Disintegration regime of industrial fan-spray atomizers through CFD simulations

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Abstract
Among all the literature devoted to the investigation of sprays, very few works deal with the influence of the nozzle’s geometry on the characteristics of the spray produced, even though it has been proved to play a crucial role in certain operating regimes. The present paper presents criteria for the determination of the dominant disintegration regime in industrial fan-spray atomizers through CFD simulations accounting for the atomizer’s geometry.

Introduction

Fan-spray atomizers were object of research in several pioneering works in the field of atomization, like those of Magnus [1], Fraser and Eisenklam [2] and Dombrowski et al. [3]. A great interest aroused for this type of atomizers due to some special features that increase the difficulty of their analysis, such as an attenuating thickness and the accumulation of liquid at the borders of the sheet. The former characteristic is a valuable advantage, since it promotes the production of very small droplets. The latter is due to the contraction of the sheet boundaries as a result of surface tension. In the absence of surface tension, the edges of the sheet would travel following straight paths from the orifice forming a sector of circle. Otherwise, at low injection pressure, edge contraction lasts until both edges of the sheet coalesce. During contraction, drops are emitted from the edge following the direction tangential to the sheet at the point where they are produced. When sheet contraction is completed drops cross over from one side to the other. This breakup mode was called “rim disintegration” [2] and in several works [4][5] it has been proved to have a great influence on the breakup of the liquid sheet. At higher injection pressure, contraction is less pronounced and the sheet disintegrates before the two edges coalesce. Two additional sheet disintegration modes were also reported in [1] for this situation: under atmospheric pressure, a large wavelength sinuous wave grows and eventually leads to the sheet disintegration; while at sub-atmospheric pressure, perforation holes appear on the sheet and extend up to the disintegration of the whole sheet.

Since then, a lot of numerical and experimental studies concerning the physics of the destabilization and break-up of different liquid streams have been developed, but very few tackle the relationship between the atomizer geometry and the spray features.

The present paper is focused on the definition of criteria determining the dominant disintegration regime of industrial fan-spray atomizers through CFD simulations accounting for the atomizer’s geometry.

Description of the atomizers

Three different designs of industrial fan-spray atomizers, henceforth named N1, N2 and N3, have been analyzed. All of them are tiny plastic units with circular section geometry ending in a hemispherical cavity with a wedge-cut orifice, in such a way that the liquid sheet formed is parallel to the major axis of the orifice. These nozzles were designed so that, under nominal operating conditions of 3 bars, provide a flow-rate of 0.8 l/min but different liquid sheet angle: N1 provides a liquid sheet of 90º, N2 of 80º and N3 of 120º. The other main differences between nozzles are the shape of the orifice and the transition between different cross-sectional areas, the latter being rounded in nozzle N1 and sharp in nozzles N2 and N3.

Liquid sheet visualizations

High-speed images of the liquid sheets produced by N1, N2 and N3 have been captured in order to determine which of the aforementioned disintegration regimes take place and their relative importance (Figure 1).
Images of the liquid sheet produced by N\textsubscript{1} nozzles reveal that spanwise perturbations appear at the exit of the atomizer and spread downstream. These perturbations are clearly distinguishable near the breakup region, due to their increasing amplitude. The fact that these perturbations appear at constant angular positions in all the pictures of each unit indicates that their origin is geometric, that is, due to irregularities in the orifice; and not the instability of the liquid sheet itself. Although they do not seem to influence the liquid sheet breakup length, looking at the droplets it is easy to identify larger droplets at the angular coordinates of these disturbances. At high pressures these perturbations are “hidden” by the amplitude of actual instability disturbances. It should be noticed that this disintegration strongly resembles that of radial liquid sheets at high Weber numbers.

Even though the predominant breakup mode is the wave mode, the role played by the rim differs depending on the operating pressure. For 1 bar, the rim destabilizes and disintegrates before the liquid sheet does. Droplets from the rim continue their path attached to the liquid sheet by thin threads and the liquid between threads recedes due to surface tension. This phenomenon leads to shorter breakup lengths at the region near the rim and a more rounded shape of the breakup front. At injection pressures over 1 bar the breakup of the rim occurs downstream of the liquid sheet disintegration, following the behavior of a jet; and therefore the breakup front is not influenced by the rim.

For high operating pressures random disturbances appear within the liquid sheet near the outlet, probably due to the presence of turbulence generated inside the tip of the nozzle. However, these disturbances are damped out as travelling downstream and do not influence the breakup length.

Some perturbations are observed in the recorded sequences that momentarily decrease the liquid sheet breakup length. However, both their number and frequency are not high enough to affect the global performance of the atomizer.

In N\textsubscript{2} liquid sheets wave and rim modes predominate over perforations, the liquid sheet emerging highly disturbed from the nozzle (Figure 1). However, while disturbances within the liquid sheet tend to damp out as moving downstream due to the effect of surface tension, finger structures appear at the borders which rapidly disintegrate into a column of droplets. In this column, a large first droplet is followed by some smaller “satellite” droplets. The inter-finger receding fluid leads to a progressive decrease of the liquid sheet angle, just like in N\textsubscript{1} at low pressures. While in N\textsubscript{1} this phenomenon takes place far away from the orifice and the liquid sheet is hardly affected; in N\textsubscript{2} it occurs right after the liquid emerges from the orifice and has increasing influence on the disintegration of the liquid sheet as the injection pressure increases.

Finally, the disintegration of the liquid sheet produced by N\textsubscript{3} is governed by the interaction of all three modes; having all of them a similar relative importance. As can be seen in Figure 1, the border of the liquid sheet is already highly disturbed just downstream of the orifice. Thus the phenomena described for N\textsubscript{2} of droplet formation and subsequent liquid retraction, and interactions between rim and sheet dynamics start taking place at smaller radial coordinates, leading to shorter breakup lengths than those of N\textsubscript{2}.
Mathematical Model

A mathematical model has been developed to study the two-phase flow that takes place inside and near the outlet of the atomizer (Figure 2). The geometry of the nozzles allows the simplification of the domain using two symmetry planes (XY and XZ). Moreover, the length of the domain is such that liquid sheet’s perturbations have very small amplitude, and a stationary solution is wanted; thus it is reasonable to assume also the symmetry of the flow and model only a quarter of each geometry. Further details on the selection of the flow domain are given in [6].

![Figure 2. Schematics of the flow domain.](image)

The fluids employed are water and air, both assumed to be incompressible and with constant properties. The Reynolds Average Navier-Stokes (RANS) approach is used to model the turbulence effects though the RNG model, while the VOF approach has been chosen to cope with the multiphase flow. Thus, flow properties like density (\( \bar{\rho} \)) and viscosity (\( \bar{\mu} \)) are calculated in terms of the averaged gas volume fraction (\( \bar{\alpha} \)) as

\[
\begin{align*}
\bar{\rho} &= \bar{\alpha} \rho_l + (1 - \bar{\alpha}) \rho_g, \\
\bar{\mu} &= \bar{\alpha} \mu_l + (1 - \bar{\alpha}) \mu_g
\end{align*}
\]

where subindices g and l refer to liquid and gas phases and overbars indicate ensemble averaged values. The governing equations of the model are

\[
\begin{align*}
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i)}{\partial x_i} &= 0, \\
\frac{\partial \bar{\alpha} \bar{u}_i}{\partial t} + \frac{\partial (\bar{\alpha} \bar{u}_i u_j \rho_j)}{\partial x_j} &= \frac{\partial}{\partial x_j} \left[ \bar{\alpha} \left( \bar{u}_i \frac{\partial \bar{p}}{\partial x_j} - \bar{u}_j \frac{\partial \bar{p}}{\partial x_i} \right) + \frac{\partial}{\partial x_i} \left( \bar{u}_j \frac{\partial \bar{p}}{\partial x_j} \right) \right] + \frac{\partial}{\partial x_j} \left( \bar{\mu} \frac{\partial \bar{u}_i}{\partial x_j} \right) + (\bar{F}_{\rho})_i, \\
\frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial \bar{\rho} u_i k}{\partial x_i} &= \frac{\partial}{\partial x_j} \left[ \bar{\alpha} \left( \bar{\rho} u_i u_j \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right) + \frac{\partial}{\partial x_i} \left( \bar{\alpha} \bar{\rho} \frac{\partial \bar{u}_i}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \bar{\alpha} \bar{\rho} \frac{\partial \bar{u}_j}{\partial x_i} \right) \right] + (\bar{F}_{\rho} k), \\
\frac{\partial \bar{\rho} \varepsilon}{\partial t} + \frac{\partial \bar{\rho} u_i \varepsilon}{\partial x_i} &= \frac{\partial}{\partial x_j} \left[ \bar{\alpha} \left( \bar{\rho} u_i u_j \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right) + \frac{\partial}{\partial x_i} \left( \bar{\alpha} \bar{\rho} \frac{\partial \bar{u}_i}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \bar{\alpha} \bar{\rho} \frac{\partial \bar{u}_j}{\partial x_i} \right) \right] + C_{1_{\varepsilon}} \frac{\varepsilon}{k} \frac{\partial}{\partial x_j} \left[ \frac{\partial \bar{p}}{\partial x_i} \right] + C_{2_{\varepsilon}} \varepsilon^2 \\
\text{with}
\end{align*}
\]

where \( S_{ij} \) makes reference to the strain rate tensor and coefficients \( C_v, C_{1_{\varepsilon}}, C_{2_{\varepsilon}}, \sigma_{\varepsilon}, \beta, \eta_{\varepsilon} \) are taken as constants. The quantities \( \gamma_k \) and \( \gamma_{\varepsilon} \) are the inverse effective Prandtl numbers derived analytically from the RNG theory. The effective viscosity (\( \bar{\mu} + \mu_{\varepsilon} \)) is derived from a differential equation, in such a way that the capacities of the model to handle low-Reynolds-number flows and near-wall flows are improved. Three new terms have appeared in the equations after ensemble averaging and need to be modeled: \( u_i' u_j' \), \( \bar{u}_i' \bar{u}_j' \), and \( \bar{F}_{\rho} \). The first term, \( u_i' u_j' \) (Reynolds stress term), has been modeled adopting the Boussinesq hypothesis. The second, \( \bar{u}_i' \bar{u}_j' \), which represents the correlation between the fluctuations of volume fraction and velocity, would provide valuable information about the influence of turbulent scales on the liquid sheet dynamics. Based on [7], one can conclude that in the region near the outlet of the atomizer, where turbulent disturbances present small amplitudes, the effects of this term on the mean flow are negligible. Consequently, it has been omitted in the mathematical model. Finally, the last term corresponding to the fluctuations on the equivalent surface tension force has been calculated directly with the mean values of the variables.
At the tip inlet, profiles of total pressure, turbulent quantities as well as the velocity direction were enforced. Values for these fields were obtained from simulations of the entire inner geometry of the nozzles under study. Conditions for flow impenetrability and no slip were imposed on the walls. Additionally, it has been considered that the pressure gradient in the direction perpendicular to the wall is zero. At the outlets, a zero-valued gauge pressure field was enforced with very small constant values of turbulent quantities.

The flow domain has been discretized with a 3 million element hybrid mesh. The CFD code Fluent V.6.3, which discretizes the flow-governing equations through the Finite Volume Method, has been used to solve the mathematical model. The SIMPLE algorithm has been chosen for pressure correction. The interpolation schemes adopted for the simulations are listed in the following table:

<table>
<thead>
<tr>
<th>Transport Eq. Terms</th>
<th>Numerical Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusive</td>
<td>2nd Order Centered</td>
</tr>
<tr>
<td>Convective</td>
<td>2nd Order Upwind</td>
</tr>
<tr>
<td>Velocity interpolation</td>
<td>Rhie-Chow [8]</td>
</tr>
<tr>
<td>Pressure interpolation</td>
<td>Staggered-grid based scheme [9]</td>
</tr>
<tr>
<td>Volume fraction</td>
<td>HRIC [10]</td>
</tr>
</tbody>
</table>

**Results and Discussion**

To elucidate the fundamental differences between the liquid sheets formed by these three designs observed in high-speed visualizations, values of turbulent intensity at the XZ symmetry plane have been investigated (Figure 3). Turbulent intensity was calculated adopting the averaged velocity at the inlet of the atomizer’s tip as the reference velocity in order to be able to appreciate the subtle differences inside the nozzles.

Firstly, it can be seen that the liquid enters the tip of N₂ and N₃ nozzles with higher turbulent intensity, especially in the near wall region, due to their sharp cross-section changes. In N₁, on the contrary, rounded cross-section transitions lead to low turbulence levels. The sudden area reduction of the orifice increases turbulence.

![Figure 3](image-url)
generation in all three designs; this increase being more significant at the end of the orifice, where the aperture is narrower.

Air interaction also creates a high turbulence region at the borders of the liquid sheet, which is concentrated near the orifice for N₁ and N₃ and extends to larger radial coordinates for N₂. This may be related to the external geometry of the nozzles, since N₂ features a longer passage between the orifice and open air (Figure 4).

![Figure 4. Schematics of the nozzle geometry between the orifice and open air.](image)

The two aforementioned effects lead to different distributions of turbulent intensity within the liquid sheet. While N₁ presents a uniform angular distribution, N₂ and N₃ have low values of this magnitude next to the symmetry axis that increase as moving toward the edge of the liquid sheet. Based on this information, a criterion to determine whether an aerodynamic or rim-influenced breakup will dominate the disintegration of the liquid is defined.

Conclusions

The inner geometry of the nozzles has been proved to play a leading role in the breakup regime of the liquid sheets. When cross-section reductions are sharp the liquid reaches the orifice with higher turbulence near the walls. This turbulence, together with that generated at the orifice, leads to a non-uniform distribution of turbulent intensity, with low values of this magnitude next to the symmetry axis that increase as moving toward the edge of the liquid sheet. Air flow creates an additional high-turbulence region at the border of the liquid sheet. The sum of these effects leads to the prompt destabilization of the rim characteristic of the breakup mechanism of N₂ and N₃.

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