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NUMERICAL DROPLET DISTRIBUTION FOR ETHANOL SPRAY WITH OPENFOAM

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Abstract. *Internal combustion engines are thermal machines that convert chemical energy contained in a fuel into mechanical energy, using combustion and a mechanical system. Because of their simplicity, ruggedness and high power/weight ratio, internal combustion engine has been responsible for supplying a significant portion of energy generation required for the daily life of our society. The new high-end concept of mixture formation for SI engine has been using a Direct Injection System, accordingly the fuel is delivered with high pressure into the combustion chamber, especially on the compression stage. The use of atomizers to deliver fluids require that the drop size distribution must have a particular form with narrow, wide, few large drops, few small drops, among others for optimal operation. No fundamental mechanism or model enables a theory on particle-size distribution to be built, consequently, a wide variety of empirical models or equations have been proposed to characterize experimental particle-size distributions, such as the Rosin Rammler model. In order to understand and analyze the numerical modeling of these phenomena, this paper illustrates the review of two available methods for modeling drop size distributions in fuel spray: the empirical classical method and Rosin Rammler method. A numerical investigation was carried out using the capabilities of OpenFoam code to evaluate the characteristic form of the fluid in the spray. The results shown that both distributions are well implemented in the software, compared to the literature. The work demonstrate that the Rosin Rammler model better reproduce the Spray droplets distribution.*

Keywords: *OpenFoam, Rosin Rammler, Ethanol, Direct Injection, Internal combustion engines*

1. INTRODUCTION

The economic development model adopted by most countries in the world requires efficient transport of goods and people between cities and also different regions of a country. This led to the rapid growth in the number of vehicles in almost all industrialized countries. Today most current vehicles use internal combustion engines which consume fossil fuels. This energy source is a nonrenewable natural resource that pollutes the planet's atmosphere mainly, among other problems, causing the phenomenon called greenhouse gases responsible for global warming.

Direct injected spray ignition engines are currently developed in industry with the objective to improve simultaneously fuel economy and performances, overcoming disadvantages associated with intake throttling in part load operation. The design and the optimization of the combustion system of direct injected spray ignition engines require many efforts due to the stratified charge working condition. Thus, the mixture preparation is a very important task and, consequently, the spray evolution and the droplets break-up process, combined with the air motion in the combustion chamber, are too Allocca (2002).

Multidimensional models for computing fuel spray dynamics have been under development for more two decades. Among the models, the Lagrangian stochastic method has been demonstrated to be computationally efficient and successful in ethanol spray predictions. This method solves the governing equations for the gas phase and the interactions between the liquid drops and the gas phase. To compute spray dynamics, discrete drops are introduced into the

computation stochastically in the form of groups or parcels of particles, and each computational parcel represents a number of droplets of identical size, velocity, and temperature.

In the computations, a model is needed to provide the drops size and size distribution information off the atomized liquid jet or sheet, and models are required to calculate the subsequent drop breakup process. Much progress has been made in modeling of the atomization processes of jet sprays. Reitz (1997) has established a methodology to model jet atomization processes in which blobs are injected with characteristic size equal to the nozzle hole diameter and the subsequent breakup of the blobs and drops is computed by a model based on the linear stability analysis of liquid jets. Han (1997)

Babinsky (2002) studied the classical method of modeling drop size distributions is empirical: a curve is fit to data collected for a wide range of atomizer nozzles and operating conditions. Curves appearing frequently become the basis for standard empirical distributions; given a sizable collection of such distributions one can be fairly certain to locate a form that fits virtually any non-pathological data set. The problem with this approach is the difficulty of extrapolating the data to operating regimes outside the experimental range. With-out additional experimentation, one can never be certain whether the extrapolated empirical correlation applies to the regime of interest; unfortunately, additional experimentation is often impractical, impossible, or prohibitively expensive.

A computational model and an experimental analysis have been performed to study the atomization processes of hollow cone fuel sprays from a high pressure swirl injector for ethanol direct injection engines. The objective has been to obtain reliable simulations and better understood structure and evolution of the spray and its interaction with air the flow field. Computed and measured spray characteristics, such main-spray structure, tip penetration and break-up phenomena, have been compared, achieving good levels of agreement.

The Computational Fluid Dynamics, CFD, has developed to the point where the complete three dimensional flow field over the vehicle and through engines can be computed expeditiously with accuracy and reliability. To achieve this requirement, the industry must investigate a range of factors that can potentially reduce engine emissions, including fuels, combustion process, chemical-kinetics, in-cylinder flow, fuel-air mixture formation, sprays, engine geometries, etc. Nowadays, computational simulations have been adopted as a key analysis tool in engine research to establish correlation with experimental studies and provide new information for designers. A significant advantage of using Computational Fluid Dynamics is the flexibility of simulation setups and the time and cost efficiencies compared to experiments. Major CFD commercial codes that are available in the market currently include Ansys CFX, Ansys Fluent, AVL Fire and CD-adapco Star-CD and Star-CCM+, whereas OpenFOAM has been chosen in this study to take advantage of its ability to simulate general flow problems. It offers different kinds of models to evaluate engine characteristics (Senthilnathan 2015).

The motivations of this project is to understand the functionality and utility of the CFD code OpenFoam in spray simulations.

2. HOLLOW CONE SPRAY MODEL

Baumgarten (2006) stated the properties and behavior of all droplets in the spray can be approximately represented by these discrete droplets. Nevertheless, in order to have the correct fuel mass in the cylinder, the mass of all droplets must be regarded. This is why every representative droplet gets a number of further droplets with identical size, temperature and velocity components etc., who have exactly the same behavior and properties like the representative one. These groups of equal droplets are called parcels.

In case of a hollow cone spray, an annular liquid sheet is produced at the nozzle orifice forming a free cone-shaped liquid sheet that disintegrates into droplets. There are several ways to describe the distribution of the particles during this stage, such as Rosin-Rammler distribution and the Exponential function, which will be discuss later on this work.

Secondary breakup models are designed to simulate the formation of smaller droplets in the downstream of a spray. The secondary break-up can be approximated to a processes of continue reduction of the radius of the droplet, Eq. 1, this is known as the Reitz-Diwakar model.

$$\frac{dr}{dt} = -\frac{r - r_{\mathrm{RD}}}{\tau_{\mathrm{RD}}} \tag{1}$$

The Eq. 1 follows the empirical equations Eq. 2 and Eq. 3 when $We_g > 0.5\sqrt{Re_g}$, Eq. 4 and Eq. 5 when $6 < We_g < 0.5\sqrt{Re}$ and the droplet radius is assumed to be constant if $We_g < 6$.

$$\tau_{\mathrm{RD}} = B_{\mathrm{RD}} \frac{r}{U} \sqrt{\frac{\rho_f}{\rho_g}} \tag{2}$$

$$r_{\mathrm{RD}} = \frac{\sigma^2}{2\rho_g U^3 \nu_g} \tag{3}$$

$$\tau_{\mathrm{RD}} = \pi \sqrt{\frac{\rho_f r^3}{2\sigma}} \tag{4}$$

$$r_{\mathrm{RD}} = \frac{6\sigma}{\rho_g U^2} \tag{5}$$

We and Re are the Weber and Reynolds number, respectively, both of which calculated for the gas phase. ρ is the density and σ is the surface tension coefficient of the fuel, ν is the kinematic viscosity, U is the magnitude of the gas velocity vector with respect to the droplet, and the subscripts g and f designate the gas and liquid fuel, respectively. The default value of the constant BRD is 20 (Chen Huang, 2014).

3. METODOLOGY

There are several methods to introduce particles in the system. In sprayFoam the particles are introduced through the injectors, with according settings specified by the user. It is important to note that in this work it was used an atmosphere pressurized chamber to simulate the Spray. Three simulation was made for two different Probability Density Function (PDF), two for the Rosin-Rammler and one for the Exponential function.

The geometry of the chamber, the mesh and pre-processing was with the software OpenFoam. The Image post-processing was done with the ParaView software and the raw data was treated with Microsoft Excel.

3.1 Geometry and Mesh

The geometry was specified to be a rectangular prism with the dimension 40x100x40 mm with the average cell size of 1mm. This was based from Mayer, R. L (2015) work, that tested the sensibility of the Mesh for Ethanol Spray.

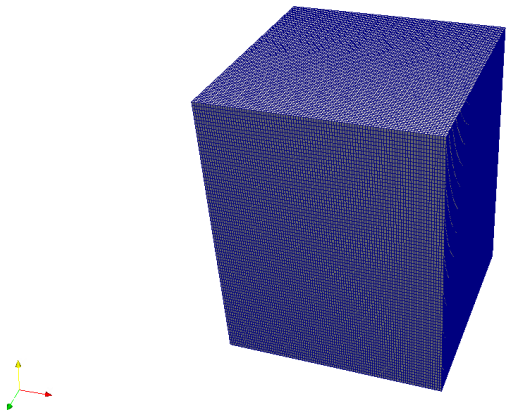

Figure 1. Numerical domain of the Spray

This prism contains 656100 hexahedra and no non-orthogonality. Another detail that was addressed is that the direction of the spray is aligned with the mesh.

3.2 Injection strategy

Within the description of the problem it is defined the inner and outer angle of the hollow cone spray. The parcels are randomly and uniformly distributed between this angle. The total inject fuel, injection temperature and injection pressure are also defined in this step.

There is also a table to inform how the fuel will be introduced in the system. The program checks the total time of injection, the total mass of fuel to be injected and normalize the average mass to be injected in each time step so that all these parameters checks with the injection table. For this work it was implemented a constant injection of 12,6 g/s during the injection time of 1,5 ms.

3.3 Numerical Model

The domain was planned so that the Parcels would not reach the boundary, therefore, do not interact with the walls. The simplest approach to modelling primary atomization involves seeding a number, Np, of different parcels at the position of the injector nozzle (Chen Huang, 2014). The diameter of the droplets in individual parcels, *x*, are determined using a suitable probability density function based upon a value between a minimum value of the diameter, *minValue*, and a maximum value of the diameter, *maxValue*. In OpenFOAM, the rosin-Rammler PDF:

$$k = 1.0 - \exp\left(-\left(\frac{maxValue - minValue}{d}\right)^n\right) \tag{6}$$

$$x = minValue + d\left(-ln(1{,}0 - yk)\right)^{1/n} \tag{7}$$

Where y is a random number for the particle diameter generated.

In this work we adapted the value of n to 3 and 2 to investigate witch one would give a better penetration fit compared to experimental data.

Another PDF function would be the Exponential PDF:

$$k = exp(-\lambda maxValue) - exp(-\lambda minValue) \quad (8)$$

$$x = -\frac{1.0}{\lambda} ln(exp(-\lambda minValue) + yk) \quad (9)$$

Where y is a random number for the particle diameter generated.

The value of lambda is the inverse of the mean diameter from the particle, therefore, lambda is 33334 for this case.

Table 1. Initial and Boundary conditions

Chamber Temperature (K)	300
Chamber Presure (Pa)	1.0E05
Injection Temperature (K)	320
Injection Pressure (bar)	100
Inner Cone Angle (°)	40
Outer Cone Angle (°)	60.1
Mean Mass Flux (g/s)	12.65
Parcels per second	8,000,000

The time step was set to be adjustable based in the maximum Courant number of 0.1 and the secondary break-up model chose for this work was the Reitz-Diwakar model.

4. RESULTS AND DISCUSSIONS

In this section, the results are showed and discussed. First, to analyze the RR model implemented in OpenFOAM, a comparison with literature are plotted in Figure 2. The graph shows that the results of the OpenFOAM model agree with the ones presented in Reis, L.M. (2015). Both indicated the same behavior and near the same penetration per time, demonstrating that the spray simulation models are well implemented, as expected.

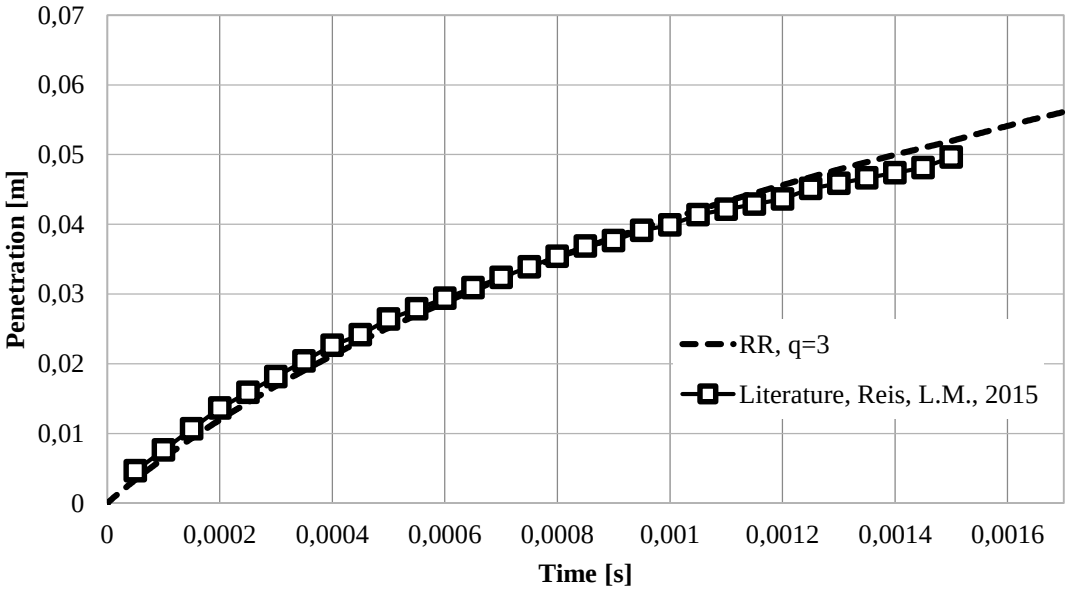

Figure 2. Spray penetration per time, comparison with literature.

Figure 3 displays the results of the analyzed models in comparison with experimental data. The plot shows agreement of numerical data and experimental data. However, the end-behavior of exponential function model

indicate an over-estimated penetration. The three models curve suggest an under prediction of penetration in region between 0,3 and 0,9 milliseconds, especially because of the experimental behavior of the spray that showed a pre-spray. This pre-spray is not modeled, consequently there are some disagreement with experimental data.

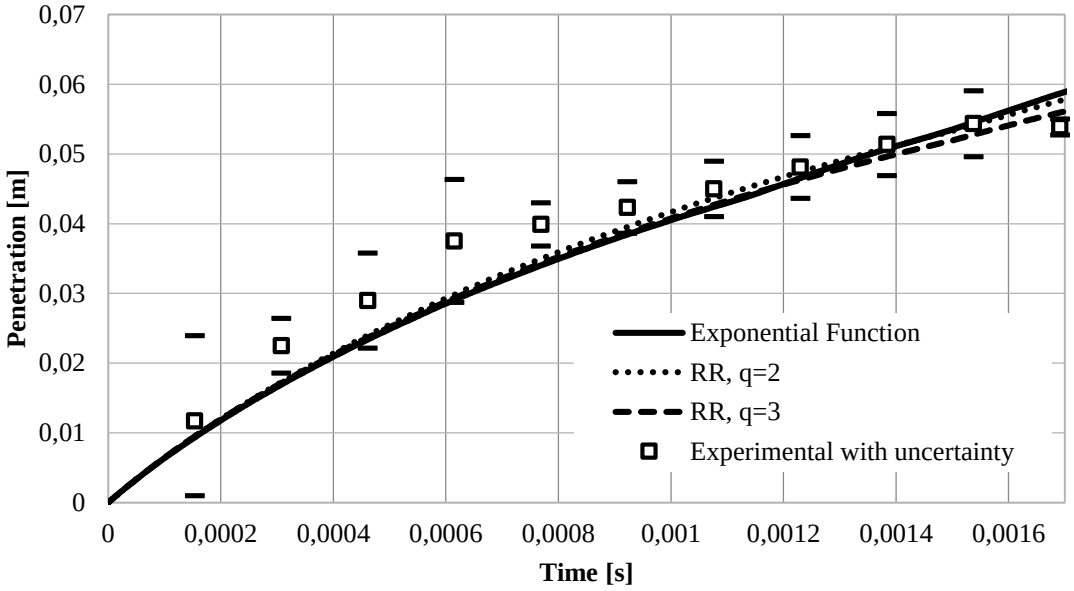

Figure 3. Spray penetration per time, models comparison with experimental data.

Figure 4 displays the results of the initial droplet distribution for ethanol spray. The plot shows the different approaches of PDF functions used in the analyzed models. As can be seen, the behavior of Exponential Function and RR are quite different. The droplet diameter dominant in both cases are different, as in EF the peak of frequency is near 0 and the RR function is near 30 μm or 20 μm depending on variable q.

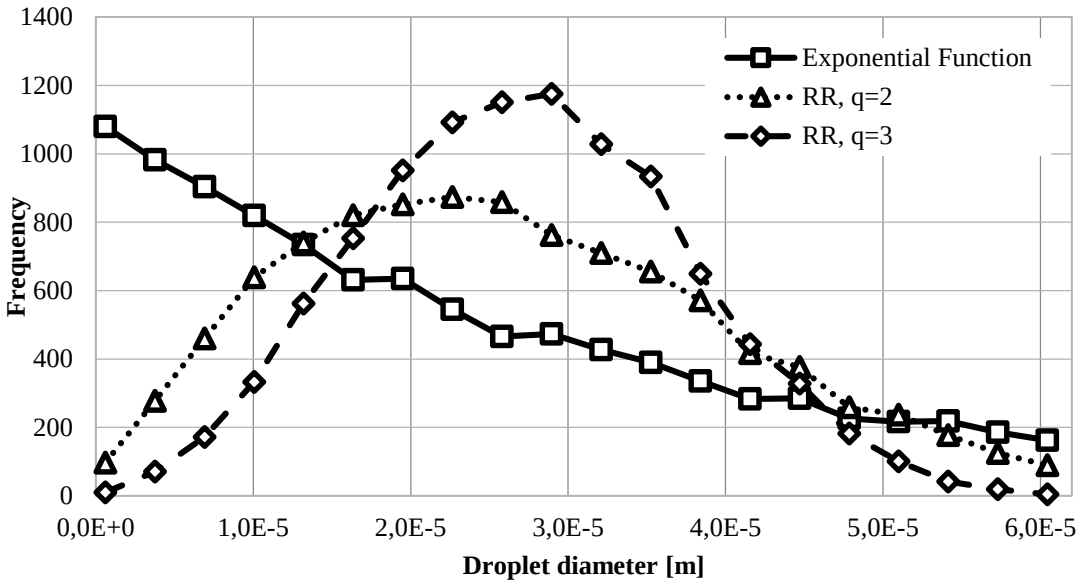

Figure 4. Droplet diameter in the parcels of the spray (Rosin-Rammler, q=2)

Figures 5, 6 and 7 display the results of the droplet diameter in the parcels of the spray at near the end of the simulation. The imagens show near the same characteristic form and growth of the fluid spray.

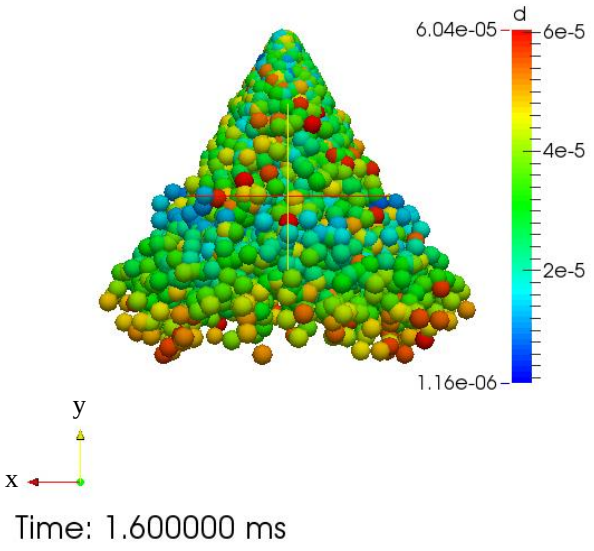

Figure 5. Droplet diameter in the parcels of the spray (Rosin-Rammler, q=2)

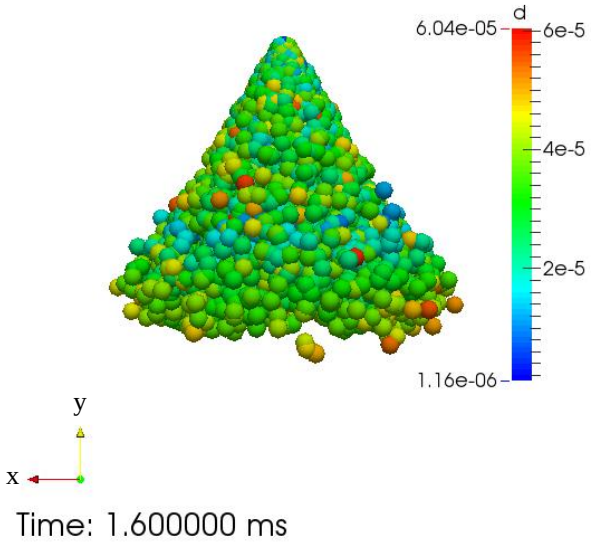

Figure 6. Droplet diameter in the parcels of the spray (Rosin-Rammler, q=3)

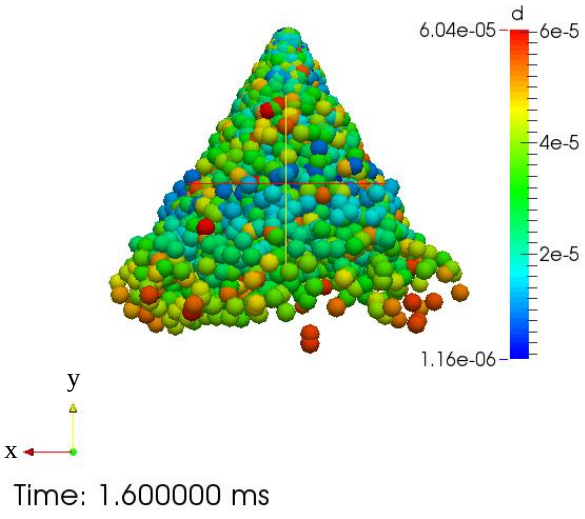

Figure 7. Droplet diameter in the parcels of the spray (Exponential function)

5. CONCLUSIONS

It's important to note that this model does not consider the pre spray, that is why the curve is a lower than the experimental data in the beginning. Both methods, Rosin Rammler and Exponential, achieved a good penetration curve, compared to the experimental data. The imagens 5 through 7 show near the same characteristic form and growth of the fluid spray. The Rosin Rammler was a better fit in the end of the curve as the Exponential curve tends to increase, therefore, is recommended to utilize this PDF method for Spray simulations.

6. ACKNOWLEDGEMENTS

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8. RESPONSIBILITY NOTICE

The authors Hélder Alves de Almeida Júnior, Roberto Ribeiro Schor, Allysson Fernandes Teixeira and Ramon Molina Valle are the only responsible for the printed material included in this paper.