

Predictions of the Spray Characteristics of Model Gasoline, Ethanol and Ethanol-in Gasoline Fuel Blends

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ABSTRACT: This paper presents predictions of spray characteristics of model gasoline, ethanol gasoline-ethanol fuel blends. Fuel breakup models and correlations between flow patterns and droplet characteristics were adopted and implemented in OpenFOAM Computational Fluid Dynamics (CFD) modeling suite 1 for direct gasoline injector using a simple cylindrical mesh structure at constant volume. The Rosin Rammler distribution model was used to generate the number of spray particles injected into the cylinder. The spray modeling and atomization employed the use of blob sheet model and KH-RT model while the numerical technique for simulating atomization process by CFD included the use of governing equations such as Eulerian for gas phase, Lagrangian for disperse phase and turbulence modeling. Spray evolution at various energizing times particle density and The Sauter Mean Diameter (SMD) relationships and particle size distribution were studied in simulation mode. The results showed that with longer injection time frame and wider injection angle, the penetration width was wider and the penetration length deeper (longer) resulting in better atomization. Concerning particle density and its distribution, as number of particle increased, the density of clusters became smaller.

KEYWORDS: SMD, Cone angle, gasohol, fuel-bled, atomization, spray.

1. INTRODUCTION

The repeated breakup of bulk liquids into an ensemble of droplets, (sprays), commonly known as atomization, is a phenomenon that plays a key role in the field of combustion science and other fields such as agricultural irrigation pesticides application, fluid catalytic cracking, spray drying waste fuel reuse and medical applications. However, in spite of the plethora of studies and publications on the subject, some aspects such as mechanisms and process paths for primary breakup are either poorly understood or remain unresolved. Worse still the focus of the existing body of knowledge is on conventional liquid fuels such as diesel and gasoline thus providing the impetus for exploring other fuels and their hybrids either in real time or as model fuels.

Studies on spray properties of various blends at ambient conditions, and spatial analysis have been conducted. However, relative to studies on diesel and bio-ethanol, much less attention has been given to atomization and spray modeling of gasoline-ethanol fuel blends.

Research efforts regarding atomization of fuels are well reported in the open literature.

Ejim et al (2007) analyzed seven biodiesels as well as their binary and ternary blends at a constant temperature. The Sauter Mean Diameter (SMD) of droplet was reported but no attempt was made regarding correlation of injector geometry, fluid properties and atomization characteristics. In Lebas et al. (2009), the atomization characteristics of sprays in the dense zone was studied by Direct Numerical Simulation (DNS) and the Eulerian-Lagrangian Spray Atomization (ELSA) models. This contribution is purely a simulation study in which experimental data drawn from previous work was used for parameter estimation. Gao et al. (2007) studied the atomization and spray characteristics of gasoline, ethanol and various blends of gasoline and ethanol. In particular blends consists of 75% gasoline and 25% ethanol (E25), 50-50% blend of gasoline and Ethanol (E50), 25% gasoline and 75% ethanol (E75) were studied under various ambient conditions, by means of high-speed Schlieren photography. Results from the study show that at high pressures, spray development patterns are not significantly different for the various blends and the zero blends. However, spray trip penetration decreases and spray angle increases with increases in ethanol fraction in the blended fuel, at low pressure.

Although, the images clearly affirm the authors' position, they were silent on the basis for volume of ethanol in the blends that were studied. In Aleifens et al (2008), a study on the study development of gasoline, iso-octane and ethanol in a spark-ignition engine was presented. According to the authors, the spray characteristics of fuels differ between hot and cold engine operation to a large extent. Regarding spray development, slight differences were noticed among all fuels at an engine head temperature of 20°C. However, spray cone angle was found to have reduced considerably at an engine head temperature of 80°C. In Hassainpour and Ninesh (2009), computational fluid dynamics (CFD) code was adopted in a study of sprays in direct injection engines. The discrete droplet method, a statistical tool was employed for spray calculations by the authors. Based on experimental validation, the authors reported that spray penetration and emission characteristics are predicted better with modeling methodologies. Other authors such as Juang et al. (2010) explained the use of CFD in complex processes. A study of droplet-gas system configured in a three-dimensional model which accounted for atomization of parent droplets was reported in Lijuan et al. (2009). Deduction from this study, point to the air-to-liquid ratio in the effervescent atomizer as having strong influence on droplet size and distribution. Soybean oil methyl ester (SME) atomization was reported by Park et al. (2009), the results showed similar SMD distribution patterns for biodiesel and diesel in comparison with experimental droplet size distribution. Park et al. (2009b) studied conditions for atomization of soybean oil Methyl ester (SME) fuel, nozzle tip and SMD were calculated. SME physical properties were used as input in KIVA code (Torres and Trujilo, 2006) for the calculation of spray characteristics. Kim et al (2010) analyzed atomization performances of three fuels. Tip penetration of spray, width spray cone angle and SMD were determined by experiment and predicted by KIVA-3V code. Deductions from their study point to droplet size as being proportional to fuel physical properties. Microscopic droplets behavior of diesel and biodiesel was studied by Hung et al. (2010). The KIVA-3V code, the Taylor Analogy Breakup (TAB) model and its modifications were used as numerical tools for quantifying experimental results. Other relevant experimental studies are those of Shinjo and Umemura (2011), Zhoulang et al (2012), Lee and Park (2014), Cipolat and Valentim (2013), Theoretical and experimental injection spray characteristics were compared in a study Zhao et al. (2012). Moreover, most of them are local to diesel fuel sprays and biodiesel. Among this category are the contribution in Kawahara et al. (2004), Jiang et al. (2012), Vita and Alloca (2012), Li et al. (2014). The merit in using open source code is that it provides a platform for preliminary study. However, the task of adopting such codes vis-à-vis editing to suit specific situations can be very time consuming, besides the computer programming expertise that is required. In the last few years, research efforts geared towards broadening the

understanding of sprays, atomization and breakup have been reported in the open literature. In Xie et al (2015), an experimental study in the macroscopic spray characteristics of biodiesel and diesel was reported. Various blends of biodiesel and diesel ranging from 0% and 100% diesel was formulated and studied at five different injection pressures and ambient pressures, in a constant volume chamber and a high speed camera was used to capture spray images. Results from the study show that ambient and injection pressures have significant effects on spray characteristics. The contribution is purely experimental, requiring high precision gadgets and no attempt has made regarding correlations or modeling applications. Yoo et al. (2017) studied the atomization and breakup characteristics of liquid jets at various spray conditions, using the large eddy simulation approach. A combined Eulerian-Lagrangian approach was employed to describe the spray field dynamics. The liquid column and the droplet breakup processes were simulated using a Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) hybrid wave breakup model. Reasonable agreement between model predictions and experimental data was demonstrated by the authors. However, TVD Range-Kutta method was used to solve the modeling equation without recourse to CFD codes. In a related work, Garai et al (2017) reported an experimental investigation of spray characteristics of kerosene and ethanol-blended kerosene using a gas turbine hybrid atomizer. The breakup length, cone angle and stream width of the fuel stream were said to have been analyzed directly from backlit imaging for various fuel and air flow rates. It was concluded that breakup occurred earlier in the ethanol-blended kerosene. A study on the spray and combustion characteristics of bio-ethanol-gasoline blended fuel based on fuel temperature was reported in Park et al (2016). The bio-ethanol test fuel was blended at volume ratios of 10%, 20% and 100% while fuel temperature were set at -7.25°C and 35°C respectively. A visualization scheme that is similar to a high speed camera was used to capture spray images. The major conclusion from the study is that it is necessary to adjust the spray strategy and ignition timing to adopt bio-ethanol blended fuel as an alternative fuel. Ghahremani et al (2016) reported an experimental and theoretical study on spray behaviours of modified bio-ethanol fuel. They employed an unnamed atomization model to study spray atomization indicators such as Ohnesorg number, atomization index number and Sauter Mean Diameter and used a high speed visualization method for capturing spray images. The major conclusion is that increasing percentage of ethanol in the fuel blend results in increase in spray top penetration and decreases the projected spray area. Feng (2016), investigated the effects of ethanol and gasoline addition on the spray and atomization characteristics of diesel spray, in a constant volume chamber and at various ambient and injection pressures. The spray tip penetration and cone angle were extracted from spray evolution process

that was recorded with high spatial and time resolution system. The results showed that the spray breakup and atomization process was promoted as gasoline blending ratio increased as gasoline blending ratio increased. However, they were silent about the optimum blending ratio and the corresponding spray characteristics.

2. Modeling of Breakup and Atomization

2.1: Blob Sheet Model

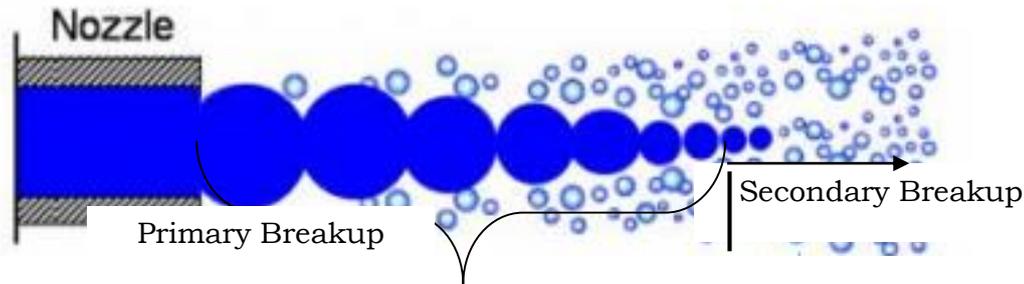


Figure 1: A typical representation of the blob-injection model

The model assumptions are:

- The length L_A :

$$L_A = C_1 \times L_t = C_2 \times L_w \quad (2)$$

The atomization scale is the linear sum of the turbulence and wave growth time scales:

Turbulence quantity dissipation rate is given as:

$$L_t^0 = C_\mu \frac{k_{avg}^{3/2}}{\varepsilon_{avg}} \quad (3)$$

$$\tau_t^0 = C_\mu \frac{k_{avg}}{\varepsilon_{avg}} \quad (4)$$

$C_\mu=0.09$ and the average quantities are estimated as:

$$k_{avg} = \frac{u^2}{8(L/D)} \left[\frac{1}{C_d} - k_c - (1-s^2) \right] \quad (5)$$

$$\varepsilon_{avg} = k_\varepsilon \frac{u^2}{2L} \left[\frac{1}{C_d} - k_c - (1-s^2) \right] \quad (6)$$

Turbulence length

$$L_t(t) = L_t^0 \left(1 + \frac{0.0828t}{\tau_t^0} \right)^{0.457} \quad (7)$$

Time scale

$$\tau_t(t) = \tau_t^0 + 0.0828t \quad (8)$$

The blob sheet model is presented in fig 1 and the breakup rate is given as:

$$\frac{dD_p}{dt} = k_l \frac{L_A}{\tau_A} \quad (1)$$

The proportionality constant k_l is subject to calibration,

L_A is the dominant length scale of atomization.

$$\text{Wave growth time scale } \tau_w = \frac{L_w}{U} \sqrt{\frac{\rho_L}{\rho_g}} \quad (9)$$

2.2: Wave Model

The wave model (KH model) is where the stability analysis of round liquid jets is developed. The droplet breakup (Kelvin–Helmholtz instability) of liquid jet has initial radius r and η_0 is an infinitesimal initial perturbation as shown in Fig 2.

Radius change of this droplet is calculated as:

$$\frac{dr}{dt} = \frac{r - r_{new}}{\tau_{bu}} \quad (10)$$

Where, τ_{bu} is the characteristic breakup time scale defined by:

$$\tau_{bu} = 3.788 B_1 \frac{r}{\Lambda \Omega} \quad (11)$$

And the new droplet radius given as;

$$r_{new} = B_0 \Lambda \quad (12)$$

Where B_0 and B_1 are constants

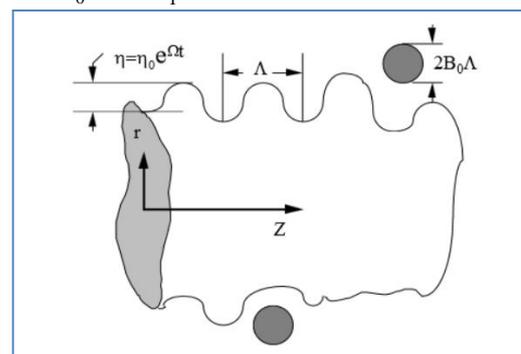


Figure 2: Kelvin–Helmholtz model

$$B_0 \Lambda \leq r \quad (13)$$

Maximum growth rate

$$\Omega = \frac{0.34 + 0.38 We_g^{1.5}}{(1+z)(1+1.4T^{0.6})} \left[\frac{\sigma}{\rho_l r^3} \right]^{0.5} \quad (14)$$

Wavelength

$$\Lambda = 9.02r \frac{(1+0.45Z^{0.5})(1+0.4T^{0.7})}{(1+0.865We_g^{1.67})^{0.6}} \quad (15)$$

Where, $Z = \frac{\sqrt{We_l}}{Re_l} = \frac{\mu_l}{\sqrt{\rho_l r \sigma}}$ Ohnesorge number,

$T = Z \sqrt{We_g}$ Taylor number, and $We_g = \frac{\rho_g r u_{rel}^2}{\sigma}$ and

$We_l = \frac{\rho_l r u_{rel}^2}{\sigma}$ are gas and liquid Weber numbers,

respectively and u_{rel} velocity of liquid droplet relation to stationary gas phase (Beale and Reitz, 1999).

2.3: KH-RT Model

This model consists of two modes of breakup: The Kelvin-Helmholtz (KH) breakup which accounts for instability in the waves growing and Rayleigh-Taylor (RT) breakup. KH instability model .Rayleigh-Taylor (RT) breakup is governed by the rapidly growing disturbances on the surface of the droplet. Wave, Ω_{RT} wavelength, Λ_{RT} were given in equation (16) and (17), respectively:

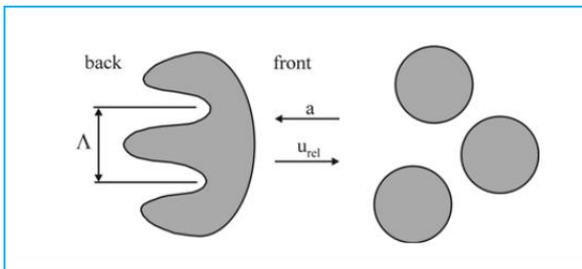


Figure 3: Rayleigh-Taylor (RT) instability.

$$\Omega_{RT} = \sqrt{\frac{2[a_d(\rho_l - \rho_g)]^{1.5}}{3\sqrt{3}\sigma(\rho_l + \rho_g)}} \quad (16)$$

$$\Lambda_{RT} = 2\pi C_{RT} \sqrt{\frac{3\sigma}{a_d(\rho_l - \rho_g)}} \quad (17)$$

$$a_d = \frac{3}{8} C_d \left(\frac{\rho_g u_{rel}^2}{\rho_l r} \right) \quad (18)$$

Where, a_d is the droplet acceleration, C_d is the injector nozzle's discharge coefficient and C_{RT} is the modeling parameter.

The breakup time scale is expressed as:

$$\tau_{RT} = \frac{C_1}{\Omega_{RT}} \quad (19)$$

Where, C_1 is the modeling constant. When the growth time exceeds the characteristic Rayleigh-Taylor (RT) time, breakup occurs and the droplet is converted into parcels of smaller droplets. The new droplets formed are taken to be of uniform diameter.

3. COMPUTATIONAL FRAMEWORK

The spray injected into a constant volume cylinder is simulated using the Eulerian-Lagrangian approach. Small computational cells composing Meshes (8900) with fluid density, velocity, pressure and enthalpy were computed and stored on each computation cell. Gas (continuous) is simulated using the Eulerian formulation in Reynolds-Averaged Navier-Stokes (RANS) equation alongside Realizable k-ε turbulence model which accounts for effect of turbulence fluctuations in the fluid phase. Similarly, the liquid (discrete or disperse) phase is treated using a Lagrangian formulation together with spray sub-models. The density, surface tension and viscosity of gasoline and ethanol fuels were computed internally and imported as input data. The inlet and exit temperatures and pressures were defined. A cylindrical system with consideration of all boundaries as walls and mesh coordinates were set to be symmetrical with an assumption of no heat loss. The mesh generation was taken to be one-quarter of a cylinder which was simulated by defining the process to be a transient compressible system where there were variations of pressure.

The reason for assuming symmetry in the cylinder is the use of cone injector model, hence it is considered a hollow injector atomizer so it can be symmetrical at 45°C per cross section. The inner nozzle diameter which was obtained from standard nozzle design is taken to be 100µm. The study of spray characteristics of gasoline fuel ((G100) - C₇H₁₆) was done by simulation using OpenFOAM source code which runs on Linux platform. This analysis was effected using SimFlow to generate meshes for the simulation and run. The mesh and results files were saved to the OpenFOAM file format and visualized in ParaView software. Further analysis was done with MatLab by saving in the MatLab directory. In the simulation, only a quarter of cylinder was used in the simulation. Two of the boundaries were set to symmetry and the remaining boundary set to wall. The spray foam solver is the solver type that was used to simulate a transient, compressible, reacting and non-combustible fuel injection process. High pressured fuel at 5MPa at 300°K was injected into high temperature (800°K) stagnant air at a velocity of 100m/s. The Turbulence Model of RANS - Realizable k-ε model, with heat transfer model of Ranz-Marshall as well as phase change model which is

liquid evaporation-boil model was adopted in boundary interaction (rebound) in secondary atomization.

The result files generated in SimFlow/OpenFOAM were post processed in ParaView. The Figures 4.a - d, show the images of the spray development for model Gasoline (G100) fuel.

4. RESULTS AND DISCUSSION

4.1 Spray Evolution of the Gasoline (G100) Fuel

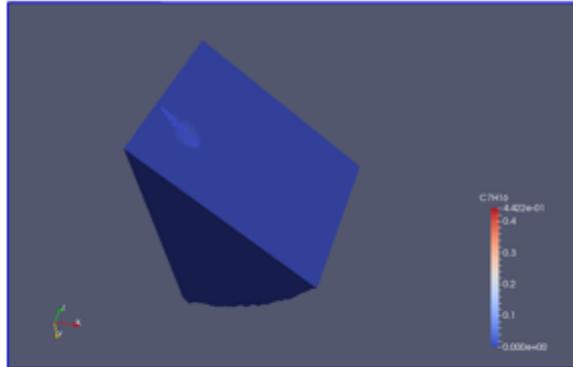


Figure 4.a: Energizing time (0.00015μs)

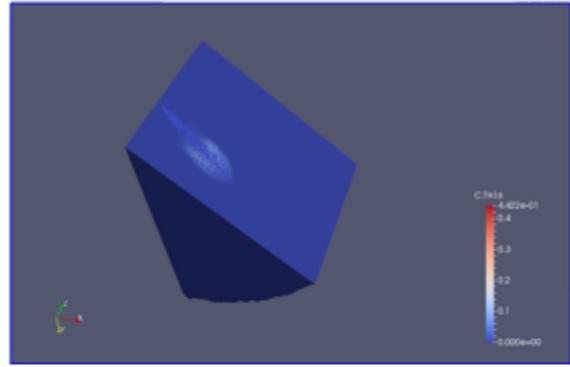


Figure 4.b Energizing time (0.00032μs)

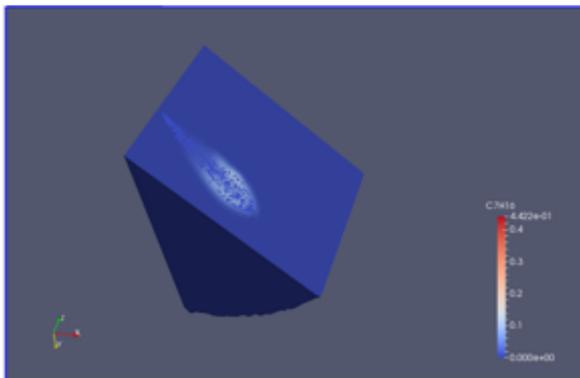


Figure 4.c: Energizing time (0.000445μs)

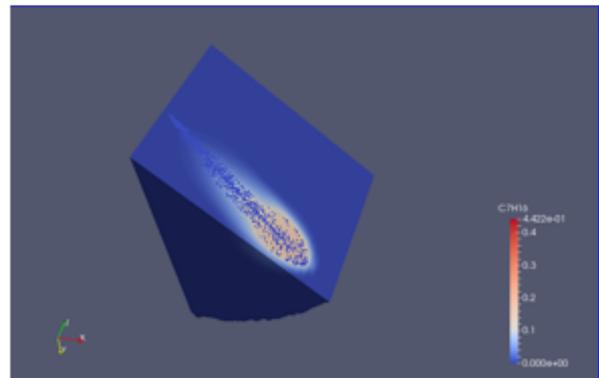


Figure 4.d Energizing time (0.0008μs)

4.2. Spray Evolution at four Cone Injection Angles at time steps of 0.0001μs, 0.0002μs, 0.0003μs and 0.00075μs respectively: Figure 5a to 5d show the spray evolution at four cone injection angles (20°, 30°, 40° and 50°) at time steps of 0.0001μs, 0.0002μs, 0.0003μs and 0.00075μs. This injection process represents time frame of injection with respect to injection angular variations. It could be deduced from the figures that with longer injection time frame and wider injection angle, the penetration width was wider and the penetration length deeper (longer) resulting in better atomization.

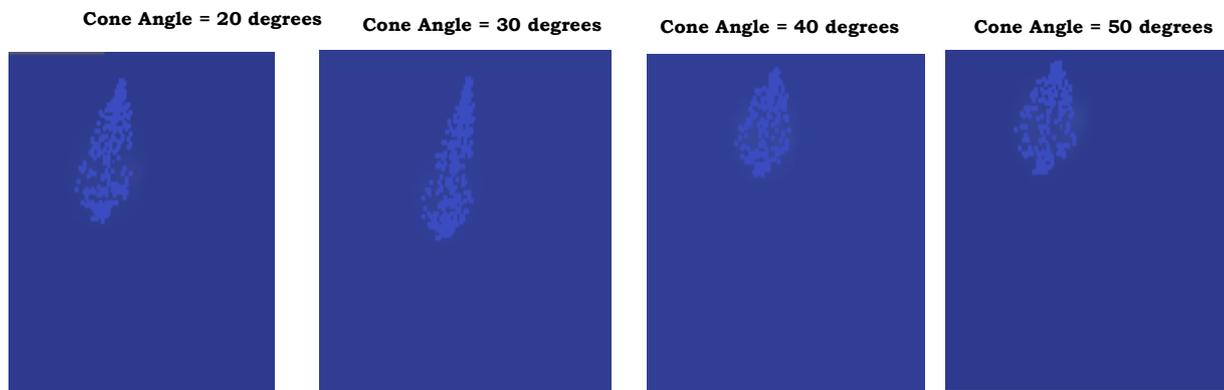


Fig 5a. 0.0001 μs after injection

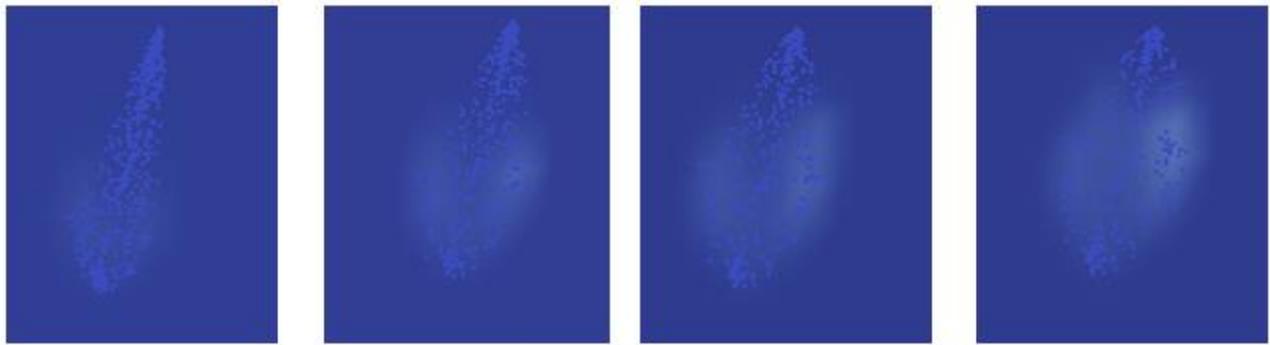


Fig 5b. 0.0002 μ s After Injection

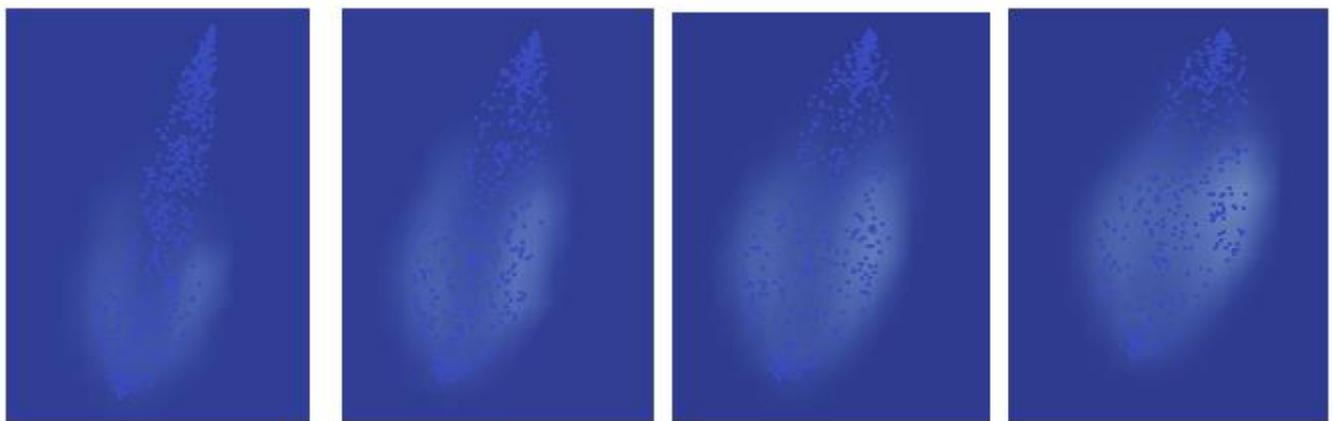


Fig 5c. 0.0003 μ s After Injection

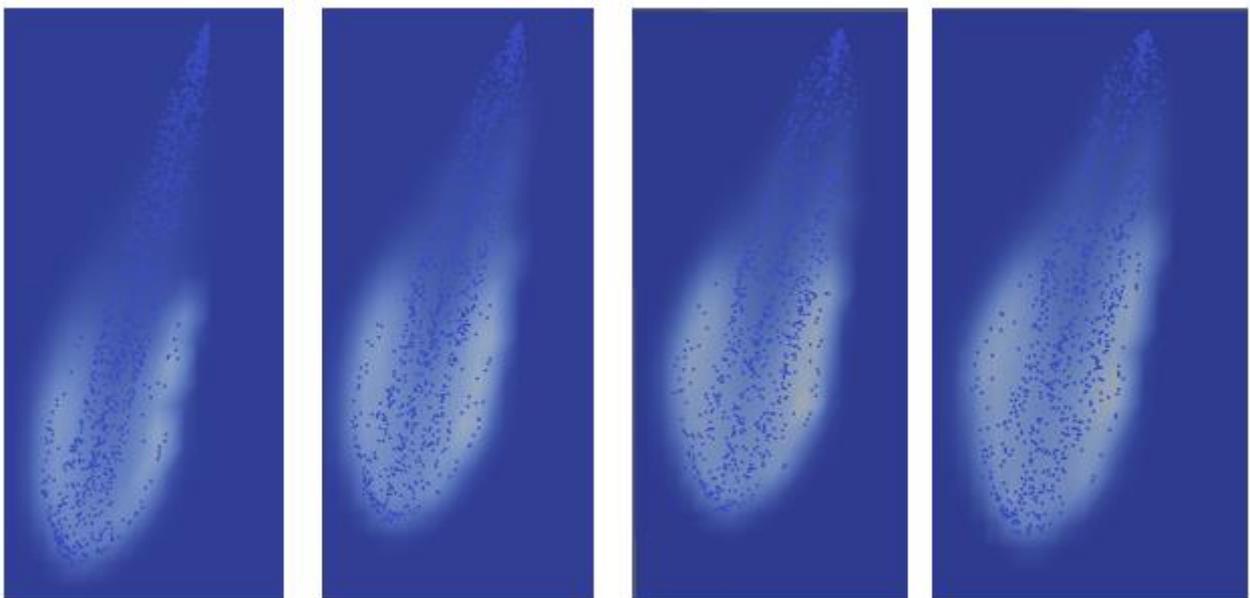


Fig 5d. 0.00075 μ s After Injection

4.3: Other Spray characteristics

Figure 6 shows the droplet diameter against number of particles. It indicates that as the droplet diameter increases the particles density decreases. This suggests that where the particle size is small the electrostatic force of attraction between them increases because the ionic radii becomes small. The droplet diameter increases up to 1.75×10^{-5} m after which it drops because the particle density even in this

range decreases. Most of the particle pumped will go out with the exhaust as without combustion taking place beyond this point which indicates that it will be waste of fuel hereafter. Again, according to figure 6, when the particle diameter is small the voidage between particles are small, hence particles tend to cluster in a particular zone. As the diameter increases, the density of the clusters become smaller. The number of particles increases while the particle

density decreases as a result of atomization. It peaks at diameter between 1.5 and 2.0 μm at particle range of 45. Beyond this point the particle density begins to build again due to coalescence. Hence the curve is a normal distribution curve which is skewed a little. The apex of this plot shows some noise before the plot descends downwards. The Rosin Rammler distribution model was used to generate the number of spray particles injected into the cylinder as shown in figure 7. Rosin Rammler distribution is adopted because its well suited for spray atomization distributions. The Rosin Rammler cumulative particle size distribution plot for spray droplets shows that with an exponential rise in the particle diameter, the cumulative effect increases which shows that there will be better combustion up to the pick $2 \times 10^{-5}\text{m}$ of droplet diameter. This figure 7 is derived from figure 6 and it is the summation of particle diameter over the range of number of particles. The curve is exponentially distributed. Figure 8 is the injected droplets profile with time at pressure of 5MPa. This plot shows the engine performance in terms of atomization. From the zero axis between 0.00 to 0.5 μs , the number of injected droplet, up to 6000 increased linearly. This means that in this region injected parcels were proportional to time of energizing (μs). Inference here is that the more the number of droplets injected the more atomization took place. Beyond this point the curve became somewhat wavy in a plateau form. This graph shows the effectiveness of atomization within a short period of time of 0.5 – 1 μs when atomization takes place close to 7000 injected droplet particles. The most essential

range to assess the extent of atomization of fuel is therefore 7000 droplet particles released into the combustion chamber. Beyond this time there is only a marginal increase in the number of particle. Figure 9 shows the Sauter mean diameter (SMD) at injection pressure of 5MPa and injection cone angle of 20°. Sauter mean diameter (SMD) decays exponentially from 100 to 50 μm shows SMD drops and experiences decay exponentially in time interval between 0 and 1000 μs . From 50 μm down to 40 μm , the SMD drops sharply- linearly and then from 40 μm to 20 μm displays negative exponential curve and does not experience any further change beyond 2000 μs . The observed trend alludes to the fact that SMD is insensitive to change with time in the value ranges of 2000 μs to 5000 μs . Despite the cone injection angle variation of 20°, 30°, 40° and 50°, the SMD profile behaves similarly with varying energizing times at 5mPa injection pressure as in figure 9. Figure 10 just like fig 9 shows four distinct atomization regimes. Reading the plot in fig 9 from the y axis show that injection angle of 30°, 40°, 50° and 20° present better atomization in that order in relation to 250 μs time after injection. Between 250 μs and 1000 μs time after injection atomization rate shows differently by presenting 30°, 20°, 40° and 50° in that order, but from 1000 μs to 1700 μs injection angles depict that 20° atomizes most, followed sequentially by 30°, 40° and 50°. The fourth and final distinct regime show that from injection time of 1750 μs through 5000 μs atomization is dominated by angular injection in the following pattern 50°, 40°, 30° and 20°.

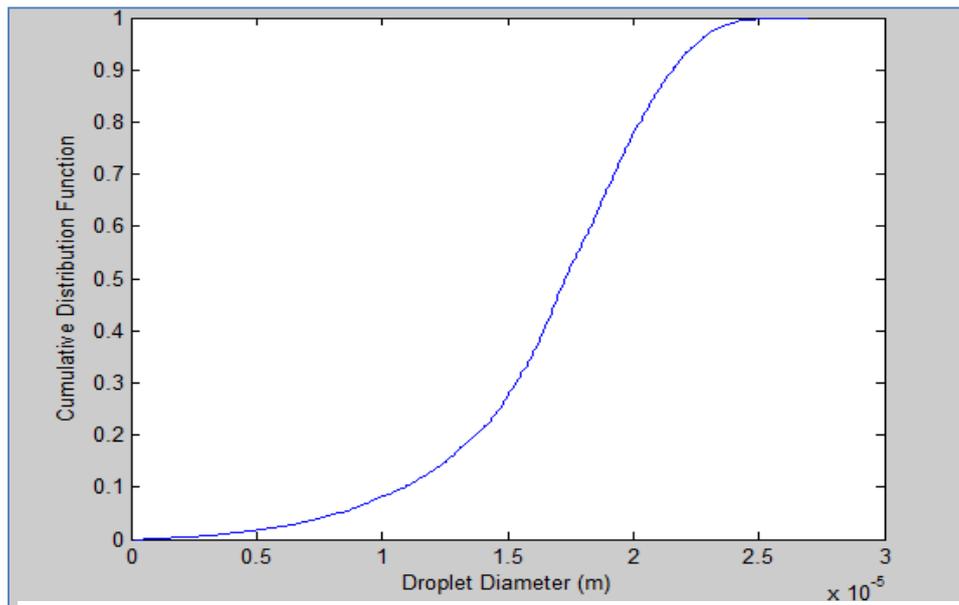


Figure 6. G100 Droplet size distribution at 5.0e-3(ms) after energizing

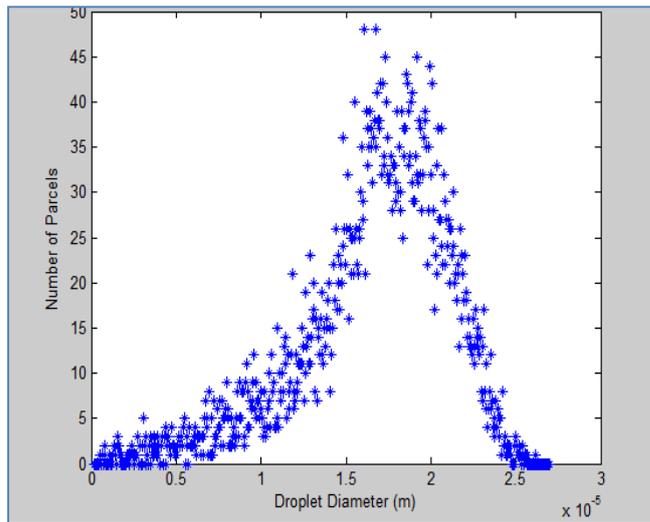


Figure 7: Rosin Rammler Distribution for the Spray droplets at 5µs after energizing.

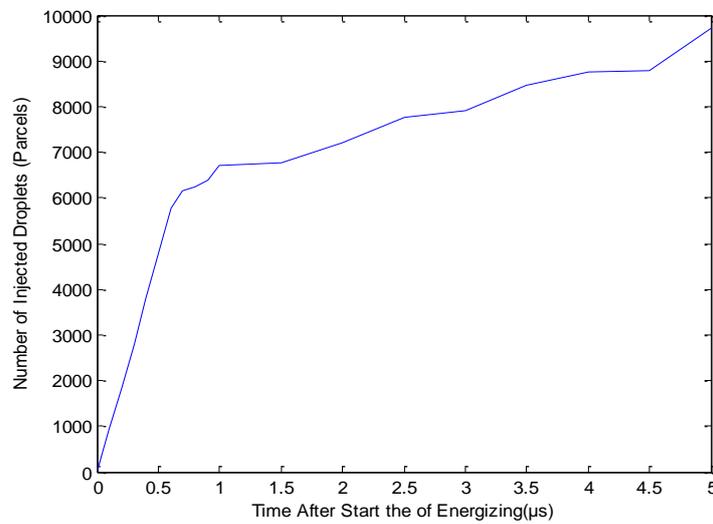


Figure 8: Injected droplets profile with time at pressure of 5MPa

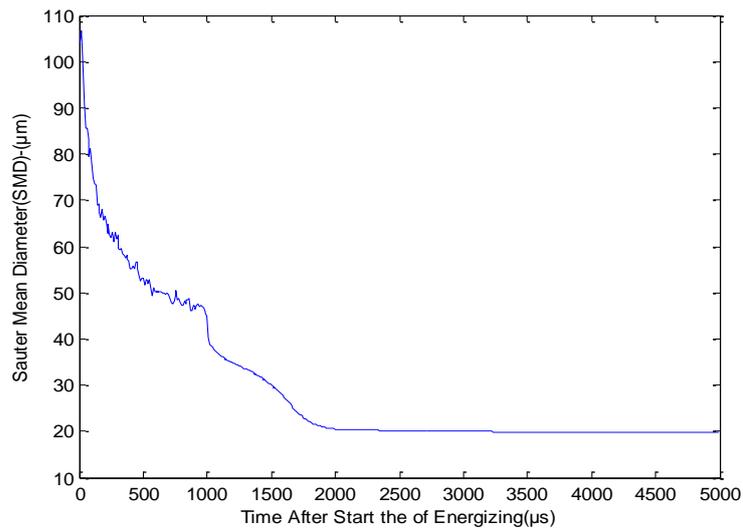


Figure 9: Sauter Mean Diameter (SMD) at injection pressure of 5MPa and injection cone angle of 20°

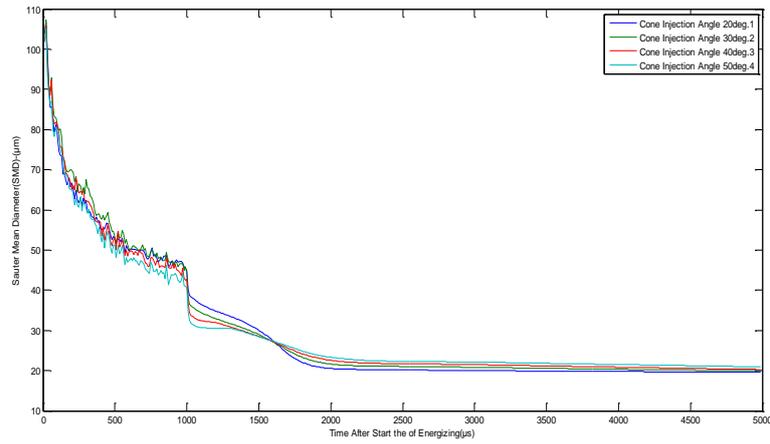


Figure 10: Sauter Mean Diameter (SMD) at injection pressure of 5MPa for four cone injection angles for gasoline

5. CONCLUSION

Predictions on the spray characteristics of model gasoline fuels and its hybrids have been presented in this paper. The observed trends revealed some valuable insights in the understanding of atomization as a precursor to combustion. It is hoped that the opinions expressed in this paper would serve as corner stones for further computation fluid dynamics (CFD) investigations around the domain of model fuels as against financially burdensome experimental investigations that demand high precision equipment. .

6: NOTATION

CFD	Computation fluid dynamics
DDM	Discrete Droplet Method
DNS	Direct Numerical Simulation
E100	Ethanol fuel
E15	15-85 % Ethanol-Gasoline blended fuel
E50	50-50 % Ethanol-Gasoline blended fuel
E85	85-15 % Ethanol-Gasoline blended fuel
ELSA	Eulerian-Lagrangian Spray Atomization
<i>F</i>	The external forces
G100	Gasoline fuel
GASHOL	Gasoline-ethanol fuels
<i>k</i>	Kinetic energy
<i>k_c</i>	Constant taking into account losses in contraction corner
<i>k-H</i>	Kelvin-Helmholtz
<i>L, D</i>	Nozzle length and diameter, ,
LES	Large Eddy Simulation
LISA	Linearized Instability Sheet Atomization
LPT	Lagrangian Particle Tracking
RANS	Reynolds Averaged Navier-Stokes
RT	Rayleigh-Taylor
<i>S</i>	Area ratio at the nozzle contraction
SMD	Sauter Mean Diameter
SME	Soybean oil methyl ester
TAB	Taylor Analogy Breakup
TAB	Taylor Analogy Breakup
3D	Three dimensional

<i>c</i>	Damping parameter
<i>d</i>	particle diameter,
<i>f(d)</i>	Probability density function of <i>d</i>
<i>k</i>	Wave number
<i>m(t)</i>	Mass of the product droplet distribution
<i>r</i>	Droplet radius
<i>t</i>	Time after start of injection,
<i>x</i>	Displacement
<i>a_d</i>	Droplet acceleration
<i>B₀, B₁</i>	Constants and the drop radius decreases
<i>C_d</i>	Nozzle discharge coefficient,
<i>C_D</i>	Drag coefficient
<i>C_d</i>	Injector nozzle's discharge coefficient
<i>C_{RT}</i>	Modeling parameter
<i>C_b, C_d, C_f, C_k</i>	Dimensionless constants,
<i>d_{max}, d_{min}</i>	Maximum and minimum droplets diameters
<i>d_{inj}</i>	Injector nozzle diameter
<i>F_D</i>	Drag force,
<i>k_s</i>	Spring's constant
<i>k_{max}</i>	Wave number corresponding to the maximum growth rate
<i>k_ε</i>	Constant for average turbulent energy dissipation, set to 0.27,
<i>K_{br}</i>	Constant – breakup regime
<i>P_a</i>	Ambient gas pressure,
<i>P_{inj}</i>	Fuel injection pressure,
<i>S₁, S₂</i>	Spray tip penetration lengths before and after breakup.

t_b	Breakup time,
μ_t	Turbulent viscosity
ε	Turbulence dissipation
$\overline{\Omega_{ij}}$	Mean rate-of-rotation tensor
ω_k	Angular velocity
ρ_L	Fuel density
ρ_a	Ambient gas density,
θ	Spray cone angle, and
ρ_g, ρ_l, σ	Gas and liquid densities and surface tension
ω_{\max}, h_b	Sheet thickness at the breakup location
ω_{\max}	Maximum growth rate
ρ_r	Air-fuel density ratio
μ	Velocity

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