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IMPROVED ATOMIZATION MODEL FOR CFD CODES

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ABSTRACT This study presents a method to improve the capability of Computational Fluid Dynamics (CFD) codes to model liquid atomization mechanisms. It is based on experimental measurements done at Laval University using the shadowgraphy technique to characterize a commercial air-assist nozzle. The software used for the numerical simulations was the CFD code FLUENT® V.6.2.16 with the mesh generator Gambit® V.2.0.4. The flexibility of the User-Defined Function implemented in the code permitted the use of empirical parameters in an existing atomization model to significantly improve the numerical simulations of a fuel spray. The drop size distributions were reproduced numerically at the exact same locations as in the experimental measurements in the spray and demonstrated very good agreement with the improved method.

Keywords: Liquid Atomization, Numerical Simulation, Sprays, Atomization model, CFD

1. INTRODUCTION

For modern industrial applications, environmental, cost, and fuel considerations are added to the fundamental complexity of combustion. CFD has proven to be a powerful tool to support the design of complex processes. The numerical modelling of liquid injection can help, for instance, to optimize atomizer design and improve spray quality in various applications.

Although the finite element/volume formulation has been well established for years in areas such as heat transfer, solid mechanics, and aerodynamics, its extension to multiphase, acoustics, and reactive flow modelling, for instance, is currently still a challenge. In order for computational models to become more reliable predictive tools for such systems, their accuracy needs to be investigated. Measurements obtained with advanced droplet size instruments can provide initial and boundary conditions for the formulation of computational models and/or validate them. The software used for the numerical simulations in the study is the CFD code FLUENT® V.6.2.16 with the mesh generator Gambit® V.2.0.4.

This study evaluated the ability of the air-blast atomization model implemented in FLUENT® to predict spray evolution of a commercial atomizer. The nozzle used in the study was the air-assist atomizer BETE XAPR-200®, which provides a solid cone spray.

2. METHODOLOGY

Models used in FLUENT® are based on the fundamental conservation equations of mass, momentum, and energy for the individual species. Accurate measurements of various parameters such as droplet size and velocity, as well as spray angle, are normally required for the formulation and/or verification of numerical models.

FLUENT® predicts the discrete phase trajectory by integrating the force balance on the droplet, which is written in a Lagrangian reference frame. In Cartesian coordinates, it can be written as follows:

$$\frac{du_{\mathrm{p},i}}{dt} = F_D\left(u_i - u_{\mathrm{p},i}\right) + \frac{g_i\left(\rho_\mathrm{p} - \rho\right)}{\rho_\mathrm{p}} + F_i \qquad (1)$$

where:

$$F_D = \frac{18\mu}{\rho_\mathrm{p} d_\mathrm{p}^2}\frac{C_D \mathrm{Re}_\mathrm{p}}{24}$$

and

$$\mathrm{Re}_\mathrm{p} \equiv \frac{\rho d_\mathrm{p}}{\mu}\left|u_{\mathrm{p},i} - u_i\right|$$

In this study, a User-Defined Function (UDF) is executed to generate random numbers from the droplet size distribution obtained experimentally at Laval University and to simulate a more realistic random process for the initialization of droplet diameters in the discrete phase model. As the name suggests, UDFs are functions implemented by the user to customize models and thus enhance the standard features of a code. In FLUENT®, UDFs are written in the C programming language and built-up using predefined macros and functions provided by the code and then, dynamically loaded within the solver. The units for the variables in the UDF must be in SI units.

3. RANDOM NUMBER GENERATION

In general, methods for generating random numbers from any distribution start with uniform random numbers. Once a uniform random generator is available, random numbers from other distributions are built-up using different techniques such as the direct, the inversion, and the rejection method. The various methods for random number generation are discussed exhaustively by Devroye [1] and Press *et al.* [2].

Pimentel *et al.* [3] pointed out the Beta density function as a suitable model to describe droplet size distribution in sprays. A Beta distribution has the following general expression:

$$f(x) = C(x-a)^{p-1}(b-x)^{q-1} \tag{2}$$

where C is the normalizing constant derived to satisfy the expression:

$$\int_a^b f(x)dx = 1 \tag{3}$$

The various methods for generating a Beta distribution and their merits are reviewed in the recent study by Mahlooji *et al.* [4]. In the present study, the Johnk's [5] algorithm, based on a rejection technique, was used because of its simplicity, accuracy, and speed to generate random numbers. The algorithm was developed the same way as presented in Devroye [1] and is as follows:

REPEAT
Generate uniform [0,1] random variables U, V.
$X \leftarrow U^{1/p}$, $Y \leftarrow V^{1/q}$
UNTIL $X + Y \leq 1$
RETURN $Z = \frac{X}{X+Y}$

Z is a Beta distribution (p,q) given by the following expression:

$$f(Z) = B_{p,q} Z^{p-1}(1-Z)^{q-1} \tag{4}$$

with $0 \leq Z \leq 1$ and $B_{p,q}$ is the Beta function:

$$B_{p,q} = \frac{\Gamma(p+q)}{\Gamma(p)\Gamma(q)} \tag{5}$$

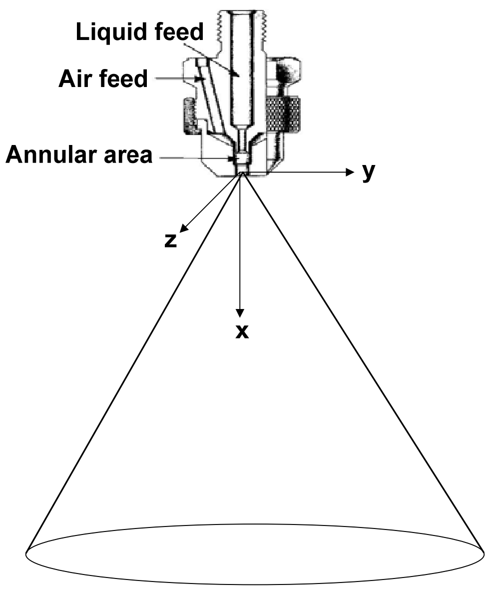
The following transformation was applied to the original Johnk's algorithm to derive the distribution in the range [*a*,*b*] instead of the range [0,1], where *a* and *b* are the minimum and maximum droplet diameters in the spray respectively:

$$Z \leftarrow Z.(b-a)+a \tag{6}$$

4. FLUENT® IMPLEMENTATION

The discrete phase model (DPM) is the only multiphase model in FLUENT® that permits the specification of a droplet distribution or includes combustion modelling in a simulation. It is therefore recommended for spray combustion applications [6].

The air-blast atomizer from the FLUENT® DPM was selected as the most suitable model to describe the atomization of the BETE XAPR-200® nozzles. Figure 1 presents the sampling positions for the measurements. The operating conditions during the experiment are presented in Table 1.



Position	x [mm]	y [mm]
Centre 1	25,4	0
Centre 2	50,8	0
Centre 3	76,2	0
Middle 1	25,4	3,8
Middle 2	50,8	6,5
Middle 3	76,2	9,0
Border 1	25,4	7,5
Border 2	50,8	13,0
Border 3	76,2	18,0

Figure 1: The BETE XAPR-200® atomizer

Table 1: Operating conditions during experiment

Flow Rate [g/s]		Pressure [kPa]	
Fuel	Air	Fuel	Air
11,30	3,52	500,3	558,6

- Fuel temperature at injection: 294 K
- Ambient pressure: 101,3 kPa
- Atomizing air temperature: 294 K
- Fuel: JP-10
- Room temperature: 294 K
- Technique for droplet sizing: shadowgraphy

In order to improve the existing air-blast sub-model in FLUENT® and to take into account the randomness of actual atomization processes, a UDF was used to simulate the variation of the droplet size in the spray following the function (Beta family) obtained in the experiments.

The following parameters of an empirical Beta distribution were used to generate the Beta random distribution:

$$a = 6,0$$
$$b = 100,0$$
$$p = 1,5$$
$$q = 11,0$$

An axisymmetric and structured grid (0,2 m x 1,0 m) with 145791 nodes was used in the simulation as illustrated in Figure 2.

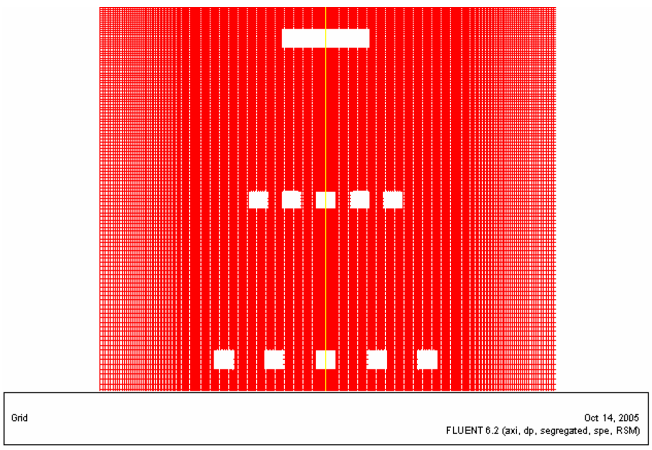


Figure 2: Sampling Position

5. THE CONTINUOUS PHASE SOLUTION

The Reynolds stress turbulence model (RSM) is the most elaborate turbulence model that FLUENT® provides, and was used to solve the continuous phase (atomizing air stream) necessary when using the air-blast model [6]. The axial and radial velocity profiles of the atomization air stream obtained by the numerical simulation are shown in Figures 3 and 4 respectively.

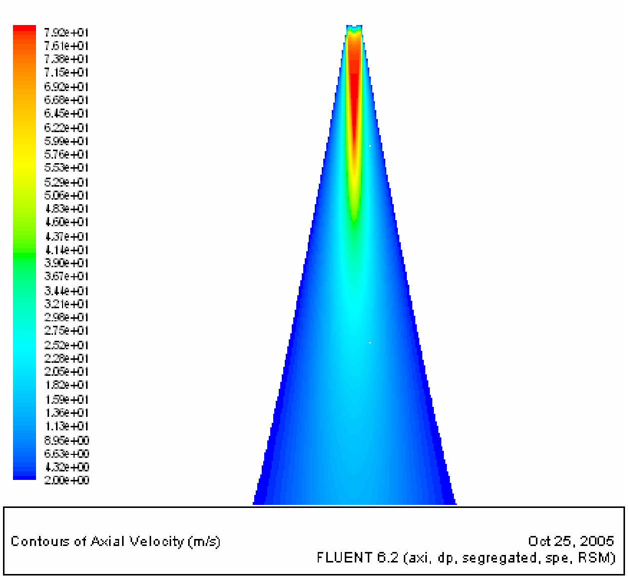


Figure 3: Axial velocity profile

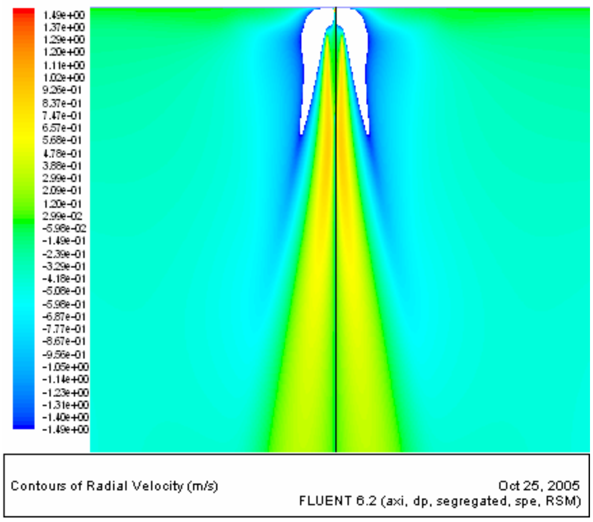


Figure 4: Radial velocity profile

6. THE DISCRETE PHASE SOLUTION

Non-evaporating liquid fuel droplets were tracked with the Lagrangian scheme using the discrete phase model. The spray downstream of the injector was validated against the experimental measurements obtained with the shadowgraphy technique. For such a validation, the sampling regions used in the experiments were generated into the grid, as illustrated in Figure 2. The sampling regions were 3,0 mm x 3,0 mm, which corresponded to the field-of-view for the optical system used during the measurements. The UDF is used to generate the initial variables for the droplet diameters and is implemented from the injection panel as shown in Figure 5.

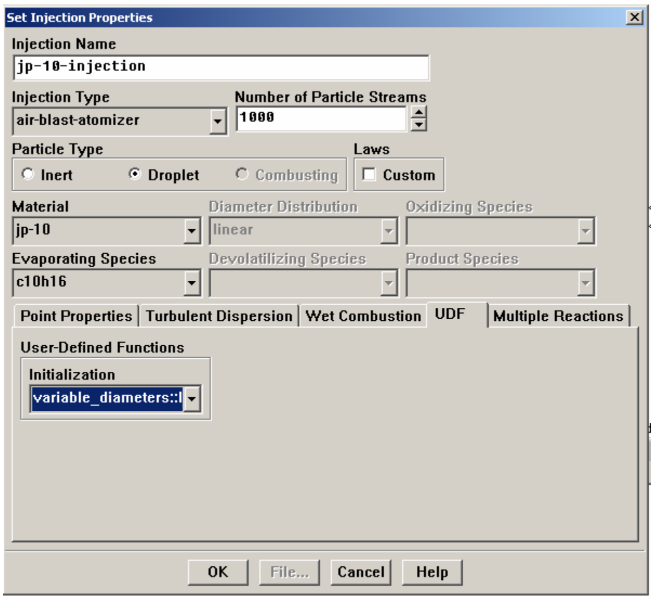


Figure 5: “Set Injection Properties Panel” in FLUENT®

The point properties necessary for the air-blast atomizer model include the “sheet” constant, set to 12 as obtained theoretically by Weber [7] for liquid jets and confirmed experimental by Dombrowski and Hooper [8], and the “ligament” constant, which was kept as 0,5. The initial velocity of the liquid sheet was estimated from the continuity law. Other parameters required for the air-blast atomizer model are presented in Table 2 as follows:

Table 2: Parameters of the Injection

Parameters	Values
X-position [m]	0
Y-position [m]	0
Temperature [K]	294
Flow rate [kg/s]	0,0113
Injector inner diameter [m]	0
Injector outer diameter [m]	0,003
Spray half angle [deg]	12
Atomizer dispersion angle [deg]	0

where:

- X and Y Positions: Coordinates of the nozzle outlet
- Temperature: Initial temperature of the sprayed liquid
- Flow rate: Mass flow rate of the sprayed liquid
- Injector inner diameter: Inner diameter of the liquid sheet
- Injector outer diameter: Outer diameter of the liquid sheet
- Spray half angle: Half of the angle of the spray as it leaves the nozzle
- Atomizer dispersion angle: The angle of initial trajectory of the liquid film leaving the nozzle

Droplets were tracked using the discrete phase model as illustrated in Figure 6.

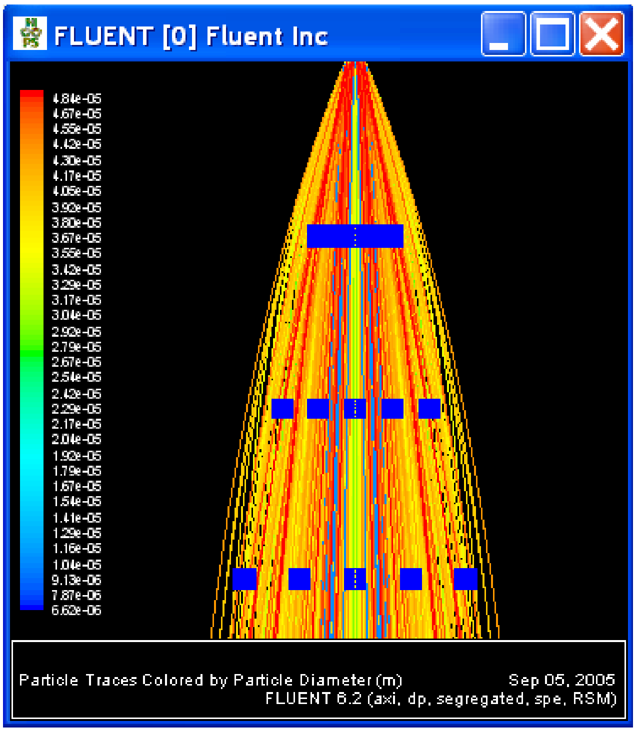


Figure 6: Validation of injection model

Figures 7 to 15 present the comparison between the droplet size distributions obtained with the numerical model and with the experiments at the nine sampling positions in the spray.

The results demonstrate that providing FLUENT® with more realistic initial conditions, the code is able to predict satisfactorily the segregation of droplets in the spray.

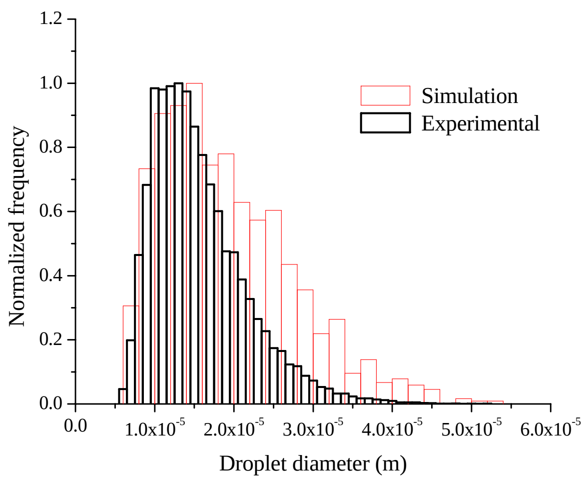


Figure 7: Droplet size distribution – Centre 1

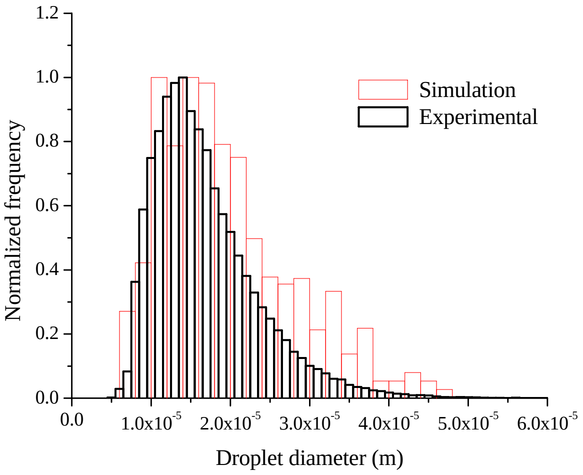


Figure 8: Droplet size distribution - Centre 2

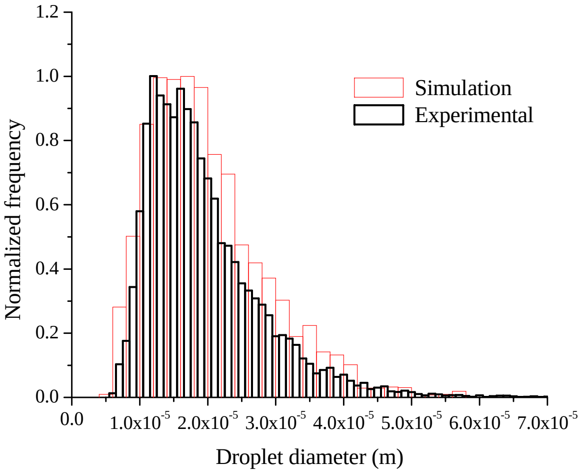


Figure 9: Droplet size distribution – Centre 3

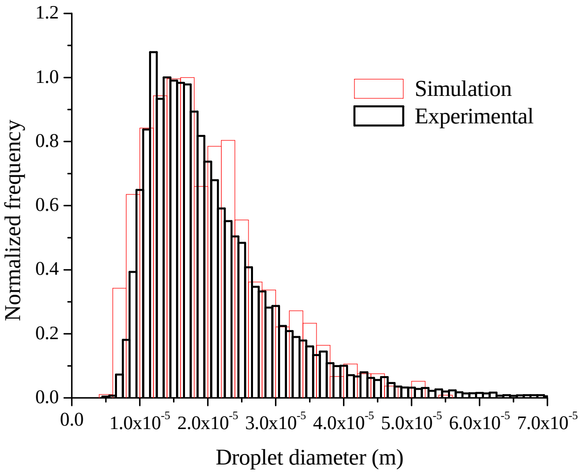


Figure 10: Droplet size distribution - Middle 1

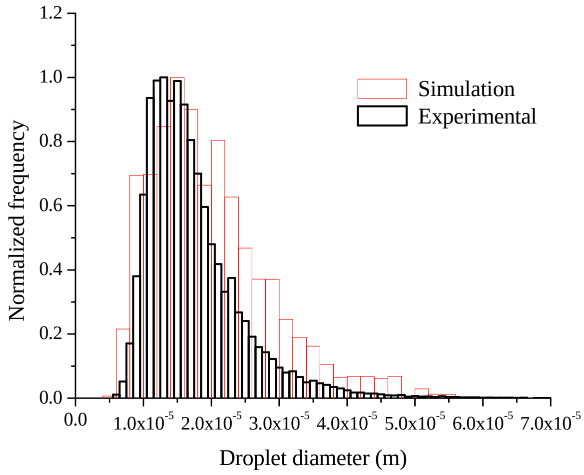


Figure 11: Droplet size distribution – Middle 2

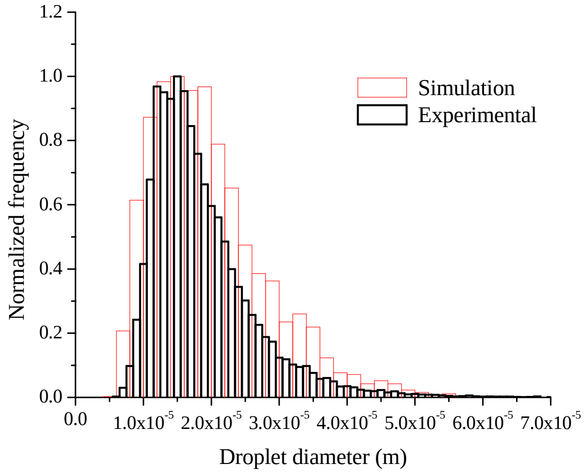


Figure 12: Droplet size distribution – Middle 3

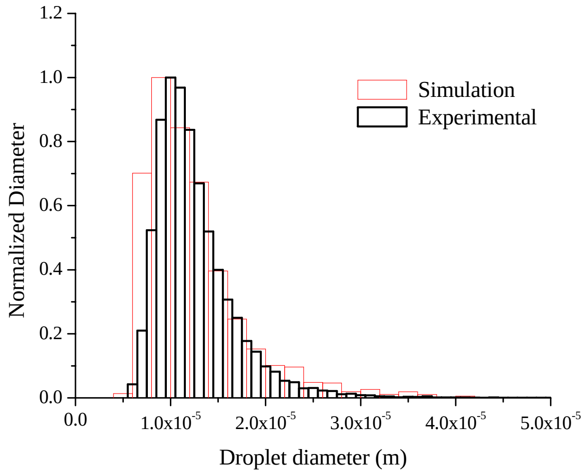


Figure 13: Droplet size distribution – Border 1

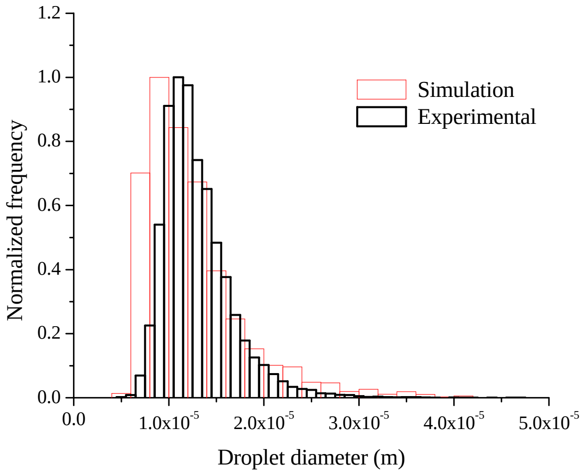


Figure 14: Droplet size distribution – Border 2

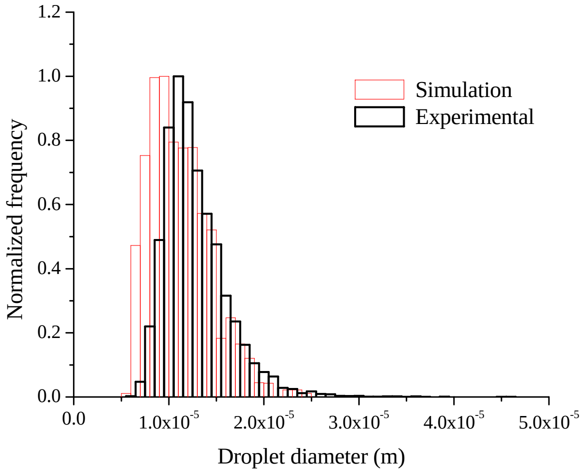


Figure 15: Droplet size distribution – Border 3

7. CONCLUSIONS

CFD is widely recognized as a powerful tool for optimizing complex systems. However, improving the accuracy of such codes for application in fields such as multiphase flows is still an issue.

This part of the study focused on improving a liquid atomization model implemented in FLUENT®. The atomizer used in the experimental part of the study was the nozzle BETE XAPR200®, which necessitated the use of the air-blast model from Fluent.

In order to provide the existing model with more realistic boundary conditions, a model is proposed to generate variable droplet distributions as an initial condition. Droplets were randomly generated following a Beta distribution which parameters were obtained experimentally by the shadowgraphy technique. For the generation of a Beta distribution, a UDF based on Johnk's algorithm was created and used within the FLUENT® solver.

The droplets generated by the UDF were further injected into an air stream and tracked at different sampling positions in the spray, the same way as done during the experimental measurements. The numerical predictions obtained with the proposed methodology demonstrated good agreement with the experiments. For further studies, the distribution of droplet velocities should be also investigated and validated.

8. ACKNOWLEDGEMENTS

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9. NOMENCLATURE

u_i	Fluid phase velocity in the direction	[m/s]
$u_{p,i}$	Particle velocity in the direction i	[m/s]
μ	Molecular viscosity of the fluid	[kg/(m.s)]
ρ_p	Density of the particle	[kg/m^3]
d_p	Particle diameter	[m]
F_D	Drag force	[N]
C_D	Drag coefficient	
Re_p	Particle Reynolds number	
Γ	Gamma function	

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