Innovative bi-fluid atomizer inner flow characterization and outer spray diffusion analysis

D Elzo, C Mazin
Fluid Mechanics Department, ICAM Toulouse, 75 Avenue de Grande Bretagne, 31300 Toulouse, France
E-mail: dominique.elzo@icam.fr

Abstract. We developed an atomizer nozzle equipping a medical device used for airborne disinfection of medical rooms. The diffusion technology of the equipment is based on the spraying of fine liquid droplets of disinfectant into the volume to be treated. The liquid phase is expelled thanks to an air assist atomizer we designed, which originality comes from the geometry we give to the throat of the micro-venturi, inner part of the atomizer nozzle. The micro-venturi throat is deviated of angle of 4° and will permit a homogeneous diffusion. We computed three dimensional numerical calculations of the inner compressible turbulent air flow through the atomizer we designed and compared the results obtained with the ones computed for a symmetrical atomizer. The modeling was done with the CFD codes STARCCM+ and Fluent, choosing the k-omega turbulent model. The modeling has been validated especially by one dimensional analytical calculations and experimental measurements of the mean axial velocity and mass flow rate circulating through the atomizer. Three dimensional numerical calculations show the vertical deviation of the flow at throat level and swirl effect generated by the deviated inner throat of the micro-venturi. These calculations allowed understanding the nature of the spray observed in experimental conditions, and the advantages to use a deviated micro-venturi throat. Indeed, micro bacteriological tests showed that the quality and the effectiveness of the diffusion are enhanced in comparison to equipments with a symmetrical micro-venturi.

1. Introduction
This paper presents analytical, experimental and numerical calculations of air flow circulating through a mixed liquid-air atomizer. The spray generated by the atomizer is used in medical applications for airborne decontamination.

First, we performed a one-dimensional analytical calculation of the hydrodynamic and thermodynamic parameters of the air phase within the atomizer. We considered a purely isentropic flow through the atomizer, a micro convergent-divergent nozzle, known as a micro-venturi and the extended diverging duct, namely the diffuser. These analytical results were confirmed by air mass flow rate and velocity measurements throughout the venturi-nozzle for a range of operating pressures. Afterwards, a Computational Fluid Dynamics (CFD) (STARCCM+ code) was used to perform three dimensional modeling of the flow. This modeling completed the analytical calculation, taking into account the specific throat deviation of angle $\psi$ (> 0) in the radial direction of the micro-venturi [1], [2], and the three dimensional aspects of the turbulent flow showing vortices generation, and boundary layer detachment.
2. Micro-venturi nozzle geometry

As we mentioned in previous papers [1], [2], a specific atomizer was designed in order to produce a spray for airborne decontamination of medical rooms.

The effectiveness of decontamination and homogeneous diffusion in the room to be treated has already been proven [3], [4], [5], and [6]. The key part of the bi-fluid atomizer is a micro convergent-divergent nozzle extended by a divergent diffuser as shown in figure [1]. We name this assembly the atomizer nozzle.

3. Analytical calculation of the flow within the micro-venturi

We considered a quasi-one dimensional fluid flow within the atomizer nozzle: the fluid follows the axial direction x. Since \( dA(x)/dx \ll 1 \), all the flow properties are a function of x only: \( A = A(x) \), \( p = p(x) \), \( \rho = \rho(x) \), \( u = u(x) \) and \( M = M(x) \).

\( A \) is the flow area of the micro-venturi, \( p \) the static pressure, \( \rho \) the density, \( u \) the axial velocity and \( M \) the Mach number. The quasi-one-dimensional isentropic flow is dictated by the area-Mach number relationship [7]:

\[
\left( \frac{A}{A^*} \right)^2 = \frac{1}{M^2} \left[ \frac{2}{\gamma + 1} \left( 1 + \frac{\gamma - 1}{2} M^2 \right) \right]^{(\gamma + 1)/(\gamma - 1)}
\]  (1)

\( M \) is the local Mach number, \( A \) the local flow area, \( A^* \) the sonic flow area, \( \gamma \) the ratio of the specific heat of the air, \( \gamma = 1.4 \). From equation (1) and from isentropic flow and normal shock tables [7], we demonstrated that the flow is subsonic in the convergent section of the micro-venturi, reaches the speed of sound (\( M = 1 \)) at the level of the throat, and continues accelerating to supersonic velocities in the divergent section. We showed that sonic flow is attained at the throat, and that we were in a situation of choked flow. It means that the air mass flow rate remains constant within the micro-venturi and is only a function of the pressure and temperature supplying the micro-venturi and of the throat area. The mass flow rate through a choked nozzle is given [7], by equation (2):

\[
\dot{m} = c(\gamma, r) \frac{p_i}{T_i^{\gamma/\gamma - 1}} A^* \cdot CD
\]  (2)

where: \( A^* \) (m²) is the sonic throat area, \( p_i \) (Pa) the absolute air pressure at micro-venturi inlet, \( T_i \) (K) the air temperature at micro-venturi inlet, \( c(\gamma, r) = 4.042 \times 10^{-2} \) the critical mass flow rate.
coefficient for air, and CD = 0.96, a corrective mass flow rate coefficient. The value of CD was
deduced from [8] who give various functions for spray cone half angle $\alpha$, as a function of the
atomizer constant K and the discharge coefficient CD. In fact, five different expressions of
theoretical functions and experimental results giving spray cone half angle $\alpha$, plotted against the
atomizer constant K allow to calculate CD from our experimental visualization of $\alpha$
The validation of the choked flow conditions and of the mass flow rate expression from equation
(2) were done with velocity and mass flow rate measurements at the air-assist nozzle outlet.
The measurements were performed with a hot wire anemometer, FLUKE 922 (± 1 m/s), with a
series of ten tests for each inlet pressure $p_i$. We performed the calculations for the air phase since
the spray is highly diluted and since the liquid phase droplets follow air phase flow streamlines
closely. Indeed, the value of the Stokes number, $S_t = \tau_r / \tau_l$ ($\tau_r$ and $\tau_l$ are respectively the droplets
and convective air phase relaxation time.) smaller than 1, indicates that the suspended liquid
droplets follow the trajectory of the air phase. Figure [2] shows especially at the absolute inlet
pressure we diffused the spray, it means $p_i = 4$ bar, a mass flow rate of the air phase of $1.2 \times 10^{-3}$
kg.s$^{-1}$. At this inlet air atomizer pressure the mass flow rate of the liquid phase is of $5.10^{-4}$ kg.s$^{-1}$,
resulting in a diluted spray. In figure [2] we can see an excellent correlation between the analytical
and the experimental results, with maximum difference of 5%. The hypothesis made about the
isentropic flow conditions and the sonic conditions at the throat, and the value of the discharge
coefficient CD of the micro-venturi were validated. These one dimensional analytical calculations
and measurements permitted to validate the numerical results we present in the following section.

![Air mass flow rate inside the air-assist nozzle](image)

**Figure 2.** Air mass flow rate through the atomizer for a range of inlet pressures $p_i$, at $T_i = 290$ K

4. Three dimensional CFD modeling of the air phase within the micro-venturi nozzle

We designed the deviated micro-venturi with the software Catia®V5, and meshed and analyzed it
with two CFD software, STARCCM+ for the pressure and velocities fields, and Fluent for the
contours of vortices (described in section 4.5). The modeling allowed describing three dimensional
phenomena not quantified with the analytical method, and gave us data like velocities (axial and radial
ones) and pressure fields, and allowed to determine the vortices magnitude of the flow.
4.1. Solver and solution method
We use a density based solver, recommended for compressible flow and high Reynolds number flow.
We choose the explicit option of the density-based solver, and each equation in the coupled set of
governing equations is linearized explicitly. It results in a system with N equations for each cell in
the domain and likewise, all dependent variables in the set will be updated at once. In other words,
the density-based explicit approach solves for all variables $(p, u_i, T)$ one cell at a time. We ran
transient simulations, using a second order implicit time integration.

4.2. Boundary layer specifications
The interior of the micro-venturi is represented by a stationary wall, adiabatic with no-slip condition
and a roughness constant equal to 0.5.
The inlet is represented by a pressure far-field condition, with a 4 bar gauge pressure, a 0.041 Mach
number and a 300K constant temperature. These boundary conditions are those of the fluid flow
during a real diffusion process. The turbulent specification method is given by the constant
intermittency (equal to 1), the turbulent intensity (1.5%) and the turbulent viscosity ratio (equal to
10). This turbulent intensity is recommended to be in the range of $[1 - 5\%]$ for high Reynolds
numbers. The outlet is represented too by a pressure far-field, with a 1 bar gauge pressure, a 0.105
Mach number and a 300K constant temperature. The turbulent specification method is given by the
constant intermittency (equal to 1), the turbulent intensity (1.5%) and the turbulent viscosity ratio
(equal to 10). This turbulence model is the one used by Launder and Sharma [4].

4.3. Venturi geometry and Mesh grid resolution
The three dimensional venturi is characterized by (figure [3]):
- a converging duct of length of 4.1 mm, height from 4.78 mm to 1.3 mm (diameter of
  the throat) with a half converging angle of 24°
- a deviated throat of length of 1.7 mm, of diameter of 1.3 mm, and of angle of deviation
  $\psi = 4^\circ$ (figure [1]),
- a diverging duct of 3.7 mm length, from 2.27 mm to 1.7 mm height, with an 8° of half
  diverging angle.
- A diverging diffuser of 4.5 mm length and of exit diameter of 6 mm.
The mesh grid is made of 51000 nodes and 161000 cells. We can see on figure [3] that the grid
adjacent to the walls is finer as compared to that in the central region. The purpose for such fine
mesh is to capture sharp gradients near the walls correctly.
For more clarity, we only represent in figure [3] the micro-venturi geometry. The diffuser geometry
has been taken into account in the modeling as it is showed thereafter (figures 4, 5, 6 and 7).
We must precise that the inner diameter of the diffuser extremity is of 6 mm, and the distance
between the exit divergent duct $(x = -9.5 \text{ mm})$ and the diffuser extremity is of 4.5 mm. The total
length of the assembly micro-venturi + nozzle is of 14 mm.
The transversal length range in the $z$ direction is identical to the ones taken for the vertical direction
since we have a revolution surface.
The fluid flows in the negative $x$ direction as shown on figure [3] below. The center of the throat is
located at $x = -4.75 \text{ mm}$ and has a radius of 1.7 mm. We only consider in the numerical models
only the air phase, the droplets being vectors of the air phase.
4.4. Numerical modeling results
The pressure and axial velocity fields obtained with the three dimensional CFD modeling can be shown in figures [4] and [5]. We can observe in figure [4] that a shock zone is sized in the divergent part of the micro-venturi. This recompression zone results in the fragmentation of the liquid phase into less than 50 micrometer droplets.
We obtain the velocity fields, reported in figure [5] through the diverging diffuser, essential information to get nozzle exit velocity fields and to compare to the analytical calculations. We report on table [1] the main fluid flow parameters obtained analytically and numerically. The comparison is done at inlet, throat and outlet sections of the micro-venturi. We report Mach number $M$, axial velocity $u_x$, absolute pressure $p$, mean mass flow rate $\dot{m}$ and local Reynolds number $R_{eD}$ (based on the local diameter $D$ of the micro-venturi). We found similar range of values along the deviated micro-venturi nozzle as for the analytical calculations. It is validating our modeling, getting further essential informations at inlet diffuser and exit nozzle location.

**Table 1.** Comparison of the analytical and numerical CFD results of the fluid flow parameters at inlet, throat and outlet section areas of the micro-venturi

| Fluid flow parameters | Analytical results | Numerical CFD results |
|-----------------------|--------------------|-----------------------|
| Mach number $M$ | Inlet | Throat | Outlet | Inlet | Throat | Outlet |
|                      | 0.041   | 1      | 2.65  | 0.02 - 0.10 | 0.91 - 1.04 | 2.44 - 2.57 |
| Axial velocity $u_x$ (m/s) | 14.1   | 311    | 586   | 2.2 - 35.4 | 240 - 300 | 472 - 508 |
| Absolute pressure $p$ (bar) | 4      | 2.11   | 0.184 | 3.8 - 4.0 | 2.05 - 2.24 | 0.13 - 0.22 |
| Mass flow rate $\dot{m}$ (kg/s) | 0.0012 | 0.0012 | 0.0012 | 0.0010 - 0.0011 | 0.0010 - 0.0012 | 0.0008 - 0.0013 |
| Reynolds number $R_{eD}$ | 2134   | 35200  | 88700 | 333 - 5375 | 36000 - 40100 | 86500 - 92000 |
To continue our analysis, we show that the throat deviation influence is definitely observed through figures [6] and [7] which show the radial velocity field $u_y$ respectively for a symmetrical and a deviated micro-venturi throat. The 3D effect becomes apparent at throat level for the deviated one, observing a significant deviation of the radial velocity profile (figure [7]).

**Figure 6.** Radial velocity $u_y$ as a function of the x coordinate for a symmetric throat nozzle

**Figure 7.** Radial velocity $u_y$ as a function of the x coordinate for a deviated throat nozzle

4.5. **Contours of vortices**

The observations done in experimental conditions showed that the spray diffused with a deviated micro-venturi nozzle exit with a rotational movement (swirl effect).
It is not observed with a symmetrical one. Therefore, we analyse the contours of vortices magnitude (as named in the STARCCM+ code) based on the rotational tensor $\Omega_{ij}$ given by:

$$\Omega_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right)$$

(3)

The effects of the deviation at throat level onto the flow at exit micro-venturi nozzle are observed onto Figure [8]. We can show at tip nozzle the mixing of the two separated boundaries layers. It gives place to the formation of more important structures able to interact with the main flow, creating at the exit of the micro-venturi vortices as observed experimentally (figure 10 below).

**Figure 8.** Contours of vortices magnitude at tip end of the deviated micro-venturi nozzle

### 4.6. Spray visualization

To complete our study, we analyze and observe the spray at exit nozzle with a video acquisition system [2] during the spray diffusion processes as shown on figures [9] and [10].

We observe (figure [9]) the lack of liquid spray phase on the lower part of the exit nozzle corresponding to the region situated below the detached boundary layer. We note also (figure [10]) periodic vortices with a vertical spray inclination due to the deviated throat. We can also compare the spray obtained with a deviated venturi, figure [11] and the one with an symmetrical one, figure [12], much more dense with no vertical inclination (resulting in an accumulation of liquid at onto the ground).

**Figure 9.** Spray diffusion visualization under CCD camera, noting a lack of liquid at bottom exit nozzle

**Figure 10.** Spray diffusion visualization, observing periodic vortices and vertical inclination of the spray
4.7. Conclusion
The analytical part showed a constant mass flow rate (choked flow) within the inner part of the air-asist atomizer nozzle, named the micro-venturi.

These calculations, under isentropic hypotheses were validated by mass flow rate measurements, and fluid mechanics equations governing continuity equation, energy conservation and oblique shock relationships for a mono dimensional flow.

We performed a three dimensional modeling of the flow with the CFD software STARCCM+ and Fluent. The precious additional information obtained from the numerical study were the observations of boundary layers detachment and vortices generation that appeared at the end part of the diverging duct of the deviated micro-venturi. It explains the vortices and the spray inclination observed experimentally. Moreover, it permits to plot the radial velocities at throat level. Conversely to a symmetric micro-venturi, this specific deviation prevents accumulation of droplets downwards the apparatus during the diffusion process and enhances the homogeneity of the spray into the volumes to be treated.

4.8. References
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