Towards A Robust Phenomenological Turbulent Jet-in-Crossflow Atomization Model

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Abstract
Jet In Crossflow (JIC) atomization models are typically based on liquid to air momentum ratio and gas Weber number. Although turbulence in a jet can significantly alter JIC atomization, the effect of turbulence is not considered when characterizing jet breakup. In this paper, we demonstrate that commonly used injectors for augmentor applications produce high levels of turbulence in the jet, while injectors commonly used in research laboratories consists of moderate to no turbulence in the jets. Thus, JIC models built using near laminar conditions will not produce accurate predictions in practical applications.

In this paper, we present the beginnings of a phenomenological JIC atomization model that can account for turbulence in the jet. High fidelity VOF simulations for JIC atomization validated against high resolution, high-speed photography will potentially be used to describe the primary and secondary breakup processes. The initial model is developed by identifying and curve-fitting non-dimensional parameters through a wide range of experimental data. Significant emphasis has been placed on minimizing the total number of correlations and maximizing the use of non-dimensional parameters throughout primary and secondary atomization. The existing model is not a phenomenological model, but has the basic framework of the desired physics-based model. Future VOF simulations may fill the gap in modeling and lead to a robust, phenomenological, turbulent JIC atomization model.

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Introduction

Accurate prediction of liquid jets penetrating and atomizing in gas crossflow is a critical technology needed for the design of current and future gas turbine augmentors. Rigorous experiments have been performed and far field measurements taken to characterize jet breakup in a wide variety of conditions (Wu et al., 1998, Becker et al., 2002, Brown et al., 2006). Numerous spreadsheet correlations exist in the literature that model the penetration and atomization of JIC in a global sense. Many of these correlations are based on hardcoded, dimensional factors without taking into account the actual physics involved. A lot of phenomenological models also exist in the literature, which are used with CFD codes to predict atomization characteristics. Typically, the models start out as physics based, but in the end, to fit with experimental data, non-physical correlations are used and the “phenomenology” ends up being left out of the model. Technically speaking, most of the models are curve-fits to experimental data and not phenomenological models.

The reliability of the models significantly depends on the care taken in deciding the curve-fit parameters. We have found that using non-dimensional atomization parameters yield the most reliable models. But in the end, the reliability of a model is, at best, as good as the reliability and applicability of the data. In this paper, we present an interesting observation regarding applicability of experimental data. Three different experimental data sets are considered, and it is shown that a seemingly minor difference in the injector’s L/D ratio can prove to be a major driver in differences in results. It is important then for JIC curve-fit model developers, to use only that data set that matches the conditions of their desired end application.

Another important factor that is often ignored in JIC atomization description is turbulence in the jet. Most JIC models and correlations define the breakup characteristics completely by liquid to air momentum ratio (q) and the gas Weber number (We). However, turbulence in the jet can significantly alter the breakup process and thus the breakup characteristics. Turbulence will alter the local relative velocity, shear and stability of the jet, and can be an important factor in determining atomization behavior. Although injectors used in most augmentor applications will have a high level of turbulence in the jet, research/laboratory injectors make a conscientious effort to minimize turbulence in the jet. We believe this is one of the reasons why curve-fit models, which match well with research data, do not match well in practical applications.

Building a phenomenological model by using experimental data alone is extremely challenging. Of the many challenges involved in experimentally resolving the phenomenology of JIC atomization, the top few are: a) the reliability and accuracy of data in the dense spray region, b) repeatability of JIC experiments for high precision processes, like ligament formation, wave growth on jet, etc. and c) measurement of local gas field turbulence and liquid jet stresses. To alleviate these challenges, we have taken the approach of developing a phenomenological JIC atomization model by using high fidelity Volume Of Fluid (VOF) simulations. VOF can accurately solve for the exact breakup process by solving the multi-phase Navier Stokes equations. Local gas phase and liquid phase properties can be precisely quantified and statistical data can be collected for a phenomenological model. Numerical simulations like VOF also do not suffer from repeatability issues and dense spray measurement problems. Smaller, highly resolved VOF cases can be setup to completely understand and model the JIC atomization process.

In this paper we present the basic model framework to incorporate the phenomenology that we will discover through VOF. Non-dimensional numbers have been used wherever possible to ensure generality. Primary and secondary atomization is included, together with various modes of each type of atomization. An important factor in the development of the atomization model is its inclusion into a CFD code from the start. This enables the model to use local conditions and not just global conditions. We have observed that JIC is highly sensitive to local details of the gas and liquid flow conditions, such as local velocity and turbulence in the gas field, local temperature gradients etc. Most augmentor applications involve fuel injection in regions of complex, three-dimensional flow (wakes, shear layers, etc.), and the local flow conditions strongly affect fuel jet penetration and atomization. The atomization model includes correlation factors based on local flow conditions (not global, freestream conditions), and thus is readily applicable to practical analysis.

The following sections describe the effect of injector on turbulence in the jet and details of the initial JIC atomization model. Predictions of mass flux and SMD are presented for a wide variety of flow conditions, and comparisons are made to far field experimental measurements. Overall good agreement between predictions and measurements is shown. The final section discusses future work needed.

Effect of Injector Geometry

While analyzing the close up snapshots and movies of JIC atomization of Brown et al. (2006), it was observed that the jet fluctuates vigorously during breakup. The flow conditions were very laminar and it was not clear on what caused such a random motion.

The disturbance right at the orifice exit (Figure 1) indicated that the liquid jet might have become turbulent inside the injector. Such a finding has not been validated
before. If the jet becomes turbulent inside the injector, the turbulence must be characterized just like the liquid to air momentum ratio (q) and the cross-flow Weber number (We) for models like the BLS model (Khosla and Crocker, 2004) and other models in the literature.

It is possible that a high level of turbulence inside the jet would cause the jet to breakup sooner when compared to a mildly turbulent or laminar jet at the same q and We. However, most experiments are conducted with injectors that have some kind of a taper to eliminate turbulence (Figure 2), while the real augmentor applications do not taper the injectors. Tapering the injector would mislead model developers, and may result in incorrect interpretation of model results and thus incorrect augmentor designs.

It was decided to run a CFD simulation of the injector in Figure 2 (with the taper, Figure 3a) and a simulation without the taper in the injector (the way it would be in practical augmentor applications, Figure 3b). Everything except the taper was kept the same in the two cases. A laminar velocity profile was applied at the inlet that corresponds to a liquid to air momentum ratio of 13.97 and crossflow Weber number of 290. No turbulence model was used and the grid resolution near the injector walls was below y+ of 2. The Reynolds number in the orifice was ~8400, which is well above the critical Reynolds number of 2300 for the flow to become turbulent given enough length. Figure 4 shows the grid for the ERC injector and Figure 5 shows the grid for injector without the taper.

Figure 6 shows the circumferential velocity contours for both the tapered and non-tapered injector. The flow becomes turbulent in the orifice in both the cases before it exits the injector. Thus our initial observation is validated that the flow inside the injector does become turbulent. The turbulence at the exit plane will affect the breakup and mixing characteristics of the liquid fuel jet when it injects in the gas crossflow. Thus, the turbulence must be characterized for use with various modeling tools that are used in augmentor design systems. In addition, it should be noted that the injector with no taper shows much higher levels of turbulence and fluctuations than the tapered injector. Thus using a tapered injector for lab experiments or building phenomenological models and then using non-tapered injector for real applications may result in erroneous model results.

We believe that the above noted findings are the first of its kind and demonstrate the importance of employing similar injector types during experiments and real applications. To quantify the effect of turbulence on jet breakup, VOF simulations of a liquid jet in gas crossflow are needed. With the help of VOF simulations we will be able to correlate the effect of turbulence on jet penetration and drop sizes. Further JIC model improvements can then be carried out to include the effect of turbulence on the liquid jet behavior. The following section discusses the current atomization model in which VOF based phenomenology will be added, if funding becomes available.

Atomization Model Description

The atomization model is implemented entirely in a Lagrangian frame of reference, i.e. the continuous liquid column is represented by discrete parcels of identical drops. For overall clarity, the term ‘drop’ is used in the discussion below for either parcels or unique drops unless a specific distinction between the two is required. This basic approach has been utilized by Reitz and Diwakar (1987). One discrete drop is injected at the orifice location with diameter equal to the orifice diameter; this drop simulates the liquid column. The velocity of the drop is determined from the liquid mass flow rate and the effective area of the orifice. Surface shear breakup and column breakup modes are both included in the model. Before the column breakup occurs, fragments may be formed by surface shearing as a function of the local Weber number, liquid to air momentum ratio, local Reynolds number and Ohnesorge number. When the jet reaches the column breakup length, the jet immediately breaks entirely into fragments. The fragments can further undergo secondary atomization based on specific non-dimensional number correlations.

An important aspect of the model is that all gas phase properties, including velocity, are calculated locally. Typical equations from experiments are a function of the bulk gas phase velocity, \( u_g \), which is fine for most laboratory experimental conditions. However, real applications often involve non-uniform free stream velocities where the definition of \( u_g \) is not clear. Local definition of \( u_g \) makes this model more general. The local gas velocity is found by averaging from a group of cells that are nearest to the current drop. To account for potential, undesirable, grid dependency, the gas cells are chosen such that the dilute multiphase limit is followed for the Lagrangian particle tracking, i.e. liquid to gas volume is less than 10%.

Since most of the available correlations/models in the literature are based on free-stream parameters, we had to develop new correlations that would account for local conditions. The following section discusses our correlations in detail.

Atomization Correlations

The model divides the atomization process into primary atomization and secondary atomization. For primary atomization, three modes can exist, depending on the flow conditions: column shearing, column breakup, or a combination of the two. For secondary atomization, two modes exist: shear and multimode. A key component in ensuring generality and robustness of the model is that, wherever possible, non-dimensional numbers have been used to develop expressions for the
various atomization processes. Correlation factors are obtained from the literature, or are determined by matching model predictions to the far field data.

**Primary Atomization**

The model divides the breakup of liquid column into column shearing and column breakup. During the column shearing stage, the liquid jet strips off its mass according to the following expression:

$$m = 15 \left( \frac{l_{\text{jet}}}{l_{\text{max}}} \right)^2 \sqrt{\frac{V_{\text{rel}}}{Oh}} \quad (1)$$

Here, $l_{\text{jet}}$ is the distance that the jet has penetrated in the flow field, $l_{\text{max}}$ is the maximum distance the jet will penetrate in the flow field, $V_{\text{rel}}$ is the local relative velocity that the jet sees, $Oh$ is the Ohnesorge number and $m$ is the ratio of the normalized mass shed by a parcel.

The resulting drops are given the same velocity magnitude as the current jet velocity, but the direction of the velocity vector is modeled as follows:

$$e_{\text{new}} = 0.3 e_1 + \left( 1 - \frac{l_{\text{jet}}}{l_{\text{max}}} \right) e_2 + 0.2(1 - \text{rnd}) e_3 \quad (2)$$

Here, $e$’s are unit vectors. $e_1$ is the vector in the direction of the jet, $e_2$ is the vector in the direction perpendicular to the jet but in the plane of the gas and $e_3$ is the vector in the direction perpendicular to both the gas and jet. $\text{rnd}$ is a random number between 0 and 1.

The drops formed from column shearing are given a SMD based on the mass that was stripped in Equation 1 as follows:

$$\text{SMD} = \left( \frac{m}{\pi \rho f g} \right)^{1/3} \quad (3)$$

The SMD follows a root normal distribution based on observations from Schmehl et. al. (2000) for drop breakup.

Based on our observations from initial VOF simulations, we now know that a round liquid jet deforms into a thin sheet as it penetrates the flow field (Figure 7). The spanwise corners of the sheets experience high shear and form ligaments and are further sheared to form small drops. To simulate the physics as closely as possible, we assumed that the jet deforms into a sheet having a 45° angle and placed the resulting drops at the distance calculated by the sheet angle. Such a drop placement is quite contrary to what is normally done and thought, but makes a huge difference in the volume flux spread in the spanwise and transverse direction.

The liquid jet keeps stripping mass till it reaches the maximum column length or the jet breakup length defined as below (Wu et al., 1997):

$$l_{\text{max}} = 3.44 d_0 \sqrt{q_{\text{inj}}} \quad (4)$$

$q_{\text{inj}}$ is the liquid to air momentum ratio at the injection location and $d_0$ is the injection diameter. When the liquid jet reaches the maximum column length, it breaks into drops having a SMD equal to the jet diameter at the breakup location and with the velocity vector of the jet at the breakup location.

**Secondary Atomization**

The drops resulting from column shearing and column breakup can further undergo secondary atomization based on their Weber number and Reynolds number. It was found that literature in public domain differs considerably on the breakup conditions for various secondary atomization modes. Also, the experimental data for secondary atomization does not cover a significant portion of the condition range that we consider important for augmentors. Based on the available experimental data for liquid jet in gas crossflow, the secondary breakup conditions were formulated as follows:

A drop will undergo shear breakup if the gas Weber number is greater than 80. While a drop will undergo multimode breakup if:

a) The gas Weber number is greater than 5, but less than 80 and
b) The liquid Reynolds number is greater than 5500 and
c) The gas Weber number is greater than square root of gas Reynolds number

The above conditions are just correlation curve fits to fit the experimental data from Taitech (Wu et al., 1998), DLR (Becker and Hassa, 2002) and CFDR/ERC (CFDR Report 8647, 2004) and are not justified at all using physics-based arguments.

When in the shear breakup mode, the drop follows the stripping rate as defined by Equation 5 (Ranger and Nicholls, 1969)

$$M_{\text{shear}} = C_{\text{shear}} \pi d \rho g \nu_{\text{cross}} A \alpha \sqrt{\frac{\pi d}{4}} \Delta t \quad (5)$$

Where,

$$A = \left( \frac{\rho_g}{\rho_f} \right)^{1/3} \left( \frac{\mu_g}{\mu_f} \right)^{1/3} \quad (6)$$
\[ \alpha = \left( \frac{8 \mu_t}{3Au_{g-cross} \rho_t} \right)^{1/2} \]  

(7)

And \( C_{sh} \) is equal to 3.

The SMD of the resulting drops is given by Equation 8

\[ \text{SMD} = 0.7 \left( \frac{\text{Re}_L}{\text{We}^3} \right)^{1/4} d_0 \]  

(8)

When in the Multimode Breakup, the drop breaks up into smaller drops that follow an SMD as given by Equation 9

\[ \text{SMD} = 0.3 \frac{V_{rel}}{\sqrt{O h}} \]  

(9)

Curve Fitting with Experimental Data

The above model was curve fitted with a wide set of experimental data. Tables 1, 2 and 3 describe the conditions for Taitech (Wu et al., 1998), DLR (Becker and Hassa, 2002) and CFDRC/ERC (CFDRC Report 8647, 2004) experiments.

It should be noted that the conditions presented in the tables, cover a wide range of conditions that are representative of augmentor operation. Figures 8-21 show the comparisons of centerline volume flux and SMD for all of the cases in Tables 1-3. Experimental data are represented by red circles (with no line) while CFD results are represented by blue diamonds (with line). The predictions were made using a grid representative of a 3D RANS solution in augmentor application. Overall, the atomization model shows a good fit to the measurements over all of the flow conditions.

Current Gaps and Future Work

The model presented here has the entire framework necessary for a robust, phenomenological, turbulent, JIC atomization model. Special emphasis was placed to minimize the number of correlations and use non-dimensional numbers wherever possible. The current gaps that exist in the model and need to be worked upon are as follows:

a) Remove random number dependence needs to be removed from Equation 2 for spanwise spread;
b) Jet spreading angle needs to be a function of non-dimensional numbers to remove the assumption of a 45° spread at all flow conditions;
c) Calculate the rate of mass loss for single drops in shear breakup regime (secondary atomization) based on sheet stripping theory instead of boundary layer stripping theory (Khosla et al., 2006);
d) Characterize the effects of turbulence in the liquid jet.
e) Identify correlations based on local flow conditions, for rate of ligament formation, mass stripping rate of ligaments and resulting drop sizes and velocity statistics.
f) Characterize atomization properties of secondary atomization modes for JIC application SMD, velocity correlations based on local flow conditions.
g) Determine onset of secondary atomization and time to breakup for JIC conditions.
h) Determine local jet vaporization statistics accounting for increased surface area of the liquid jet because of its deformation into a thin sheet.

The current model is significantly reliant on experimental data alone. More fidelity can be added to the model by using highly resolved VOF simulations. Future work will focus more on using VOF to address some of the gaps mentioned above, if funds become available. Significant emphasis will be placed on the effect of turbulence in the jet that is typical of augmentor conditions.

Nomenclature

\( l_{jet} \) jet penetration distance
\( l_{max} \) maximum jet penetration distance
\( V_{rel} \) local relative velocity
\( e \) unit vector
\( q \) liquid to air momentum ratio
\( d \) drop diameter
\( Oh \) Ohnesorge number
\( Re \) Reynolds number
\( We \) Weber number
\( \mu \) Dynamic viscosity
\( \rho \) density

Subscripts

\( g \) gas
\( l \) liquid
\( \text{cross} \) crossflow component
\( 0 \) initial value

References

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Table 1. Wu et al.’s (1998) test matrix and corresponding figure numbers. Liquid is water and gas is air.

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Table 2. Becker and Hassa’s (2002) test matrix and corresponding figure numbers. Liquid is kerosene and gas is air.

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Table 3. CFDRC/ERC test cases (2004) and corresponding figure numbers. Liquid is a Jet-A simulant and gas is air.

**Figure 1.** Snapshot of a Jet in Crossflow experiment (Brown, McDonell, 2006)
Figure 2. Close-up of liquid injector used in Figure 1 (Brown, McDonell, 2006)

Figure 3. Left: Brown, McDonell (2006) injector, Right: Flat face injector

Figure 4. Left: Brown, McDonell (2006) injector grid front view through centerline, Right: Grid at injector exit
**Figure 5.** Left: Flat face injector grid front view through centerline, Right: Grid at injector exit

**Figure 6.** Comparison of circumferential velocity between the tapered (left) and flat face (right) injectors. Top: Front view through centerline, Bottom: Injector exit (side view)
Figure 7. Jet In Crossflow atomization snapshot using VOF simulation

Figure 8. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 1 in Table 1

Figure 9. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 2 in Table 1
Figure 10. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 3 in Table 1

Figure 11. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 4 in Table 1

Figure 12. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 5 in Table 1
Figure 13. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 6 in Table 1

Figure 14. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 1 in Table 2

Figure 15. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 2 in Table 2
Figure 16. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 3 in Table 2

Figure 17. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 4 in Table 2

Figure 18. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 5 in Table 2
Figure 19. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 6 in Table 2.

Figure 20. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 1 in Table 3.

Figure 21. Comparison of centerline volume flux (Left) and SMD (Right) between experiments and model predictions for case 2 in Table 3.