Comparison of numerical simulation to experiments for a jet nebulizer

N. Lelong * (1), L. Vecellio (1), A. Junqua-Moullet (2), Y. Sommer de Gelicourt (3), C. Tanguy (4), P. Diot (5), H. Suzanne (2)
(1) – DTF Aerodrug, Faculté de Médecine, Tours, France
(2) – CEA Le Ripault, Monts, France
(3) – ANSYS France, Montigny le Bretonneux, France
(4) – Dantec Dynamics, Nozay, France
(5) – INSERM U1100 – EA 6305, Faculté de Médecine, Tours, France
nicolas.lelong@etu.univ-tours.fr, vecellio@med.univ-tours.fr,
alexandra.junquamoullet@cea.fr, yann.sommerdegelicourt@ansys.com,
christian.tanguy@dantecdynamics.com, diot@med.univ-tours.fr, herve.suzanne@cea.fr

Abstract

The development of jet nebulizers for medical purposes is an important challenge of aerosol therapy. However the increase of the output rate of smaller droplets through experiments has reached a plateau. The purpose of this study is to design a numerical model simulating the nebulization process and to compare it with experimental data obtained from various measurement methods. Such a model allows a better understanding of the atomization process and a determination of the relevant physical parameters influencing the nebulizer output. A model based on the Updraft nebulizer (Hudson) was designed with ANSYS Workbench. Boundary conditions were set with experimental data and the relevant model parameters were determined through a 2D axial simulation. Two air flow rate (2L/min and 8 L/min) were tested to consider different turbulence regimes. Experimental methods such as laser diffractometry, phase Doppler anemometry and CCD camera were used to characterize the spray output. Observations made with CCD camera showed similar patterns as numerical results like film formations or droplet spreading. Droplet sizes predicted by numerical results are close to distributions obtained from image processing. However, size is overestimated in relation to PDA and diffractometry. The simulation provides a good modeling of the phenomena causing droplet atomization and could help predicting nebulizer output with defined parameters.

Introduction

Aerosol therapy is traditionally used in medicine to deliver drugs into respiratory ways. It targets the affected organs, which increases therapeutical effects and reduces side-effects. The main drawback of the technique is the low fraction (10 %) of the delivered dose actually reaching the targeted area. Jet nebulizers are widely employed in this field because of their low cost but provide relatively low output and their development is still empirical. The size of the produced droplets affects their ability to be deposited in the human lung. The current challenge is to manufacture devices with a higher liquid flow rate of micrometric particles, especially with a diameter less than 5 µm. The improvement of nebulizer performances through experimental research seemed to have reached its maximal potential, so a new approach was introduced. A numerical simulation of the nebulization process was developed in order to understand the behavior of the liquid into the device and the influence on nebulizer output of relevant parameters regarding geometry, gas (pressure, flow rate), and liquid (viscosity, surface tension).

Numerical simulation has been employed to model the collision, coalescence or breakup of droplets in other domains [1]. Particle tracking is available in software like ANSYS Fluent [2]. Therefore the nebulization process, in particular the fragmentation of liquid in particles from 1 to 200 µm, is an unsteady phenomenon characterized by a micrometric size scale and an air velocity up to 400 m/s in the fragmentation area. A discretization of such a process needs high computation power. The CEA made available the supercomputer TERA to compute this model with reasonable time. A model based on the geometry of the Updraft II Optineb (Hudson) jet nebulizer has been designed with ANSYS Workbench and relevant numerical models were set on ANSYS Fluent.

Various measurement methods have been developed to evaluate aerosols characteristics produced by nebulizer, especially particle size. Laser diffraction is a robust and reliable method to evaluate medical aerosols, providing a volumetric size distribution over the whole nebulizer size range [3]. Phase Doppler Anemometry

* Corresponding author: nicolas.lelong@etu.univ-tours.fr

(PDA) can be used to characterize simultaneously droplet sizes and velocities from medical aerosols [4], allowing an accurate measurement in a localized area. Unlike laser diffraction, PDA provides a number distribution.

CCD Camera allows a visualization of the liquid behavior during the process and, through post-processing software, a determination of the size of the produced droplets [5].

The purpose of this study is the comparison between data obtained from the model and from experimental methods in terms of phenomenology and particle size. Numerical computations and experiments were made at two different air flow rates to account for turbulence regimes.

Material and Methods

Device

A jet nebulizer produces micrometric droplets by aspirating a liquid into a nozzle with compressed air through Venturi effect (figure 1). The ejected liquid hits a baffle and fragment into droplets. The Updraft II Optineb (Hudson) nebulizer was chosen to design the geometry of the simulation domain. It has a hemispheric baffle and its axial symmetry enabled a 2D-axisymmetric preliminary in order to set physical and numerical models.

Two air flow rates were considered, corresponding with different turbulence regimes at the output: 2 L/min (low turbulence: Re ~ 4000) and 8 L/min (high turbulence: Re ~ 16000).

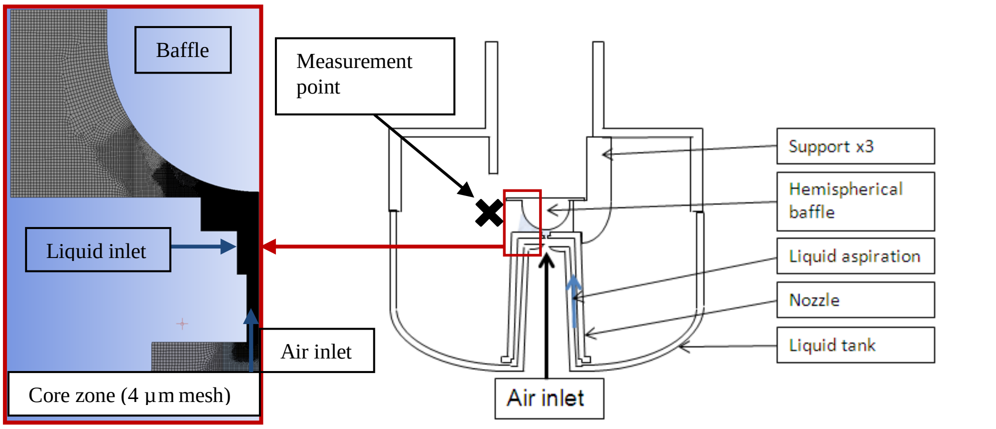

Figure 1 : Updraft nebulizer - simulation domain

Numerical study

The 3D simulation domain was designed with ANSYS Workbench based on the geometry of the Updraft. It regroups the areas where the liquid goes from a continuous phase to a discrete droplet phase, from the nozzle to the nebulizer outlet (figure 1). Because of its axial symmetry, the considered domain could be reduced to a 15° angular sector. Mesh size was 4 µm in the central zone (based on Pope criterion), where the liquid fragmentation takes place. The whole mesh held 4 million cells.

Preliminary simulations were made in FLUENT 13.0 with a 2D domain to set boundary conditions: air velocity and pressure, liquid velocity due to aspiration through venture effect in the nozzle. 2D axisymmetric simulations were used to determine which physical and numerical models in FLUENT 13.0 best predict the behavior of the liquid, the formation and transportation of the droplets. Multiphase model was selected, using the Euler-Euler approach (both phases being treated as continuous) and the Homogeneous Volume Of Fluid-model (VOF/free surface). A single set of momentum equations is shared by the fluids, and the volume fraction of each of the fluids in each computational cell is tracked throughout the domain. The gas/liquid interface was obtained via a piecewise linear interpolation scheme. Large Eddy Simulation with Dynamic Subgrid model has been used as the turbulence model to account for the wide range of Reynolds regimes in the process. After setting all relevant parameters, the 3D calculations were run in parallel on TERA. FLUENT was executed on 60 cores, the case having good scalability. At 2 L/min the average time step was 60 ns, while at 8 L/min the model was more unstable and the time step was decreased to around 7 ns. 2 L/min computations were run during 4 months, which is around 100 ms nebulization. 8 L/min computations were run during 2 months and are still in progress. 4 ms have been computed so far.

A User Defined Function (UDF) in C language function was added into the model to count droplets in and determine their diameter and center position. With the high number of detected particles (over 10 000), statistics could have been made.

Experimental methods

Various experimental methods were used to get accurate qualitative and quantitative data to be compared with numerical results. In order to characterize the droplets ejected from the hemispherical baffle of the Updraft, its plastic cover was cut so that laser beams (PDA & Laser diffractometer) and CCD camera could reach the area. The measurements were made as close as possible to the baffle to minimize influence of the modified airflow (figure 1).

CCD camera

To visualize liquid fragmentation and measure droplet size and velocity, a Photron Fastcam SA1 CCD camera was used. The camera was equipped with 2x zoom and a Nikon 200 mm macro objective, placed at 1 m from the camera to increase magnification as much as possible. This setup has an overall magnification of 13.3 (measured with a calibrated target), meaning that on the 1024x1024 pixels camera sensor, one pixel is 1.35 µm. The nebulizer was connected to an air compressor and observed through shadowgraph method. A 400 W Dedolight HMI spot followed by a convergent lens was set in alignment with all other devices to provide very high lighting to the measured area.

Images were acquired through the camera viewer software (Photron Fastcam Viewer). Preliminary tests allowed the determination of optimal settings to observe the droplets. The frame rate must be sufficient to see the trajectory of a droplet on many images but the frame size and resolution decreases with higher frame rate. Acquisitions were made at a frame rate of 10 000 images/s (768x768 pixels) for the 2L/min case and 30 000 frames/s for the 8L/min case, the droplets moving faster at higher flow rate. The shutter speed must be high to get accurate droplet contours but strong lighting is necessary. Droplet velocity in that area being around 5 m/s, optimal shutter time is 0.27 µs. The shutter time was set at its minimal value: 10^{-6} s.

In the viewer, brightness and contrast were set to enhance image quality. To ensure reproducibility, 3 sets of 100 images for each flow rate were then imported from 3 different acquisitions in the Dynamicstudio software (Dantec Dynamics), providing around 4 000 droplets for 2 L/min and 7 000 droplets for 8 L/min. Important background noise was obtained because only a minority of droplets was in the narrow depth of field (~1 mm), which is an important limitation of the method. After subtracting the pixel mean value for each image, a shadow processing analysis was made to mark droplet boundaries. The software allows the detections of droplets bigger than 3 pixels, so 5 µm minimum. Size distribution histograms were then plotted.

Furthermore, the liquid phenomenology in the transient phase was also acquired with the CCD camera, with direct lighting this time. The magnification was lowered to 5.5 to widen the field in the sphere area. Frame rate was increased to 40 000 frames/s.

Laser diffractometry

Laser diffraction characterizes particle sizes produced by nebulizers. The Spraytec (Malvern) laser diffractometer uses the Mie theory to determine the particle geometric diameter (diameter of the sphere containing the droplet) and provide instant particle size distributions within a 1 cm beam. The nebulizer was connected to an air bottle equipped with a flowmeter and was set so that the laser beam crossed the baffle exit area. The device was placed 10 cm from the receiver to avoid droplets to reach the lens and 6 acquisitions were made with each flow rate. The distribution obtained from the Spraytec is volumetric, so it was turned into a number distribution to be compared with the other methods. The size range of the Spraytec allows the detection of droplets down to 0.5 µm, so all droplets less than 5 µm had to be removed to do relevant comparisons.

Phase Doppler Anemometry

A PDA system provided by Dantec Dynamics was used in this study. PDA allows a measurement targeted in a localized area, counting and characterizing each particle flowing through a small control volume (2.10^{-4} mm^3). The measurements are performed at the intersection of two laser beams, and the nebulizer is set on a support, so that the beams intersect as close as possible of the sphere. The multiple detectors on the receiver, which is placed at an off-axis location, detect the light scattered by particles. Size and velocity are determined respectively from phase differences between detectors and frequency of the Doppler burst. Sizes down to 0.5 µm could be determined [6]. The obtained particle size distribution is then a distribution over a definite time (up to 10 000 drops) whereas laser diffraction provide instant distribution over a definite volume. With this method, the size homogeneity of the aerosol cloud could be verified. The used mask allows droplets up to 80 µm to be detected. The obtained particle size histograms were then cut after 5 µm to be compared with other methods.

Results

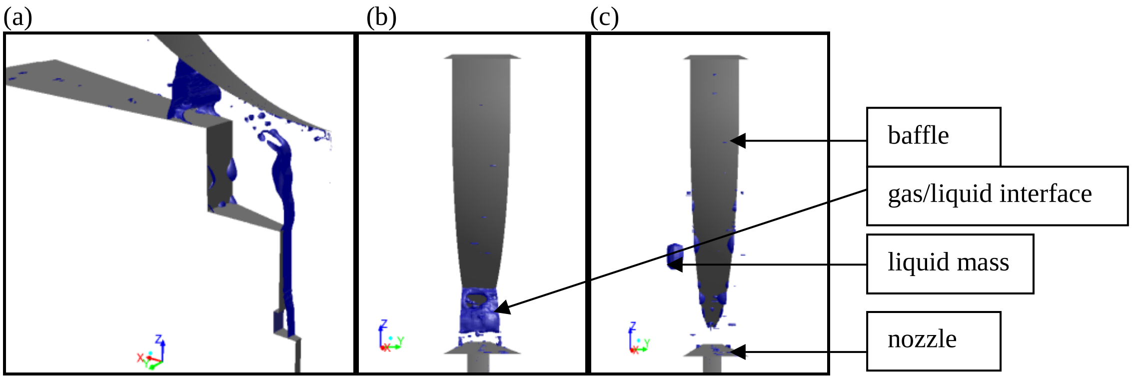

Figure 2 : Free surface images at 2 L/min – film formation (a), stretching (b), droplet formation (c)

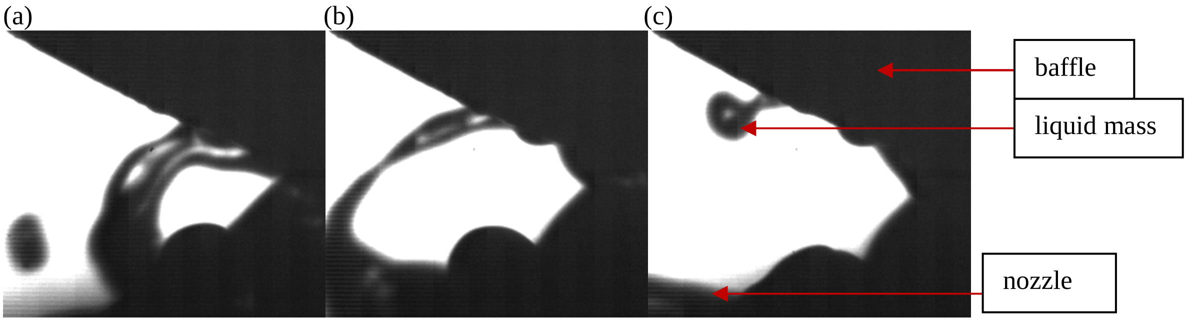

Figure 3 : CCD camera images at 2 L/min - Film formation (a), stretching (b), droplet formation (c)

Regarding liquid phenomenology during the nebulization process, both numerical results and camera observations showed similar patterns. Figures 2 and 4 display the gas/liquid interface (in blue in the figures) between the nozzle and the spherical baffle, which correspond to cells with a volume fraction of 0.5, representing the contour of liquid masses and droplets. Figures 3 and 5 show images obtained with the CCD camera

At 2 L/min, the flow had low compressibility (Ma = 0.3). The formation of liquid films between the sphere and the nozzle was observed in both cases (Figure 2 and 3). Many droplets impacted on the sphere, then spread and coalesced to form bigger masses on the solid surface. These masses were submitted to a balance of gravity and air thrust. When the mass became important enough, it slid towards the axis and formed a film bridging nozzle and baffle. Then the pressure of air blocked behind blew up the film into many droplets with size up to 150 µm. According to simulation results, this process was periodic and most of the droplet volume was produced during the film breakup. The total volume of liquid inside the domain was in constant increase during the computed 100 ms of nebulization, showing that the process was in a transient phase. The film formation was observed 4 times, each separated by around 23 ms.

A small amount of droplets were generated through rebound and breakup of faster liquid masses. The camera observations showed also film formations and breakups into large drops. However, no temporal periodicity or axial symmetry was recorded, these phenomena occurred simultaneously and randomly around the sphere.

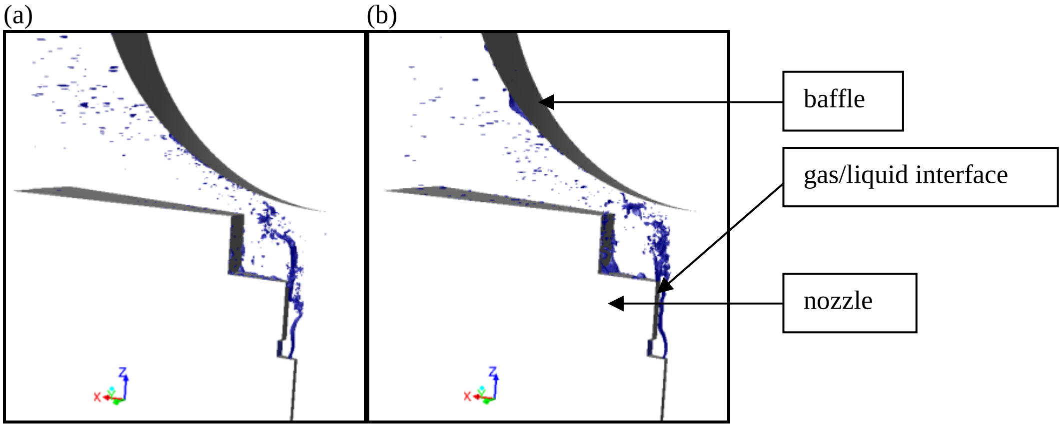

Figure 4 : Free surface images - 8 L/min – fragmentation of droplets (a), formation of an annular liquid layer (b)

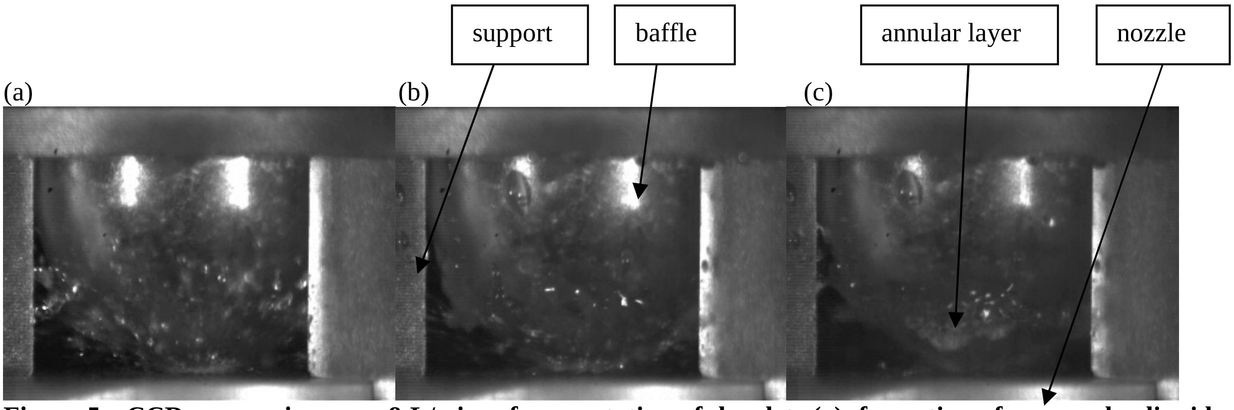

Figure 5 : CCD camera images - 8 L/min – fragmentation of droplets (a), formation of an annular liquid layer (c)

At 8 L/min, no film could be formed. The air velocity at the nozzle hole was 400 m/s. The air flow was in supersonic regime (Ma ~ 1.4), velocity peaks up to 700 m/s and shocks were recorded at the exit of the nozzle. Both observations and simulation showed that the low amount of liquid that spread on the sphere was not sufficient to compensate the air flow. Droplets came continuously from the nozzle hole (figure 4a & 5a). An annular liquid layer formed on the sphere where the air flow could not reach it (figure 4b & 5c). It was constantly fed with liquid spread on the surface and small droplets were ripped off from it. Camera images showed that this process is repeatable around the sphere axis. The total volume of liquid reached a plateau very quickly. From 2 ms of computed nebulization, the volume plot showed a slow increase, which only regarded the outer part of the domain.

	Numerical results	**Camera**	**PDA**	**Spraytec**
2L/min	**26.5 ± 20.6 µm**	**21.2 ± 18.6 µm**	**17.7 ± 20.6 µm**	**8.9 ± 5.7 µm**
8L/min	**17.1 ± 9.1 µm**	**14.1 ± 8.2 µm**	**8.6 ± 7.5 µm**	**8.7 ± 4.8 µm**

Table 1 : Particle size obtained with CFD and experiments - Mean ± SD

Table 1 shows mean and standard deviation obtained from numerical post-processing and particle size measurement methods, each for 2 L/min and 8 L/min. Several thousand droplets were considered for each value to avoid statistical errors. No droplet count could be done with the Spraytec but the beam size and the measurement time was sufficient to consider a large amount of droplets. For all methods, the mean droplet size became lower at higher flow rate, as well as the standard deviation. The overall order of magnitude was the same. CFD and CCD camera, which consider the same size range and have similar limitations (mesh size / image resolution), provided similar values. The difference between the mean values was about 20 % and standard deviations were similar.

Figures 6 and 7 show particle size distributions obtained with the simulation and the three measurement methods. For both flow rates, the simulation and camera plots showed similarities, especially at 8 L/min. The maximal amount of droplets was reached between 10 and 20 µm in numerical results but was always under 10 µm with experimental methods, even with CCD camera. This was certainly an effect of the computational grid chosen here: 4µm. PDA and laser diffractometry, which take into account droplets with a diameter less than 5 µm, provided much smaller values. At high flow rate, these methods had the same distributions.

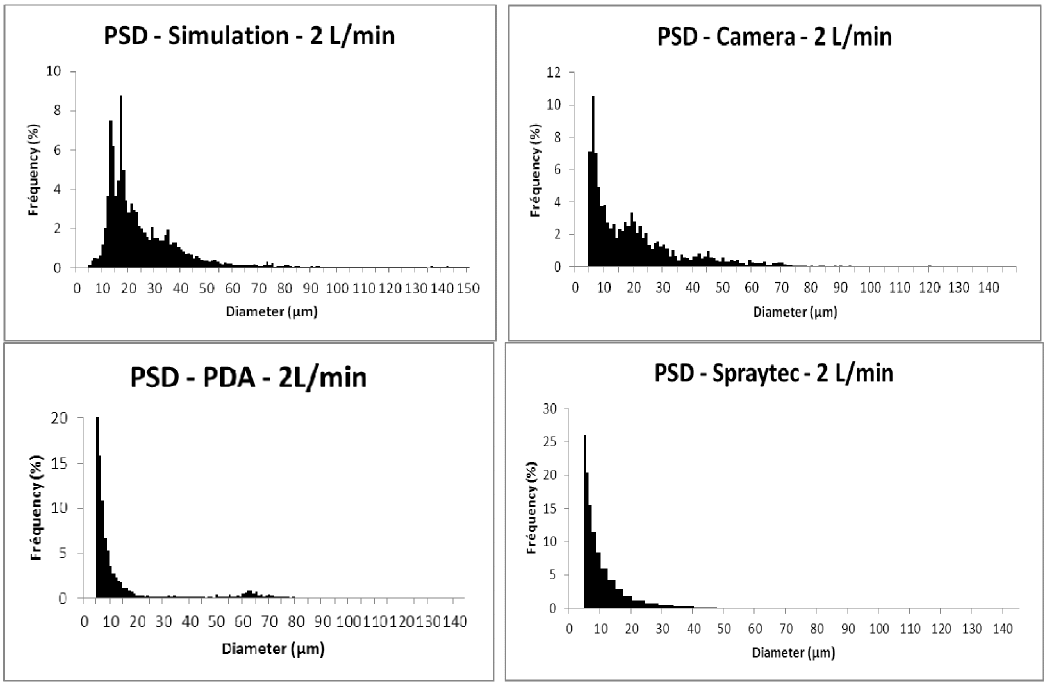

Figure 6 : Particle Size Distributions obtained with numerical and experimental methods at low flow rate

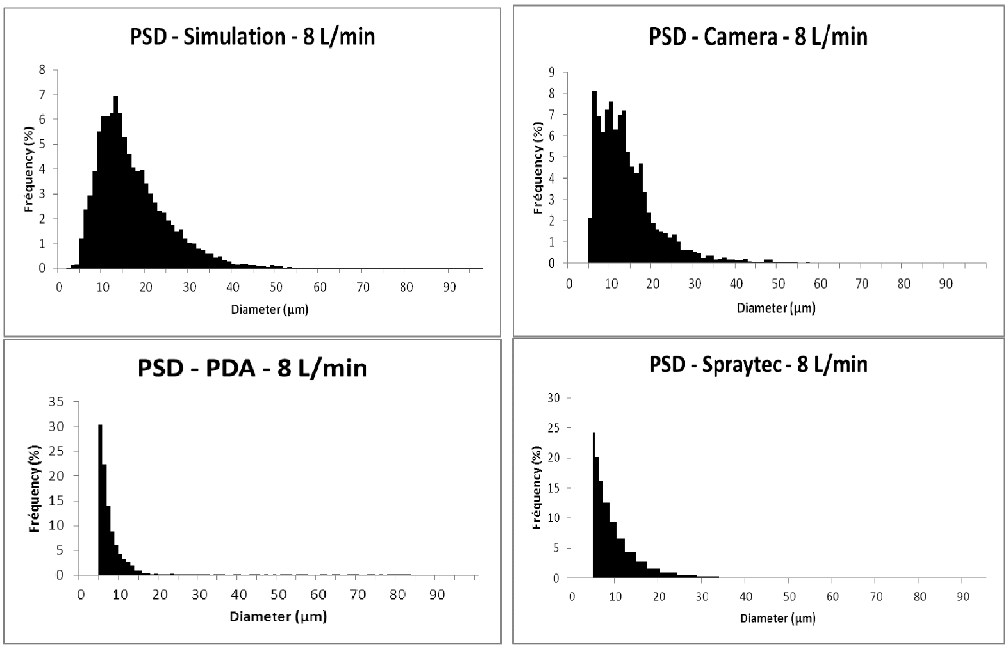

Figure 7 : Particle Size Distributions obtained with numerical and experimental methods at high flow rate

Discussion

For both considered flow rates, the liquid patterns predicted by numerical images could be observed with the camera. At 2 L/min, the formation and stretching of liquid films between nozzle and sphere, which occasionally burst into larger droplets, appeared randomly around the sphere. The CFD model only predicted liquid behavior on a 15° angular sector for CPU time purpose, and the formation of these patterns was periodic. Experimental images showed that the axial symmetry of liquid patterns cannot be established at low flow rate. Numerical results could not be extrapolated on the whole volume. The model did not consider the three supports around the sphere, which fix its distance from the nozzle. These pieces disrupt the airflow and bring surfaces on which the liquid could spread, but are necessary to maintain the distance between the sphere and the nozzle. Furthermore, a circular water film around the sphere would block the airflow and cause pressure increase inside the film. The noticed periodicity showed that every phenomenon which could occur should have been observed in the transient phase.

At 8 L/min camera images showed a continuous production of small droplets and the progressive formation of a liquid ring on the sphere surface. The observed pattern was then axially symmetric and was also predicted by the model on the angular sector. At high flow rate numerical results could be widened to 360°. The transient phase was much shorter than at 2 L/min, the air was supersonic and the fragmentation of liquid was more important. The larger masses and droplets were broken up before they could reach a surface. The liquid could only spread on the sphere where the airflow could not reach it, forming a ring around the sphere.

Particle size measurements over thousands of droplets had similar distributions in both camera measurements and simulation results. However, the differences obtained between CFD and camera mean values (26 µm vs. 21 µm; 17 µm vs. 14 µm) were in the same orderof magnitude as mesh size (4 µm) or image resolution (1.35 µm/pixel). Given these limitations, CFD provided a good estimation for particle size.

With a 4 µm mesh, smaller droplets, which only correspond to a few cells, are prone to numerical diffusion. The detection of the droplet boundary was set when the volume fraction was equal to 0.5, so diffuse boundaries could lead to larger droplets in the simulation. The CCD camera is the most adapted experimental method to compare nebulizer output in terms of particle size given by the model. The camera allows the visualization of liquid fragmentation and measures droplets detected in a wide frame with a small field depth at the exit of the sphere, which approximately corresponds to the output of a 15° angular sector. Particle sizing through image processing considers the particle shape and avoid sphericity errors [5]. In both cases, droplets under 5 µm are not considered, because of mesh size or image resolution.

PDA and laser diffraction provided smaller distributions, with a frequency of droplets decreasing exponentially with the size. For both methods, the measure point was further from the sphere and some evaporation could occur. These measurement methods take into account a large amount of droplets less than 5 µm. PDA characterizes droplets passing in a narrow area, but measurements in different points showed similar distributions. Only 40 % of the 10 000 droplets in PDA measurements had a diameter larger than 5 µm. Droplets measured by PDA must be spherical, so an accurate measurement must take place far enough from the fragmentation area. The phase difference measured by the receiver depends on the radius of curvature of the droplet. In that study, up to 30 % were detected as non-spherical droplets. Laser diffraction is suited to measure volume distributions, which is the relevant characteristic for medical aerosols. A small volume frequency detected for a small size corresponds to a large number of droplets. The exponential width of the size classes for the obtained distribution could lead to approximations for larger diameters. With this method, droplets with a diameter less than 5 µm account for a very large fraction of the total number of droplets. Only 0.07 % of the total number of detected droplets was considered in the plotted distributions.

Conclusion

The CFD modeling of the nebulization process predicted phenomena recorded by camera CCD. At low flow rate, liquid films formation, stretching, droplet spreading on the sphere and breakup of films into smaller droplets were recorded. At high flow rate, fragmentation of droplets before impinging on the baffle and formation of an annular liquid layer on the sphere were observed. The size distributions and mean values obtained from camera and numerical results matched with a 20 % relative error equivalent to the mesh size.

Particle size obtained with other experimental methods like PDA and laser diffraction was significantly lower but these methods consider a lower size range and have other experimental limitations like sphericity errors. CCD camera was the most adapted method to validate the numerical model.

Simulation is the only possible method to determine how the liquid interacts with air inside the nozzle and when impinging onto the spherical baffle. The validation of the model at a coarse level, for droplets with a diameter over 5 µm, allows the understanding of the primary atomization process. However, in order to optimize nebulizer performance, particles under 5 µm are concemed. A refinement of the mesh in the current model would be too time-consuming with the currently available computing power. Nevertheless, droplets between 0.5 µm and 5 µm are subject to same dynamics as larger particles. The fact that the generation process of these droplets is similar as with larger droplets would be a reasonable assumption. Then, by modifying the physical parameters in the model, ways to increase the flow rate of small droplets and thus the nebulizer output could be determined.

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