A Comprehensive Model to Predict Simplex Atomizer Performance

The pressure swirl atomizer, or simplex atomizer, is widely used in liquid fuel combustion devices in the aerospace and power generation industries. A computational, experimental, and theoretical study was conducted to predict its performance. The Arbitrary-Lagrangian-Eulerian method with a finite-volume scheme is employed in the CFD model. Internal flow characteristics of the simplex atomizer, as well as its performance parameters such as discharge coefficient, spray angle, and film thickness, are predicted. A temporal linear stability analysis is performed for cylindrical liquid sheets under three-dimensional disturbances. The model incorporates the swirling velocity component, finite film thickness and radius that are essential features of conical liquid sheets emanating from simplex atomizers. It is observed that the relative velocity between the liquid and gas phases, density ratio, and surface curvature enhance the interfacial aerodynamic instability. The combination of axial and swirling velocity components is more effective than only the axial component for disintegration of liquid sheet. For both large and small-scale fuel nozzles, mean droplet sizes are predicted based on the linear stability analysis and the proposed breakup model. The predictions agree well with experimental data at both large and small scale.

Mean droplet size and the size distribution are even more difficult to predict theoretically or numerically than other performance parameters mentioned above as the physics of the complex atomization process is not clearly understood. So far, in most spray applications, empirical correlations for mean drop sizes are employed, which are discussed in Lefebvre (1989).

The understanding of the atomization process has benefited greatly by the pioneering work of instability analysis of liquid sheets by Squire (1953). Extensive research has been conducted thereafter, for example, Hagerty and Shea (1955), Dombrowski and Johns (1962), Clark and Dombrowski (1972), and Li and Tantin (1991). Forces such as the inertial force, surface tension, aerodynamic force, viscous force, and centrifugal force are involved in the disintegration process. Some of them resist the disintegration process while others promote it. It is the competition among these forces that determines the stability of liquid sheets. It is now generally agreed that the aerodynamic instability of the liquid sheet is responsible for the disintegration process. Based on linear stability theory, Dombrowski and Johns (1963) proposed a breakup model for a plane liquid sheet. The predicted mean drop sizes agree well with experimental measurement. The two-dimensional instability model was extended later by Cropper et al. (1975), Meyer and Weihs (1987), Lee and Chen (1991), Dumouchel et al. (1993), Panchagnula et al. (1996), and Shen and Li (1996) for annular liquid sheets.

The objective of the present paper is to develop a comprehensive model to predict the performance of a simplex atomizer. In the CFD model, the Arbitrary-Lagrangian-Eulerian method with a finite-volume scheme is employed to compute the internal flow field and the initial properties of the liquid sheet emanating from the nozzle. Discharge coefficient, spray angle, film thickness, and velocity at the nozzle exit are predicted. The computational model has been validated by comparisons with experimental measurements (Holtzclaw et al., 1997; Jeng et al., 1998). The instability model considers an inviscid, swirling annular liquid sheet under three-dimensional disturbances and different gas velocities. A parametric study has been carried out to understand the specific roles of various forces, fluid properties, and geometrical conditions in the disintegration process. By incorporating the essential features such as axial and tangential

1 Introduction

Atomization is a process of generating a large number of droplets from a bulk liquid. The performance of a liquid fuel atomizer has direct effects on combustion efficiency, pollutant emissions, and combustion stability. Understanding the underlying mechanisms of the atomization process is crucial for improvements in liquid-spray combustion. Because of its advantages such as small power consumption, good spray quality, and simple geometry (Bayvel, 1993), the pressure swirl atomizer, or simplex atomizer, is widely used in gas turbine engines and in furnaces in the power generation industry. Figure 1 shows a typical geometry of a simplex atomizer. High pressure liquid enters through the swirler inlet slots. Due to the swirling motion of the liquid, an air core is developed inside the nozzle and liquid emanates in the form of a conical liquid sheet. The flow features inside the nozzle and the disintegration of the liquid sheet determine the characteristics of the resultant spray. Since the spray angle, mean drop size, and droplet size distribution from the liquid sheet disintegration control the subsequent heat and mass transfer in a convection environment such as in spray combustion, they have a direct effect on combustion efficiency, pollutant emission, and stability. Understanding factors that affect the atomizer performance parameters is important for both practical atomizer design and improvement. However, predictions of the atomizer performance still remain a challenge.

According to Giffen and Muraszew's (1953) maximum flow principle, discharge coefficient, spray angle and film thickness depend only on the geometry constant K, which is defined as

\[ K = A_s/D_s \]

Although the theory provides correct trends, it is based on the assumption of inviscid flow and the features of the internal flow are ignored. Recent studies (Yule et al., 1997; Holtzclaw et al., 1997) show that the performance parameters depend not only on nozzle geometry but also on internal flow features.

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velocity, attenuating film thickness and finite radius of the liquid sheet issuing out from a simplex nozzle, the present model is used to calculate the maximum growth rates and the most unstable wave number (wavelength). This wavelength is then incorporated into the breakup model, based on Rayleigh's theory, to predict mean droplet sizes, while the maximum growth rate is employed to determine the location of the liquid sheet breakup.

2 Mathematical Formulation

2.1 Computational Model. The flow is assumed to be axisymmetric and incompressible. The governing equations are the continuity and Reynolds averaged Navier-Stokes equations expressed below.

\[ \frac{\partial (\rho U)}{\partial x} + \frac{\partial (\rho V)}{\partial r} = 0 \]  

\[ \rho \frac{\partial U}{\partial t} + \rho U \frac{\partial U}{\partial x} + \rho V \frac{\partial U}{\partial r} = (\mu + \mu_t) \left( \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial r^2} \right) \]  

\[ \rho \frac{\partial V}{\partial t} + \rho U \frac{\partial V}{\partial x} + \rho V \frac{\partial V}{\partial r} = (\mu + \mu_t) \left( \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial r^2} \right) \]  

The turbulent eddy viscosity is determined by the algebraic equation model proposed by Baldwin and Lomax (1978).

Boundary conditions are prescribed at the swirl chamber inlet, tip (outflow of computational domain), solid boundary and liquid/gas interface. To compare the CFD model with the experimental configuration comprised of a finite number of square inlet slots, the radial and tangential velocities and the width of the equivalent annular inlet slot are determined by equating the total mass flow rate, angular momentum and kinetic energy of the two cases. No-slip boundary conditions are prescribed at the solid boundary. At the tip, the second derivative of pressure with respect to \(x\) is set to 0. At the gas-liquid interface, the normal stress is balanced as

\[ P = P_\infty + \sigma (1/R_1 + 1/R_2) \]  

where \(P_\infty\) is the ambient air pressure and \(R_1, R_2\) are the principal radii of curvature at the interface. The velocity gradients of liquid normal to the interface are assumed to be zero since shear stress is small due to the large density and viscosity ratios between the liquid and gas phases.

The above governing equations and boundary conditions are discretized by a finite-volume scheme. The Arbitrary-Lagrangian-Eulerian method (ALE) with an adaptive grid generation technique is used to track the position of the interface. The details of the computational procedures of ALE are described in Jeng et al. (1998) and are not repeated here for brevity. The steady state solution is achieved when the normal velocity component at the interface becomes zero.

2.2 Linear Stability Analysis. A swirling annular liquid sheet subject to concurrent inner and outer air streams is considered. The geometrical and flow conditions are shown in Fig. 2. Both the liquid and gas phases are assumed to be inviscid and incompressible. The inviscid assumption is based on Shen and Li's study (1996), which found that viscosity has only a small influence on the growth rates of disturbances at high Weber number. Basic flow velocities for the liquid and inner and outer gas are assumed to be \((U_i, 0, A/r), (U_o, 0, 0)\), and \((U_s, 0, 0)\), respectively. A temporal linear instability analysis is performed

\[ \text{Nomenclature} \]

\[ A = \text{vortex strength, m}^2/s \]
\[ A_p = \text{total inlet area, m}^2 \]
\[ C_d = \text{discharge coefficient} \]
\[ D = \text{mean droplet diameter, m} \]
\[ D_L = \text{ligament diameter, m} \]
\[ D_s = \text{slot diameter, m} \]
\[ D_0 = \text{swirl chamber diameter, m} \]
\[ D_e = \text{exit orifice diameter, m} \]
\[ FN = \text{flow number (} = m_i/\Delta P \rho_i \text{), m}^2 \]
\[ g = \text{density ratio between gas and liquid} \]
\[ h = \text{ratio of inner and outer radii} \]
\[ K = \text{atomizer geometric constant} \]
\[ k = \text{axial wave number, } 1/m \]
\[ m_i = \text{mass flow rate, kg/s} \]
\[ n = \text{azimuthal wave number} \]

\[ P = \text{mean pressure, N/m}^2 \]
\[ p_b = \text{absolute pressure, N/m}^2 \]
\[ \Delta p = \text{pressure differential, N/m}^2 \]
\[ R_i, R_o = \text{inner and outer radius of liquid sheet, m} \]
\[ R_1, R_2 = \text{radii of curvature, m} \]
\[ r = \text{radial coordinate, m} \]
\[ t = \text{time, s} \]
\[ t_b = \text{film thickness at breakup, m} \]
\[ U = \text{mean axial velocity, m/s} \]
\[ V = \text{mean radial velocity, m/s} \]
\[ W = \text{mean tangential velocity, m/s} \]
\[ U_i = \text{disturbance axial velocity, m/s} \]
\[ u = \text{disturbance radial velocity, m/s} \]
\[ v = \text{disturbance tangential velocity, m/s} \]
\[ W = \text{disturbance tangential velocity, m/s} \]
\[ \text{We} = \text{Weber number (} = \rho U^2 R/\sigma \text{), m} \]
\[ x = \text{axial coordinate, m} \]

\[ \text{Greek Letters} \]
\[ \eta = \text{displacement disturbance, m} \]
\[ \lambda = \text{wave length, m} \]
\[ \theta = \text{azimuthal angle or spray cone half angle} \]
\[ \phi = \text{fluid density, kg/m}^3 \]
\[ \omega = \text{temporal frequency, } 1/s \]

\[ \text{Subscripts} \]
\[ l = \text{liquid phase} \]
\[ i = \text{inner gas} \]
\[ o = \text{outer gas} \]
\[ m = \text{at maximum condition} \]
\[ s = \text{based on swirling component} \]
for the annular liquid sheet under three-dimensional disturbances with the normal mode method. The approach to the problem is similar to that of Panchagnula et al. (1996).

The governing equations in a cylindrical coordinate system are

\[
\frac{V}{r} + \frac{\partial V}{\partial r} + \frac{1}{r} \frac{\partial W}{\partial \theta} + \frac{\partial U}{\partial z} = 0 \tag{6}
\]

\[
\frac{\partial U}{\partial t} + V \frac{\partial U}{\partial r} + \frac{W}{r} \frac{\partial U}{\partial \theta} + U_0 \frac{\partial U}{\partial z} = - \frac{1}{\rho} \frac{\partial p}{\partial r} \tag{7}
\]

\[
\frac{\partial V}{\partial t} + V \frac{\partial V}{\partial r} + W \frac{\partial V}{\partial \theta} + U_0 \frac{\partial V}{\partial z} = - \frac{1}{\rho} \frac{\partial p}{\partial \theta} \tag{8}
\]

\[
\frac{\partial W}{\partial t} + V \frac{\partial W}{\partial r} + W \frac{\partial W}{\partial \theta} + U_0 \frac{\partial W}{\partial z} + \frac{VW}{r} = - \frac{1}{\rho} \frac{\partial p}{\partial z} \tag{9}
\]

The disturbances are assumed to have the forms of

\[
(U, v, w, p') = (\eta(x, \theta, t), \eta(x, \theta, t), \eta(x, \theta, t)) e^{i(kz + \omega t - \omega_{0} t)}, \tag{10}
\]

where \( \eta \) indicates the disturbance amplitude which is a function of \( r \) only. For the temporal instability analysis, the wave number \( k \) and \( n \) are real while frequency \( \omega \) is complex. The imaginary part of \( \omega \) reflects the growth rate of the disturbance. The displacement disturbance at the inner and outer interfaces are

\[
\eta_i(x, \theta, t) = \eta_i e^{i(kz_{i} + \omega_{i} t)} \tag{11}
\]

To obtain linearized disturbed equations, let

\[
U = \bar{U} + u, \quad V = v, \quad W = \bar{W} + w, \quad p = \bar{p} + p', \tag{12}
\]

where the over bar represents the assumed mean flow quantities and prime indicates disturbance. Substituting Eq. (12) into Eq. (6), (7), (8), and (9) and neglecting second order terms, we get the linearized disturbed equations for the liquid flow as

\[
\frac{\partial u}{\partial t} + \frac{A}{r^2} \frac{\partial u}{\partial \theta} + U \frac{\partial u}{\partial z} = - \frac{1}{\rho} \frac{\partial p'}{\partial t} \tag{13}
\]

\[
\frac{\partial u}{\partial t} + \frac{A}{r^2} \frac{\partial u}{\partial \theta} + U \frac{\partial u}{\partial t} = - \frac{1}{\rho} \frac{\partial p'}{\partial \theta} \tag{14}
\]

\[
\frac{\partial u}{\partial t} + \frac{A}{r^2} \frac{\partial u}{\partial \theta} + U \frac{\partial u}{\partial t} - \frac{2Aw}{r^4} = - \frac{1}{\rho} \frac{\partial p'}{\partial r} \tag{15}
\]

The linearized disturbed equations for the inner and outer gas flow can be written in vector form as

\[
\nabla \cdot \mathbf{u} = 0 \tag{16}
\]

\[
\frac{\partial u'_i}{\partial t} + U \frac{\partial u'_i}{\partial x} = - \frac{1}{\rho_i} \nabla p'_j \quad j = i, o, \tag{17}
\]

where \( \mathbf{u}_j = (u' v' w') \).

The boundary conditions are

**For the Inner Gas,**

\[
\frac{\partial n_i}{\partial t} + \frac{\partial n_i}{\partial t} + U \frac{\partial n_i}{\partial x} = 0 \quad r = R_i \tag{18}
\]

**For the Outer Gas,**

\[
\frac{\partial n_o}{\partial t} + \frac{\partial n_o}{\partial t} + U \frac{\partial n_o}{\partial x} = 0 \quad r = R_o \tag{19}
\]

**For the Liquid Phase,**

\[
\frac{\partial n_s}{\partial t} + \frac{\partial n_s}{\partial t} + U \frac{\partial n_s}{\partial x} = 0 \quad r = R_s \tag{20}
\]

The dynamic boundary conditions are

\[
p'_i - p'_o = \sigma \left( \frac{\eta_i}{R_i^2} + 1 \frac{\partial^2 \eta_i}{R_i^2 \partial \theta^2} + \frac{\partial^2 \eta_i}{R_i^2 \partial^2 \theta} \right) - \rho_i \frac{A_i^3 \eta_i}{R_i^3} \tag{21}
\]

\[
p'_i - p'_o = - \sigma \left( \frac{\eta_o}{R_o^2} + 1 \frac{\partial^2 \eta_o}{R_o^2 \partial \theta^2} + \frac{\partial^2 \eta_o}{R_o^2 \partial^2 \theta} \right) - \rho_o \frac{A_o^3 \eta_o}{R_o^3} \tag{22}
\]

In order to determine the role of the various forces, fluid properties and geometric parameters, the above equations are nondimensionalized by introducing the following dimensionless parameters:

\[
W_{e_i} = \frac{\rho_i U_i^3 R_i}{\sigma}, \quad W_{e_o} = \frac{\rho_o U_o^3 R_o}{\sigma}
\]

\[
W_{e_s} = \frac{\rho_o W_o^2 R_o}{\sigma R_s}, \quad W_{e_s} = \frac{\rho_o U_o^3 R_o}{\sigma}
\]

\[
g_i = \frac{p_i}{\rho_i}, \quad g_o = \frac{p_o}{\rho_o}, \quad h = \frac{R_s}{R_i}, \quad k = kR_s, \quad \omega = \frac{\omega R_s}{U_i}
\]

\[
\frac{U_i}{U_s} = \frac{\sqrt{\frac{W_{e_s}}{W_{e_i}}} \sqrt{g_i}}{W_{e_s} \sqrt{g_i}} \quad \frac{U_i}{U_o} = \frac{\sqrt{\frac{W_{e_o}}{W_{e_i}}} \sqrt{g_i}}{W_{e_o} \sqrt{g_i}} \quad \frac{A}{U_i} = \frac{\sqrt{\frac{W_{e_i}}{W_{e_o}}} \sqrt{g_i}}{W_{e_i} \sqrt{g_i}}
\]

The final dispersion equation is a polynomial of fourth order of the form

\[
a_4 \omega^4 + a_3 \omega^3 + a_2 \omega^2 + a_1 \omega + a_0 = 0.
\]

The detailed derivation of the above dispersion equation is available in Liao (1999). The coefficients \( \{ a_i \} \) depend on wave number \( k \) and \( n \), flow conditions, fluid properties, and geometric parameters and are given in the appendix. The dispersion equation is solved using Mathematica™. For each pair of \( \{ k, n \} \) and given dimensionless parameters, we look for the root with the maximum imaginary part which represents the growth rate of the disturbance.
2.3 Breakup Model. The breakup model of a conical liquid sheet is essential for understanding the atomization process and the prediction of droplet sizes in practical simplex atomizers. The current breakup model assumes that the most unstable wave is detached at troughs to form a ring of half wavelength width ($\lambda/2$) as shown in Fig. 3. Dombrowski and Johns (1963) originally proposed this assumption for the breakup of plane liquid sheets. The most unstable wavelength is determined by the above instability model. The ring immediately evolves into a ligament of diameter $D_L$. Drops of equal diameter are formed from one wavelength intervals on the resultant ligament (Rayleigh, 1879). By conservation of liquid mass, the diameter of the ligament is given by

$$ D_L = \left( \frac{2}{\pi} \frac{\lambda}{2} \right)^{0.5} = 2 \left( \frac{t_i}{k_r} \right)^{0.5} $$

(27)

and the mean drop diameter is related to the diameter of the ligament as (Lefebvre, 1989)

$$ D = 1.89 D_L. $$

(28)

Substituting Eq. (27) into Eq. (28) leads to the equation of mean drop diameter as follows:

$$ D = 3.78 \left( \frac{t_i}{k_r} \right)^{0.5}. $$

(29)

It should be noted that $t_i$ in Eq. (29) represents the film thickness at the point of breakup. The breakup length is first calculated based on the maximum growth rate. Knowing the spray cone angle, the film thickness at the point of breakup is then determined through conservation of mass.

3 Results and Discussions

3.1 Computational Model. The CFD model was first validated by detailed comparison with experimental data. All the experiments to validate the CFD model were carried out on large size prototype atomizers with an exit orifice diameter of 18 mm and a swirl chamber diameter of 76 mm. The working fluid was water. The Reynolds number for the flow based on the exit orifice diameter and the mean exit velocity varied from $2.7 \times 10^3$ to $3.5 \times 10^3$. The corresponding pressure drop in the injector varied from 69 to 345 kPa. The details of the apparatus and the experimental methodology are available in Holztclaw et al. (1997) and are not repeated here for brevity.

The computational results were obtained with a grid of 71 points in the $x$-direction and 21 points in the $r$-direction. In the radial direction, the grid points are distributed nonuniformly with a fine grid near the wall and at the gas-liquid interface where higher gradients are expected; a coarser grid is used in the central region. In the $x$-direction, the grid points are distributed as follows: seven in the inlet section, 29 in spin chamber, 22 in the converging section, six in the exit orifice section, and seven outside the nozzle orifice. In the Lagrangian step, the solution was considered converged if the maximum relative error in cell mass between two iterations was less than $10^{-4}$.

To test grid independence of the computational solutions, results were obtained by doubling the grid in both directions for two cases corresponding to the minimum and the maximum value of the atomizer constant. The results for film thickness, spray cone angle and the discharge coefficient were essentially unchanged (less than 1 percent).

Figure 4(a) shows that the mean film thickness at the orifice is directly proportional to $K$. Note that the experimental and computational results match to a good extent, while the analytical model (Rizk and Lefebvre, 1985) clearly underestimates both. In Fig. 4(b), it is observed that spray cone half angle increases with increasing $K$. Note that the experimental and CFD results are in good agreement, while the analytical model (Giffen and Muraszew, 1953) overestimates the results for this case. An increase in the atomizer constant can be effected by increasing the inlet swirl slot area. For a given mass flow rate, this results in decreasing the swirl inside the spin chamber resulting in lower centrifugal force and corresponding lower cone angle and higher film thickness. Giffen and Muraszew's model is based on an inviscid flow assumption, and therefore it does not provide accurate predictions. Figure 4(c) shows that the discharge coefficient increases with increasing $K$. Again, an excellent agreement between the computational and experimental results is clearly evident, and this validates our computational model.

We note that the dimensionless flow parameter governing the flow phenomena inside the atomizer is the Reynolds number. The range of Reynolds number considered here is the same as that typically encountered in small-scale fuel injectors in aircraft engines. Therefore, the results of the computational model are also valid for small-scale atomizers.

It is evident from Fig. 4 that the geometry parameter $K$ plays an important role in determining the atomizer performance. Other dimensionless geometry parameters such as $L/D$ and $D/d$, also influence the atomizer performance. We have used the validated computational code to evaluate the effect of two such parameters $L/D$ and $D/d$, on the film thickness at the orifice exit. $L/D$, was varied from 0.1 to 1.5 and $D/d$, from 3.5 to 6.5. For these cases, the mass flow rate, inlet slot area and the exit diameter were all held constant. Figure 5(a) shows the variation of film thickness with $L/D$. The film thickness is seen to increase with this parameter. At low values of $L/D$, there is a sharp increase in film thickness with $L/D$, followed by a gradual increase. For a given spin chamber diameter, increasing $L$, may result in high friction losses and therefore lower exit velocities and corresponding higher film thickness. Figure 5(b) shows the variation of $D/d$, with the film thickness. It is seen from the figure that the film thickness increases with decreasing $D/d$. For a given $D_s$, a decrease in $D/d$, can be achieved by increasing $d_s$. With a large $d_s$, fluid is no longer squeezed through a narrow orifice and the film thickness increases. At present, reliable correlations are not available to predict the influence of these geometric parameters on the performance of the atomizer. The CFD model allows us to predict the effect of geometry changes on the film thickness, spray cone angle, and in conjunction with the stability analysis and the breakup model, the mean drop sizes.
3.2 Linear Stability Analysis. Based on the derived dispersion equation, a parametric study has been carried out to isolate the effects of the axial and swirl velocity, gas-to-liquid density ratio, and surface curvature on the instability of liquid sheets. The frequency with the maximum imaginary part is the most unstable mode, hence, it will dominate the liquid sheet breakup process. For the simplex atomizer using this model, the inner and outer gas velocities are set equal to zero. The disturbance growth rate $\omega$ is plotted in terms of dimensionless parameters such as axial Weber number, $W_e$, swirl Weber number, $W_s$, axial wave number, $k$, azimuthal wave number, $n$, the ratio of inner and outer radii, $h$, and the gas-to-liquid density ratio, $\rho_g$.

It is seen from Fig. 6, that there exists a finite range of wave numbers with positive growth rate. The wave number that corresponds to the maximum growth rate is called the most unstable wave number. This behavior is explained as follows. The instability mechanism can be thought of as a frequency-selective amplifier. The mean flow is its energy supply, and its gain and frequency characteristics depend upon flow conditions and fluid properties. When the axial velocity is very low, the axisymmetric mode ($n = 0$) dominates the competition of disturbance growth. As the axial velocity increases, both the maximum growth rate and the range of wave numbers with positive growth rate (unstable wave number range) increase. The corresponding most unstable wave number or frequency shifts to a higher value. Furthermore, the importance of helical modes become comparable with the axisymmetric mode. This behavior has also been validated by previous studies (e.g., Panchagnula et al., 1996).

Figure 7 shows the instability of a purely swirling (i.e., with a zero axial velocity component) annular liquid sheet. As the swirl strength increases, i.e., as the swirl Weber number increases, the aerodynamic force increases, thus, promoting instability. This is manifested in the increased growth rate and the increased range of unstable wave number. More interestingly, the dominating mode shifts from the axisymmetric mode to the helical mode at moderate swirl Weber number. This is explained by the fact that the helical mode extracts more energy from the
unstable wave number range and the growth rates increase with increasing gas density. Since an increase in gas density increases the aerodynamic force, it enhances the aerodynamic instability of liquid sheets as expected. This implies that the higher the ambient pressure, the smaller the drops produced. This conclu-

mean swirling flow field than the axisymmetric mode for the case where swirl is stronger. This illustrates the superior performance, at moderate injection pressure differential, of a simplex atomizer compared to plain pressure atomizer where liquid swirl is absent. This performance is partly due to the destabilizing effect of swirl.

The influence of the gas-to-liquid density ratio on the instability of the annular liquid sheet is presented in Fig. 8. Both the
modes become the dominating mode and are responsible for the disintegration of the liquid sheet.

Surface curvature has a remarkable effect on the growth rate of unstable waves as shown in Fig. 9. For both axisymmetric and helical modes and decreasing inner radius (for fixed outer radius), the growth rate increases, while the unstable wave

![Image](image_url)

**Fig. 8** Growth rate versus wave number for n = 0, 1, 2 mode at h = 0.77: (a) g_u = 0.00125, We_g = 1000, We_a = 0, (b) g_u = 0.0125, We_g = 1000, We_a = 0, and (c) g_u = 0.0125, We_g = 1000, We_a = 1000

... experimental study of the effect of ambient density on drop size formation. Furthermore, when there is no swirl and gas density increases, the importance of helical modes becomes comparable with the axisymmetric mode. However, for weak swirl, helical

![Image](image_url)

**Fig. 9** Effect of surface curvature on instability for first three modes at g_u = 0.00125, We_g = 20, We_a = 20: (a) n = 0, (b) n = 1, and (c) n = 2
Table 1 Geometry details and performance parameters of three large scale atomizers

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Atomizer constant</th>
<th>Orifice diameter (mm)</th>
<th>Pressure differential (Ps)</th>
<th>Mass flow rate (kg/s)</th>
<th>Spray cone angle (degree)</th>
<th>Orifice film thickness (um)</th>
<th>Breakup location (mm)</th>
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<tbody>
<tr>
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number range is unaffected. These results are consistent with Lee and Chen (1991) and Shen and Li (1996). However, Crapper et al. (1975) claims the unstable range also changes with increasing surface curvature.

3.3 Mean Drop Size Prediction. Using the CFD model, the stability analysis and the breakup model, we have calculated mean drop sizes for both large scale and small scale (aero-engine scale) atomizers. The large-scale results were compared with our experimental data for a number of atomizer geometries and flow conditions. For the small-scale results, extensive comparisons of our predictions have been carried with correlations of experimental data available in the literature for small-scale atomizers. Properties of water ($\mu = 0.001$ kg/ms, $\nu = 0.0734$ kg/s², $\rho = 1000$ kg/m³) were used in the predictions of mean droplet sizes for both large and small scale atomizers.

3.3.1 Large Scale. The mean droplet size and spray cone angle were measured by optical techniques and the liquid film thickness at the orifice exit was measured by an ultrasonic transducer. The film thickness and spray cone angle measurements were used to validate the CFD model as described earlier. A video recording of droplets was obtained using a high speed CCD camera at a vertical distance of 0.5 meter from the nozzle orifice. This distance was chosen to assure that liquid sheets were well atomized and no ligaments were present in the measurement window. The size of measurement window varied from case to case and had a value of about 30 mm by 30 mm. A large number of images were analyzed to obtain the sauer mean diameter (SMD). The spray angle was determined by digitizing and processing images of the spray obtained by the CCD camera. An ultrasound transducer was mounted at the nozzle exit. The liquid film thickness measurements were based on the time delay in signal reflected from the water-Plexiglas interface and that from the water-air interface. The details of the experimental apparatus and procedure are available in Benjamini et al. (1998).

The axial and tangential velocity components, film thickness and cone angle were taken from the CFD results. The breakup point of the liquid sheet was located experimentally by observing the occurrence of discontinuities in the liquid sheet with stroboscopic lighting at 450 Hz and by analyzing spray images. The mean droplet sizes were then calculated using the breakup model.

Table 1 summarizes the performance parameters of three large-scale atomizers under three different operating conditions. We note that the liquid film thickness at the orifice exit were rather large (about 2 mm) due to large orifice diameters (15–29 mm). Also the breakup length shortens as pressure differential (discharge velocity) increases.

In Table 2, the predicted SMD values obtained using the present theory are compared with measurement data and with those by Couto et al. theory (1997) and existing empirical correlations (Lefebvre 1989). It is seen that the present theory correctly predicts the trend for SMD; that is, the SMD decreases with increasing mass flow rate. Quantitatively, the present theory gives an overall error of about 20%. The discrepancy at the lowest flow cases may be caused by non-stationary flow at very low pressure. However, SMD is significantly overestimated by the Babu et al. correlation and significantly underestimated by the Couto et al. theory and correlations of Jasuja, Lefebvre, and Wang, and Lefebvre. It is evident from Table 2 that, for large-scale atomizers, Radcliffe's correlation and the present theory give the best predictions.

3.3.2 Small Scale. There is considerable experimental data at small scale for film thickness, spray cone angle, and drop sizes available in the literature. Unfortunately, these studies do not provide geometric details of the small-scale atomizers used. Therefore, the CFD code could not be utilized to calculate the properties of the liquid sheet emanating from the atomizer. These were obtained from the available data as follows. The axial and tangential velocity components were calculated using Eq. (30) and (31), respectively.

$$U = \frac{m_t}{\rho(A_x - A_y)} = \frac{4m_t}{\rho r(4d_y d_x - 4t^2)} \quad (30)$$

$$W = U \tan (\theta), \quad (31)$$

where $r$ is the film thickness at orifice exit and is estimated by the equation below (Lefebvre, 1989).

Table 2 Comparison of SMD predicted by existing theory and empirical correlations

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amplitude reaches \( r^2 \) as suggested by Dombrowski and Johns (1963). Hence, the breakup length (or time) can be readily calculated from the maximum growth rate and the film thickness at the breakup point is thus determined via conservation of mass. The effect of attenuating film thickness is considered in the breakup model by employing the film thickness at the point of breakup in Eq. (29).

The present model was employed to predict SMD for small-scale atomizers and compared with the experimental data of Wang and Lefebvre (1987), the aforementioned theory and correlations. The three small atomizers used by Wang and Lefebvre had a 60 deg spray cone angle with flow numbers of 6.25, 12.5, and \( 25 \times 10^{-4} \text{m}^2 \), respectively. The pressure differential varies from 0.35 MPa to 2.07 MPa. As shown in Fig. 10(a) and 10(b), for atomizers with the FN of \( 6.25 \times 10^{-4} \) and \( 12.5 \times 10^{-4} \), SMD predictions by Lefebvre's correlation and the present theory are very close to experimental data while others either significantly overestimate or underestimate them. For the atomizer with the FN of \( 25 \times 10^{-4} \), as shown in Fig. 10(c), the discrepancy between Lefebvre's correlation and measurement data becomes larger than those in Fig. 10(a) and (b). Our model predicts drop sizes with experimental data with a somewhat more gradual variation of SMD with mass flow rate than that measured. This is because the slope of the curve is highly dependent on the predicted film thickness from the correlation. Therefore, accurate film thickness measurements at small-scale would improve the agreement. We note that Radcliffe's correlation, which appears to provide reasonable prediction at large scale, gives errors of over 100 percent at the small scale! Results from present analysis are consistently close to measurement data for both large and small-scale atomizers.

4 Conclusions

A comprehensive model to predict the performance of a simplex atomizer has been established. The CFD model based on the ALE method can accurately predict the internal flow features and properties of the liquid sheet emanating from the nozzle. It is found that the atomizer geometric constant \( K = \sigma_0/(D_0 d_0) \) and other geometric parameters (\( L_o/D_o \) and \( D_0/d_0 \)) significantly affect the atomizer performance. As atomizer geometric constant increases, discharge coefficient and film thickness at the orifice increases while spray angle decreases. The film thickness was found to increase with \( L_o/D_o \) and decrease with \( D_0/d_0 \).

A temporal linear stability analysis was performed for cylindrical liquid sheets under three-dimensional disturbances. The instability model incorporates swirling velocity components, finite film thickness, and radii that are essential features of conical liquid sheets emanating from simplex atomizer. It is observed that the relative velocity between the liquid and gas phases, gas-liquid density ratio, and surface curvature enhance the interfacial aerodynamic instability. As Weber number and density ratio increase, both the wave growth rate and unstable wave number range increases. The combination of axial and swirling velocity components is more effective than the single axial component for disintegration of the liquid sheet. It not only enhances the interfacial instability, but also shifts the dominating mode from axisymmetric to the helical mode. Based on the proposed breakup model and stability analysis, mean drop size are predicted for both large and small-scale atomizers. Our predictions agree well with experimental data at both large and small scales.

Acknowledgment

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References


APPENDIX

Coefficients in the dispersion equation, Eq. (26), are listed below.

\[ a_4 = C_4 \frac{C_1}{C_4} + C_{10} \]
\[ a_5 = C_5 \frac{C_1}{C_5} - C_{12} \]
\[ a_9 = C_9 \frac{C_1}{C_9} - C_{11} \]
\[ a_2 = -C_1 \frac{C_1}{C_2} - C_{12} + C_{11} \]
\[ a_2 = -C_1 \frac{C_1}{C_2} - C_{12} + C_{11} \]
\[ a_1 = C_2 \frac{C_1}{C_2} + C_{12} + C_{11} \]
\[ a_0 = C_0 = C_2 + C_{12} \]
\[ C_1 = -B_a + g_a \frac{k}{G} \]
\[ C_4 = -g_a \frac{H_a}{C_a} \]
\[ C_6 = \frac{1}{h} \frac{H_a}{C_a} - \frac{1}{h^2} \frac{H_a}{C_a} + \frac{k}{h} \frac{H_a}{C_a} \]
\[ C_{10} = \left( \frac{h}{h^2} \frac{H_a}{C_a} + k \right) \frac{H_a}{C_a} \]
\[ C_{11} = \left( \frac{h}{h^2} \frac{H_a}{C_a} + k \right) \frac{H_a}{C_a} \]
\[ C_{12} = \left( \frac{h}{h^2} \frac{H_a}{C_a} + k \right) \frac{H_a}{C_a} \]

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