the liquid particles/droplets are not well dispersed in the radial direction as in the previous cases i.e. for pressures of 1.10 and 14.8 atm. The particles/droplets have to travel against the high drag force and are confined to a region that is close to the nozzle/cylinder axis. Once again, this can be attributed due to the high back pressure. The particles are reduced from maximum size of 3.6 mm to a minimum size of 0.36 mm. The jet atomizes completely by traveling a very small distance.

Figure 20(a) SMD Contours for the Gas Turbine Combustion Chamber Case (Chamber/Back Pressure 10MPa)

An interesting observation was the different ranges of the turbulence kinetic energy. So far, a similar trend has been observed regarding the magnitude of the turbulence kinetic energy. The trend has been that with an increase in back/chamber pressure, the magnitude of the turbulence kinetic energy has increased. The turbulence kinetic energy in case 3c (back pressure 14.8) has a maximum value of 30 m²/s². Even though the pressure in case 4 was increased to a significantly high value of 10 MPa (approximately 100 atm) there was an insignificant amount of rise in the turbulence kinetic energy. As shown in Figure 20b the
maximum value of the turbulent kinetic energy for case 4 is $38.62 \text{ m}^2/\text{s}^2$. Hence, there was a very small difference of $8.62 \text{ m}^2/\text{s}^2$ between the two cases (148 atm and 100 atm).

Figure 20(b) Turbulence Kinetic Energy Contours for the Gas Turbine Combustion Chamber Case (Chamber/Back Pressure 10MPa)
The pressure jet atomizer was numerically simulated using ANSYS-CFX 12.0 for three different flow conditions/cases. There were five different parameters, JetA particle traveling time, Sauter Mean Diameter (SMD), Weber Number (We) and turbulence kinetic energy.

For case 1a, which has the lowest back pressure of 1atm as compared to cases 1b and 2, the liquid jet/spray penetration depth is deeper and the time taken for the jet to penetrate is faster (see Figure 9a and 12a). As opposed to case 1a, in case 1b and 2 the liquid jet/spray penetration depth is shorter and the time taken is longer (see Figure 9b, 11 and 12b). This is because of the high back pressure. Due to the high back pressure, the gas density increases since the gas density is directly proportional to the pressure inside the chamber. This increases the drag force and the particles have to travel at a higher velocity to overcome the drag force. As pointed out by Kleinstreuer et al. [21], the particles reach equilibrium i.e. no break-up occurring, in much shorter distances (see Figure 10a, 10b and 10c) than under low back pressure due to the expedited break-up process brought about by an elevated back pressure.

For a low back pressure in case 1a, referring to Figure 14a, the particle Weber Number break-up regime ranges from sheet stripping kind of break-up (at the nozzle exit) to bag break-up (at the cylinder outlet). As shown in Figure 14b, for higher back pressure, in case 1b, the particles experience a catastrophic break-up regime due to high Weber Numbers. The Weber Numbers for the pressure jet and the air-blast atomizer were in the same range for all the cases.

All experimental measurements and numerical simulations so far compare the particle
velocity with the radial distance. In this thesis, the particle velocity was compared to the axial distance. Numerical errors were encountered in comparing the velocity to the radial distance. The trend in the particle velocity shows (see Figure 16a and 16b) that the particle velocity reduces with the axial distance.

The turbulence kinetic energy for the pressure jet atomizer is more intense near the exit of the nozzle due to the momentum transfer and shear stress experienced by the particles and the gas (see Figure 17a, 17b and 17c). However, as stated by Kleinstreuer et al [21] the kinetic energy along the nozzle axis is smaller than the nearby regions due to the lack of shear stress. Contradictory to the pressure jet atomizer, the turbulence kinetic energy was higher downstream of the liquid jet. There was a significant difference between the magnitudes of the turbulence kinetic energy for the two atomizers.

Simulation of the atomization process using an air-blast atomizer presents many challenges. The recommendations include:

1. The accuracy of the numerical model varies with chemical kinetic mechanisms, turbulence models, numerical schemes, grid topology, etc. It should be mentioned that the grid quality plays a crucial role in simulations success. The ANSYS-CFX 12.0 license at Embry-Riddle Aeronautical University has a limit for the number of nodes in a grid. Running simulations for a grid size of more than 512000 nodes are highly recommended.
2. It is recommended for future simulations, that a highly fine structured grid should be used and the simulations should be performed on a high performance computing cluster.
3. To study the atomization characteristics of biofuel, future work should be carried out by incorporating a blend of JetA liquid fuel along with biofuel.
4. Along with the atomization characteristics the next step would be to study the process of
5. Transient state analysis should be carried out since liquid jet/spray dynamics is a time evolution process.

6. A sophisticated multiphase model like the Eulerian-Lagrangian Spray Atomization model (ELSA) coupled along with Reynolds-Averaged Navier Stokes (RANS) should be performed to accurately model the atomization process. Performing large-eddy simulations (LES) and direct numerical simulations of gas-liquid two-phase flows for atomization and sprays would be extremely helpful and is highly recommended.

While noting that there is room for further improvements, this study shows that CFD numerical simulation of JetA liquid fuel jet atomization and break-up via ANSYS-CFX 12.0 can adequately supplement theory and experiment.
REFERENCES


