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A STUDY OF THE ATOMIZATION PROCESS USING NUMERICAL SIMULATION

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Abstract. *The liquid droplets atomization process plays an important role in several industrial processes and in many aspects of the combustion engines performance, gas turbines, diesel engines and rocket motors. The use of Computational Fluid Dynamics (CFD) to study the atomization process is relatively new and this work studies the atomization spray field using pressure swirl atomizers and the computation simulations was done by the using of the commercial software CFX 15. The parameter analyzed was the semi-angle of the spray. Particles were placed at the entrance and different settings for the primary and secondary breakup were studied. Two models for the primary breakup (BLOB and LISA models) were* *tested and two other for the secondary breakup (Reitz and Diwakar model and TAB model). The numerical results were compared with experimental data and showed acceptable compatibility.*

Keywords: *numerical simulation, CFD analysis, oxidizer injection profile, spray semi-angle*

1 INTRODUCTION

The liquid droplets atomization process has sort of important application in several industrial processes and in many aspects of the engines combustion performance, as gas turbines and rocket motors. This phenomenon has been applied, successfully, also in agricultural, metrology and medicine field. Spray atomizers are the devices responsible to transform a liquid flow in a bulk spray and other physical dispersions of small particles and at the end of the process we have a gaseous flow. The combustion and chemical reactions efficiency depends on the way that the liquid flow is atomized. In general aspects, the small droplets generated through atomizers devices increases the specific surface area of the fuel leading to mixture ratio and evaporation as near as possible of the design desired.

The main fundamental process in the atomization phenomena are: (i) droplet formation; (ii) liquid jet (non)impingement; (iii) fan formation; (iv) secondary breakup (v) coalescence; and (iv) liquid mixing and reaction. In this work we focus in the primary and secondary breakup once that they are important classical multiphase flow problems. Primary breakup involves the initial formation of drops and others liquid fragments at the surface of a liquid. Primary breakup is important because it controls the initial dispersion of liquid into the gas phase and, through the strong effect of drop sizes on interphase transport rates, the subsequent mixing properties of the sprays. Secondary breakup involves any subsequent breakup of drops or liquid fragments present as dispersed liquid. Secondary breakup is important because drops after primary breakup are intrinsically unstable to secondary breakup, which affects subsequent mixing rates by influencing drop size as well, Wu at al. (1999).

Lacava et al. (2004) did an evaluation performance of pressure-swirl atomizers, primarily to be applied in gas turbine and liquid propellant rocket engine. They carry out a comparison between theoretical and experimental design procedures in order to obtain experimentally the liquid mass flow rate, the discharge coefficient, the spray semi angle, the Sauter Mean Diameter (SMD) and the droplet size distribution. To measure the spray semi-angle they used a fast velocity commercial camera with an initial minimum exposure time to obtain the best instant picture and after a maximum exposure time (and no flashlight) in order to obtain the spray mean boundaries. By the use of a commercial graphic editor software the picture with longer exposure time were converted to negative form, then using the AutoCAD® software, they determined the spray semi-angle. In order to analysis the spray droplet size distribution and the Sauter mean diameter (SMD), Lacava et al. (2004) used a laser scattering system (Malvern Mastersizer X®). To obtain the droplet size distribution it was applied the Fraunhofer diffraction theory.

Bertoldi (2007) did an experimental study of a N_2O liquid oxidizer and paraffin-based hybrid rocket. The work investigates the impact of a pressure swirl atomizer of the paraffin grain over the fuel regression rate. It was shown that using a single pressure swirl atomizer in a 250 N lab-scale hybrid motor it was possible to increase around 26% the fuel regression rate in comparison with a showerhead injector. Kumar et al. (2013) investigates numerically the effect on regression rate in a hybrid rocket motor assuming invariance in azimuthal direction to reduce the computational domain to a 2D axis-symmetric domain. They observed that the effect of swirl is high near the head end and reduces downstream.

In other hand, the use of Computational Fluid Dynamics (CFD) to study this phenomenon is relatively new. An important step in this area was done by Brinckman et al. (2008) that developed a methodology to predict vaporization in a compressible flow. Others recent works in atomization were done by Fung (Fung et al, 2009; Fung et al 2012) who did the numerical model of a nasal spray and Solanki (Solanki, et al 2013) that developed a numerical study of a diesel fuel spray.

This work is an initial study in the atomization spray field using a pressure swirl atomizer. At this research point, we conduct a computation simulation using the commercial software CFX 14.5 which uses the finite volume method. For the advection scheme, we use the High Resolution Scheme. The turbulent model chose was the k-ε and was used different models for primary and secondary breaking and the best models are discussed later in this paper. The understanding of the behavior of the atomization process is important, in the context of this research, once the pressure swirl atomizer seems to be a good option for a hybrid rocket motor under development at the University of Brasília.

2 METODOLOGY

The disintegration of a continuous phase that dispersed liquid droplets is called atomization and the resulting droplets of the system are named the spray (Solanki et al., 2013). The spray forming is usually divided into two consecutives and fundamental steps: primary and the secondary breakup. Figure 1 shows the schematic of droplets formation.

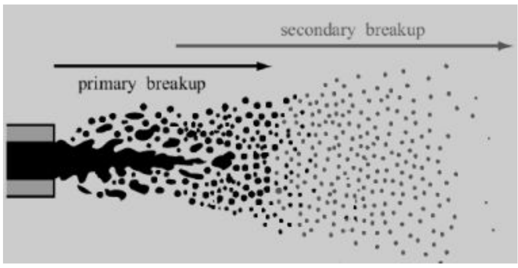

Figure 1: Breakup of a liquid jet.

In this work we use an approach where discrete phase (water) has a Lagrangian approach and the continuous phase (air) is Eulerian. So, in the Lagrangian-Eulerian method the governing equations for the fluid phase are given by the continuity and momentum equations, respectively:

$$\frac{\partial \alpha_g}{\partial t} + \frac{\partial\left(\alpha_g \boldsymbol{u}_i^g\right)}{\partial x} = 0 \tag{1}$$

$$\frac{\partial\left(\alpha_g \boldsymbol{u}_i^g\right)}{\partial t} + \boldsymbol{u}_i^g \frac{\partial\left(\alpha_g \boldsymbol{u}_i^g\right)}{\partial \boldsymbol{x}_j} = -\frac{\alpha_g}{\rho_g}\frac{\partial p_g}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\alpha_g(\nu+\nu_t)\left(\frac{\partial \boldsymbol{u}_i^g}{\partial x_j} + \frac{\partial \boldsymbol{u}_j^g}{\partial x_i}\right)\right] + \frac{1}{\alpha_g \rho_g} M_p \tag{2}$$

where α is the void fraction, $\boldsymbol{u}$ the velocity, t the time, $\boldsymbol{x}$ the displacement, ρ density, p the pressure, ν and ν_t kinematic and eddy viscosity, respectively. The subscripts g and p are the gaseous phase and particle.

For the discrete phase (spray droplets) the two-way coupling is applied in the model and there is a coupling between continuous and discrete phase. The force balance equation is (Fung *et al.*, 2012):

$$\frac{du_p}{dt} = \frac{18\mu}{\rho_p d_p^2}\frac{C_D Re}{24}\left(u_g - u_p\right) + \frac{\boldsymbol{g}\left(\rho_p - \rho_g\right)}{\rho_p} + \boldsymbol{F} \tag{3}$$

where Cd is the drag coefficient, given as $C_D = a1 + \frac{a2}{Re} + \frac{a3}{R3}$.

In Eq. (3), d is the droplet diameter, μ is the dynamic viscosity, $\boldsymbol{g}$ and $\boldsymbol{F}$ the gravitational and additional acceleration terms.

Different models were studied for the primary and secondary breakup. To the primary breakup were used BLOB and LISA models. The BLOB model is one of the simplest and most popular approaches to define the conditions for injecting particles. It ignores the detailed description of the atomization process within the primary breakup zone of spray. More details of the method can be found in Bhatt (Bhat*et al.*, 2011). The LISA (Linear Instability Sheet Atomization) was the other model applied. This model is able to simulate the effects of primary breakup in pressure-swirl atomizers. More information can be found in Fung (Fung et al., 2012). For the secondary breakup it was used the Reitz *and* Diwakar model and TAB model. The first considers only bag and stripping breakup. In the TAB model we assumed that the droplet is similar to the spring-mass system, for the forced, damped and harmonic oscillation. More information is found in Solanki (Solanki et al., 2013) and ANSYS (ANSYS, 2012).

The computational domain used was a cylinder with 0.1 m diameter and 0.1 m high. The discretization of the domain was performed using CFX-Mesh with 1182922 million mesh elements predominantly hexahedral. We did a mesh study where 2017000 elements mesh were used and, once that the error associated with the length of the element was negligible, it was chosen to use the mesh with lower computational cost.

Figure 2 illustrates the discretization of the domain and the boundary conditions used. The liquid and gas properties were based on Lacava et al. (2004) experimental case studies. These properties are shown in Table 1. Twenty particles were injected in the domain in order to obtain the spray particle opening semi-angle.

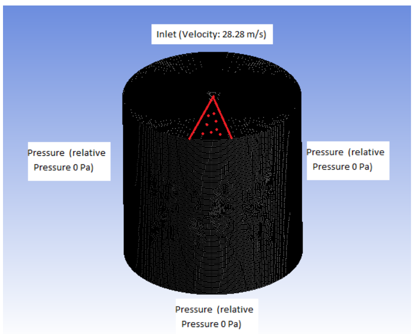

Figure 2: Geometry mesh and boundary conditions.

3 RESULTS

In this research were tested two models for the primary breakup (BLOB and LISA) and two other for the secondary breakup (Reitz and Diwakar model and TAB model). As it an initial study, we are not concerned about trying to recover all the characteristics of the spray and, at the moment, this parameter in only estimated at the beginning of the computational simulation. In order to measure the spray semi-angle it was used the Meazure software.

The first tested configuration was conducted with BLOB and Reitz and Diwakar model. As it can be shown in Figure 3, the results are coherent; however, the spray semi-angle was underestimated, reaching the value of 28.2°. When the secondary breakup model is changed to the TAB, it was not find any difference related with spray semi-angle.

Table 1. **Properties of the liquid and gas phase, based Lacava (Lacava et al., 2004)**

		Properties of spray	
Density	1000 kg/m³	Surface Tension	0.072 N/m
Viscosity	0.001 kg/m·s	Mass Flow Rate	0.006 kg/s
Spray Angle (estimated)	34.89°	Droplets Mean Diameter	45 µm
	Properties of Air		
Density	1.185 kg/m³	Viscosity	1.83e-05

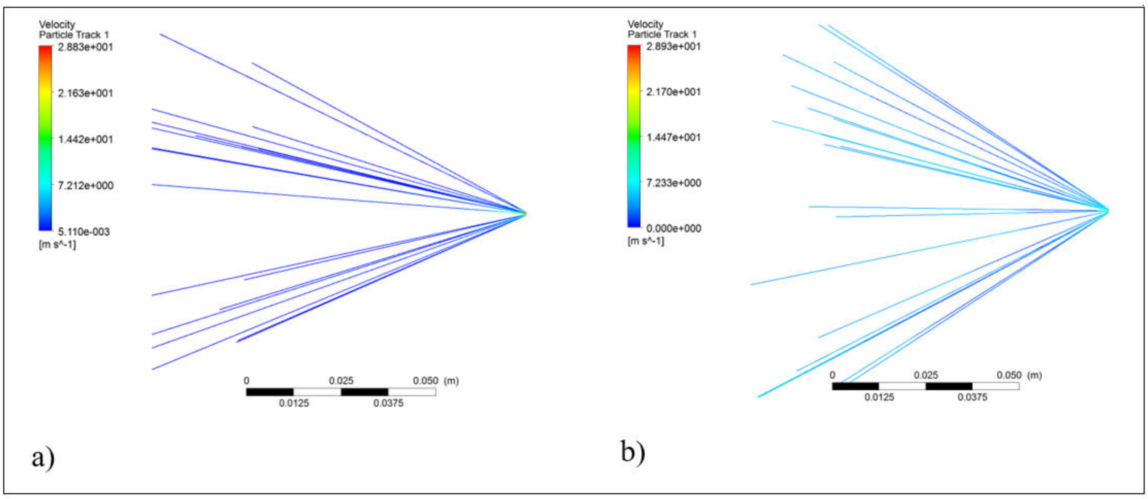

Figure 3: Displacement of the injected particles into the domain, BLOB e Reitz and Diwakar configuration (a) and LISA and Reitz and Diwakar configuration (b).

To perform the simulations with LISA model are necessary some more parameters, as pressure drop, in this case 4 atm, and the Density Probe Normal Distance, took to be the average diameter of the particle, 45 μm. Analyzing the simulation results with LISA model and Reitz *and* Diwakar model, presented in Figure 3b, it is possible to see a significant improvement in the analyzed parameters, once that the spray semi-angle found was 33.4°. This difference can be explained by the simplification that the BLOB model does when ignore the jet breakup process (Fung et al., 2009).

When we use the TAB model to the secondary breakup there aren't any noticeable changes in the spray semi-angle. Thus, for the realized test, it is possible to affirm that the primary breakup model is the most important model to be determined.

4 CONCLUSION

In this initial research phase was simulated different models in order to capture the atomization phenomena with accuracy. The liquid droplets atomization process plays an important role in several industrial processes and in many aspects of the combustion engines performance, as gas turbines, diesel engines and rocket motors. However, determining the distributions of drop size and velocity theoretically is an extremely difficult problem. In general, the influence of the aerodynamic forces on the breakup of jets and the secondary breakup of drops is so complicated as to be beyond realistic analysis, Culick and Yang (1995). However, nowadays, with the advance of the computation power and metrologies implemented in various commercial and noncommercial programs in the last 20 years we have computational tools that can simulate a sort of complex physical phenomena realistically.

Due of the importance of the theme, the aim of this research was determined the best models set to obtain the spray semi-angle. In all of the configurations tested in this study, the LISA model showed best results for the primary breakup when compared with BLOB model. For the secondary breakup both models, Reitz and Diwakar model and the TAB model, presented similar results. The value of the spray semi-angle found with LISA model and Reitz *and* Diwakar model was 33.4°. It showed a good agreement with the research performed by Lacava et al. (2004) that obtained the value of 34.9° (theoretical analyses) and 34.5° (experimental results). The set BLOB and Reitz and Diwakar model gave the underestimated value of the 28.2° form the spray semi-angle.

With the intuit to continue the present study the next target for future works will be perform a transient analysis of the problem.

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