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Analyse of the Atomization Process Using Computational Fluid Dynamics

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Abstract

The process of liquid atomization is largely used in the aerospace engineering field once that the combustion efficiency is directly related with the injector system design. However, the experimental study of this process in the propulsion system design phase increases drastically the cost of the project. In this context, the computational fluid dynamics is one of the best solutions because it can give high quality results with low cost, observing that to achieve this purpose it is necessary refinements in the models and, mainly, perform an extended study of the boundary conditions. Thus, in this work it was used the software CFX17 to study the atomization process with different models and boundary conditions. A comparison between the computational and experimental results was preformed in order to analyse the prediction of each model tested with the geometrical parameter of the spray.

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 [1].

Lacava et al. [2] 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), it was used a laser scattering system (Malvern Mastersizer X®). To obtain the droplet size distribution it was applied the Fraunhofer diffraction theory [2].

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Bertoldi [3] 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 20% the fuel regression rate in comparison with a showerhead injector.
Kumar et al. Investigate 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 [4].
In the atomization phenomena, the determination 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 [5].
Nowadays with the advance of the computation power and metrologies implemented in various commercial and non-commercial programs in the last 20 years we have computational tools that can simulate a sort of complex physical phenomena realistically. 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 [6] that developed a methodology to predict vaporization in a compressible flow.
Others recent works in atomization were done by Fung ([7], [8]) who did the numerical model of a nasal spray and Solanki [9] that developed a numerical study of a diesel fuel spray.
Here, we used the software CFX 17 for the numerical analysis. This program uses the finite volume method and mesh structured and unstructured. The turbulent model utilized is the k-ε and different models for primary and secondary breaking. This is the principal part of this study. In the moment, the University of Brasilia is development the hybrid rocket motor using the pressure swirl atomizers and this initial study is part of this project.

2. Pressure Swirl atomizer design considerations

Humble et al. [10] affirm that the propellant injectors are the heart of the thrust chamber and it is falls into two broad categories: impinging and non-impinging. A typical injector assembly can incorporate dozens and even hundreds of individual injectors [11]. For the hybrid systems, a priori it is possible to use any liquid engines injector types. The oxidizer can be directly injected down the port and also can be injected into a pre-combustion chamber, where it is largely gasified and heated before flowing down the port. In this paper was used a particular oxidizer injection device that promotes a swirling effects by the use of a pressures–swirl atomizer. In this case, the liquid is brought into rotation in a small auxiliary chamber by means of tangential orifices and at the exit of the injector we observe a conical sheet made up of fine droplets [12].
In this sort of atomizer the required data for the design are: the liquid properties (density, surface tension and viscosity), the discharge ambient characteristics (ambient pressure and density) and the liquid injection conditions (mass flow rate, injector pressure differential and others). The first pressure–swirl characteristic that could be find is the flow number, FN, expressed as:

$$FN = \frac{\dot{m}_L}{\sqrt{\rho_L \Delta P_L}} \tag{1}$$

Where $\dot{m}_L$ is the liquid oxidizer mass flow rate, ρ_L is the liquid oxidizer density and ΔP_L is the injector pressure differential. It is necessary to take into account the manufacture process limits and the following dimensionless group, i.e., $(A_p/D_s \cdot D_0)$ and (D_s/D_0) - figure (1) – due its importance on the discharge coefficient, C_d [2]. The discharge coefficient can be calculated by:

$$C_d = \frac{\dot{m}_L}{A_{or}\sqrt{2 \cdot \rho_L \Delta P_L}} \tag{2}$$

The Eq. (3) brings the derivation of the discharge coefficient in function of the injector dimensions and the liquid properties [13].

$$C_d = 0.45 \cdot \left(\frac{D_0 \cdot \rho_L \cdot U_0}{\mu_L}\right)^{-0.02} \cdot \left(\frac{L_0}{D_0}\right)^{-0.03} \cdot \left(\frac{L_s}{D_s}\right)^{0.05} \cdot \left(\frac{A_p}{D_s \cdot D_0}\right)^{0.52} \cdot \left(\frac{D_s}{D_0}\right)^{0.23} \tag{3}$$

In the design procedure, the critical atomizer dimensions are accepted or not, depending on the calculated values of the spray semi-angle (θ) and the mean drop diameter. The semi-angle can be estimated by the expression developed by [14] for a pressure-swirl atomizer.

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$$\sin\theta = \frac{(\pi/2)\cdot C_d}{K\cdot(1+\sqrt{X})} \tag{3}$$

Where $K = A_p/(D_s D_0)$ and X is the ratio between the air core area (A_a) and the injector nozzle orifice exit area(A_0), estimated by the equation (5) below,

$$D_0 = 2\cdot\sqrt{\frac{FN}{\pi(1-X)\sqrt{2}}} \tag{4}$$

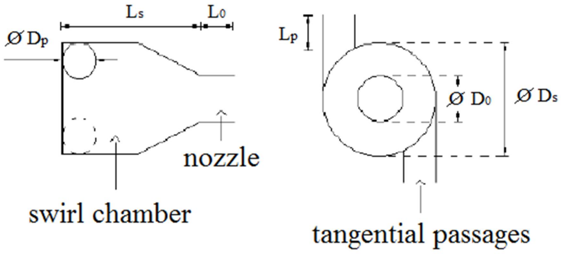

Figure 1: Pressure–swirl atomizer schematics [2].

3. Metodology

The disintegration of a continuous phase that dispersed liquid droplets is called atomization and the resulting droplets of the system are named spray [9]. The spray forming is usually divided into two consecutives and fundamental steps: primary and the secondary breakup. Figure 2 shows the schematic of droplets formation.

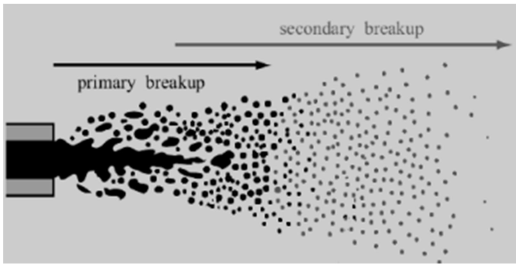

Figure 2: Breakup of a liquid jet

In this work we use a procedure 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:

$$\frac{\partial\alpha_g}{\partial t} + \frac{\partial(\alpha_g \boldsymbol{u}_i^g)}{\partial x} = 0 \tag{5}$$

$$\frac{\partial(\alpha_g \boldsymbol{u}_i^g)}{\partial t} + \boldsymbol{u}_i^g\frac{\partial(\alpha_g \boldsymbol{u}_i^g)}{\partial x_j} = -\frac{\alpha_g}{\rho_g}\frac{\partial p_g}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\alpha_g(\nu+\nu_t)\left(\frac{\partial \boldsymbol{u}_i^g}{\partial x_j} + \frac{\partial \boldsymbol{u}_j^g}{\partial x_i}\right)\right] + \frac{1}{\alpha_g\rho_g}M_p \tag{6}$$

Where α is the void fraction, u the velocity, t the time, 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,

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$$\frac{du_p}{dt} = \frac{18\mu}{\rho_p d_p^2}\frac{C_D Re}{24}\left(u_g - u_p\right) + \frac{g(\rho_p - \rho_g)}{\rho_p} + \boldsymbol{F} \tag{7}$$

Where C_D is the drag coefficient, given as $C_D = a1 + a2/Re + a3/R3$ [8].

In Eq. (7), 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 [15]. 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 atomizer [8].

For the secondary breakup it was used the Reitz and Diwakar model and TAB model. The first considers only bag and stripping breakup [8]. In the TAB model we assumed that the droplet is similar to the spring-mass system, for the forced, damped and harmonic oscillation [16].

In this study, we used as domain a cylinder, Figure (3). This geometry has 0.1 m of the diameter and 0.1 m of the length. The study utilized a mesh (performed by CFX-Mesh) with 1182922 million of elements. These elements are predominantly hexahedral. We did a mesh study and with this configuration, the results are satisfactory.

The boundary conditions used were based on the experimental case, found in [2]. All properties used are shown in Table 1. For determination of the spray semi-angle, we inject particles in the domain.

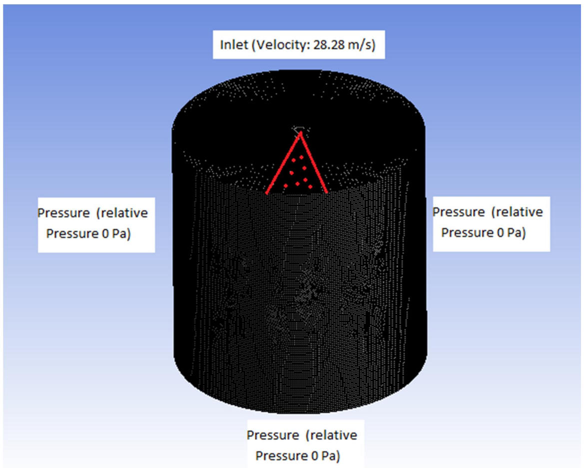

Figure 3: Discretization of the geometry, mesh and boundary conditions.

Table 1. Properties of the liquid and gas phase [2].

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 kg/m·s

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4. Results

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.
We inject particles in the domains to determine the spray semi-angle. The first question is the number sufficient of the particles for the best result with lower computational cost. We test different configurations with twenty, sixty and hundred particles. The results of the spray semi-angle are similar for different quantities of infected particles. By requiring less computational cost, it used in the work twenty inject particles.
In this research were tested different models for the primary and secondary breakup. We test the BLOB and LISA (primary breakup) and, Reitz and Diwakar model and TAB model (secondary breakup).
The first tested configuration was conducted with BLOB and, Reitz and Diwakar model. As it can be shown in figure (4) 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.

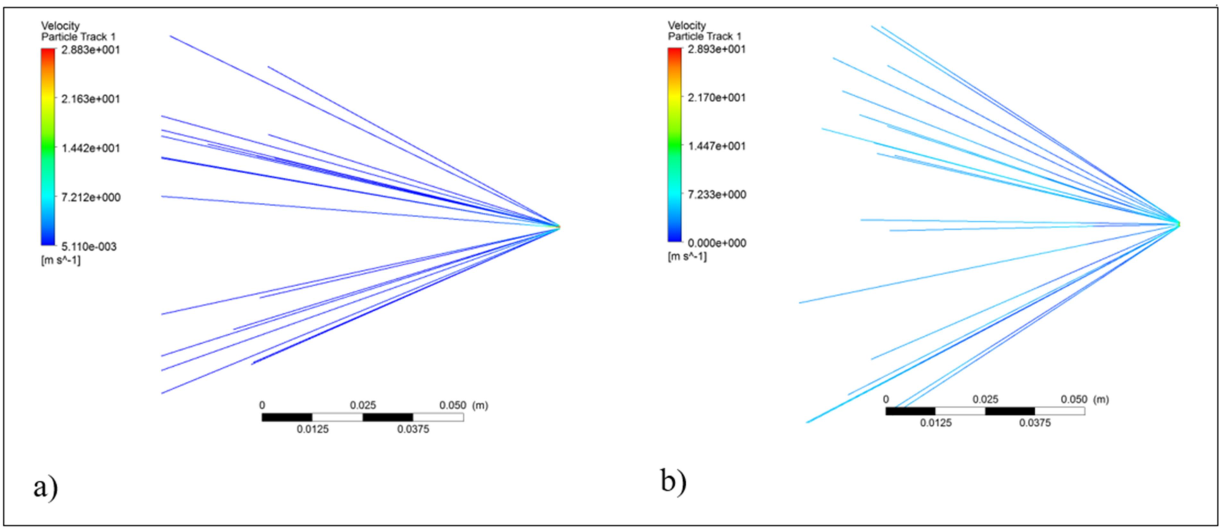

Figure 4: Displacement of the injected particles into the domain, BLOB e Reitz and Diwakar configuration (a) and LISA and, Reitz and Diwakar configuration (b).

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 (4b), 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 [7].
When we use the TAB model to the secondary breakup there are not 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. The increase in computational cost can be disregarded because all simulations had very similar times.

5. Conclusion

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 [2] 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° for the spray semi-angle.
Another important conclusion is the quantity of the particles injected. With only twenty particles is possible to determine the spray semi-angle.

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In order to continue the present study, the next target for future works will be perform a transient analysis of the problem and also insert the fuel grain that will be used in the University of Brasilia hybrid rocket, to study the influence of the spray collision with the fuel wall on the flow pattern.

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