Numerical Simulation of Aerated-Liquid Injection into a Supersonic Crossflow

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ABSTRACT

Numerical simulations of an aerated-liquid jet in a Mach 1.94 crossflow are presented. The numerical method includes solving the Reynold’s averaged Navier-Stokes (RANS) equations with the shear stress transport (SST) turbulence model coupled to a Lagrangian droplet tracker to simulate the structures of the discharged plumes. Effects of turbulent dispersion and secondary break-up are considered. A simplified injection model is proposed where a spherical cone is used to specify the injection region given user specified spray angle, mean droplet diameter, and droplet size distribution. To compare with available experimental data, water is chosen as the liquid for each case. A grid refinement study was conducted to determine appropriate resolutions. Comparisons are made to phase Doppler particle analyzer (PDPA), shadowgraph, and laser-sheet imaging. Results suggest reasonable agreement between the chosen model conditions and the experimental data available. Particular attention is made to consider the biases within each experimental technique and how to best evaluate the simulated results with these considerations in mind.

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**Introduction**

Liquid jets in crossflows are important in several applications. These flow fields can be found in propulsion systems, agricultural sprays, and painting sprays. Aerated-liquid injection is a subset of injection strategies that precondition the liquid by injecting small amounts of gas upstream of the nozzle’s injection location within a specifically-designed injector body. This small amount of gas mixes with the liquid to create two-phase structures prior to discharge. It has been shown in Ref. [1] that the discharged two-phase flows are capable of delivering favorable plume characteristics, such as increased penetration height, enhanced atomization, and a widened the spray plume.

A few different approaches to modeling liquid jets in crossflows have been proposed. These include, but are not limited to, the Eulerian-Eulerian approach, where the dispersed and continuous phases are expressed and solved in a Eulerian framework [2, 3], the mixture model, where a volume fraction represents the percentage of liquid and/or vapor residing in each cell [4], or the Eulerian-Lagrangian method, where the continuous phase is solved in the Eulerian framework and the dispersed phase is solved in the Lagrangian framework through the injection of Lagrangian droplets [5]. Promising capabilities of the Eulerian-Lagrangian approach in predicting the average properties of sprays in crossflows have been demonstrated in the Refs. [6, 7].

A significant challenge in modeling an aerated-liquid jet in a crossflow is the injector exit’s boundary condition. Through the experimental efforts of Lin et al. it was observed that the aerated-injector’s nozzle exit yields a core-annular flow structure [8]. This was further analyzed through high resolution simulations that utilized interface capturing techniques to better understand the two-phase flow field [9]. These efforts motivated a set of derivations by Lin et al. that characterize the one dimensional properties of the aerated-injectors across the nozzle region [10]. These derivations assumed a well-mixed two-phase flow and exclusively utilized x-ray fluorescence data and nozzle geometry to calculate gas, liquid, and mixture properties of density, velocity, volume fraction, pressure, and Mach number. It was found that the compressible two-phase flow at the nozzle exit can be choked for an injection condition requiring a high injection pressure. Based on this observation, the two-phase flow condition at the nozzle exit can probably be reasonably modelled without details of the two-phase flows within an aerated-liquid injector.

Therefore, assuming a choked flow, it is possible to specify the pressure, temperature, and velocity of the droplets at the injector exit plane given a specified liquid mass flow-rate ($\dot{m}_L$), gas-to-liquid mass ratio (GLR), and temperature of the incoming mixture. This simplified approach, proposed by Kim et al. [11], yields reasonable injection conditions as compared to results proposed by [9] where the entire injector is simulated in an ILES framework. Unfortunately, information regarding injector spray angle and droplet sizes are not calculable using this method and in the context of this paper must be selected via alternative methods.

In the present study, we propose the use of the Eulerian-Lagrangian method to simulate an aerated-liquid jet injected into a supersonic crossflow environment with efforts to model the nozzle exit flows using relevant information provided by previous measurements. Measurements within the discharged liquid plumes, including, shadowgraph images, laser-sheet images, and phase Doppler particle analyzer (PDPA), will be used to validate the present numerical simulations.

**Experimental Methods**

Experiments were conducted in Research Cell 19 (RC19) at the Air Force Research Laboratory (AFRL), Wright-Patterson Air Force Base. An aerated-liquid injector was flush mounted to the bottom floor of the high-speed tunnel. The facility is a continuous-run open-loop rectangular supersonic wind tunnel. A complete description and characterization of the tunnel was presented by Gruber et al. [12]. Rectangular windows give visualization access to both the side and top walls of the tunnel. The test section has a height of 127 mm, a width of 152 mm, and a length of 762 mm.

Stagnation conditions were set at 206.8 kPa (30 psia) and 260°F (50°C). A supersonic nozzle with a performance Mach number of 1.94 supplies the supersonic air stream.
The aerated-liquid injector uses an outside-in aerating scheme where the gas is injected into the liquid crossflow through 16 pairs of aerating orifices located along the mixing chamber of the injector. The injector’s internal mixing chamber diameter is 2.0 mm (0.08 in). A nozzle adapter with a smooth contour is attached to reduce the 2.0 mm diameter to 1.0 mm. It has a length to diameter ratio of 10.0. Figure 1 shows the schematic of the injector. Water and aerating gas were supplied into the aerated-liquid injector at desired flow rates to form the liquid jet. For the case considered here the liquid mass flow rate \((m_l)\) is held at 18.2 g/s with a gas-to-liquid mass ratio \((GLR)\) of 4%.

Three types of diagnostics were used to characterize the spray structures. A conventional shadowgraph imaging setup with a high-speed camera was used to capture details of the temporal evolution of the liquid plume as well as the penetration height of the plume. A two-component PDPA was also used to determine the properties of the droplets and the spray plume. Details of this technique can be found in Ref. [13]. Droplet size, velocity, number density, and volume flux were measured at a distance of 100 diameters downstream of the injector \((x/d_0)\). These measurements were done on the cross-section \((Y-Z)\) plane normal to the freestream direction \((X)\) to get cross-sectional structures of the spray plume. Lastly, laser sheet imaging was used to look at instantaneous cross-sectional structures of the spray plume at several \(x/d_0\) locations. These images qualitatively characterize regions of the spray with large amounts of interfacial surface area. Each of these techniques has its own limitations and biases in depicting an optically dense spray. Nonetheless, these measurements will be used together in the present study in order to have a better understanding of the entire plume structure.

**Numerical Methods**

Loci/CHEM’s Lagrangian Particle Tracking

Loci/CHEM is a solver utilized heavily in the literature [1-4]. Here we will just describe its use in the application of aerated-liquid jets in crossflows with emphasis on its droplet tracking techniques. The gas phase crossflow is governed by the RANS equations considering a single species air model (non-reacting) flow field. Turbulence effects are taken into account via Mentor’s Shear Stress Transport (SST) model. Loci/CHEM handles the dispersed liquid phase as a set of parcels containing many particles of the dispersed phase. The governing equations for the particle movements are derived using the Basset-Boussinesq-Oseen assumption that the density of the particle is much larger than the continuous phase and that the size of the particle is small compared to the turbulence length scale. It is also assumed that shear forces on particle motion is negligible. The particle equations are as followed:

\[
\frac{dx_p}{dt} = u_p \tag{1}
\]
\[
\frac{du_p}{dt} = \left( \frac{f_1}{\tau_p} \right) (u - u_p) + g \tag{2}
\]
\[
\frac{dh_p}{dt} = \frac{f_2Nu}{3Pr} \left( \frac{C_p}{\tau_p} \right) (T - T_p) + h_{app} \frac{m_i}{m_p} \tag{3}
\]

where \(u_p\), \(h_p\), and \(T_p\) are the particle velocity, enthalpy per unit mass, and temperature. The gas-phase properties are interpolated to the particle location. These include velocity \((u)\), temperature \((T)\), Prandtl number \((Pr)\), and heat capacity \((C_p)\). The \(f_1\) and \(f_2\) functions are corrections to Stokes drag given by Clift and Gauvin [14] and a correction for evaporating droplets. Breakup models are facilitated by a simple Weber stochastic breakup model first proposed by Chryssakis and Assanis [15]. The Sawford turbulence scattering model [16] is used to solve for the particle acceleration term and obtains the fluctuating velocity from integration.

**Aerated-Injector Boundary Condition**

In the present study, efforts to simulate the internal two-phase flows within the injector were not carried out. Instead, relevant measurements on initial plume
spreading angle and droplet populations were used to specify the injector boundary condition. In order to account for the initial expansion processes of the discharged aerated-liquid jet, which typically exhibits a spray cone angle, the injector’s nozzle exit boundary is defined by a spherical cone. This conical surface is defined based on a user’s specified spray angle ($\theta$) at the injector nozzle exit (see Figure 2). Observations from the near field x-ray imaging of the present injection condition injected into a quiescent environment from previous experiments of Lin et al. are utilized to specify the spray angle [17]. For the conditions considered here, this is specified as 64 degrees.

Properties of pressure, temperature, and velocity are specified based on a simple control volume analysis assuming a choked injector [11]. Primary break-up is assumed to be mitigated due to the efficient mixing of the aerated-injector. The presence of including a secondary break-up model is considered and discussed. Droplet properties for each case are obtained by assuming a mean droplet diameter and specifying a log normal distribution. The mean droplet diameter from each case is determined from the PDPA data at the first available $x/d_0$ location and is specified as the flux-averaged Sauter mean diameter (SMD) at the injector face. The log normal distribution’s standard deviation is specified as 0.4 for the results presented. The mean droplet diameter is scaled according to the choice of standard deviation to maintain the flux-averaged SMD. Based on the PDPA measurements at the $x/d_0 = 100$ location, flux-averaged SMD and mean droplet diameter are 15.16 $\mu$m and 10.16 $\mu$m, respectively, for the present injection condition. The size, location, and angle of each injected particle is stochastically determined based on the input parameters. The gaseous portion of the two-phase mixture is assumed to be choked and is injected normal to the cell face.

**Computational Grids**

The structured meshes used for the simulations described in this work were developed using GridPro (Program Development Company). The walls of the tunnel all maintain a $y^* < 1$. Three grid resolutions were tested. The coarse, medium, and fine cases include cell counts of 1.65, 12.5, and 87 million cells. Only the bottom wall in each simulation is clustered. The exit boundary is specified as a supersonic outflow 125 diameters downstream of the injection location. A separate simulation of the Mach 1.94 tunnel was conducted to generate an appropriate inflow condition with a developed turbulent boundary layer.

Figure 2. Schematics for the present approach to model the boundary condition at the exit of an aerated-liquid injector.

Figure 3. Grid refinement study with centerline slices colored by Mach number with overlaid droplet field colored by droplet diameter. Primary cell values are plotted for the centerline slice.
Results and Discussion

Grid Refinement Assessment

Simulations of the aerated-liquid jet into a Mach 1.94 crossflow were conducted on a series of grids with varying refinement levels. In Figure 3, centerline slices colored by Mach contours with overlaid droplets colored by droplet diameter are presented for the three different mesh resolutions. The centerline Mach contours are plotting the primary value in each cell to accentuate the differences between the solutions. Upon refinement, it was found that the averaged data changed little between the medium and fine resolutions. Therefore, the medium resolution, with approximately 12.5 million cells was selected for comparison to the experimental results.
Comparison with Near-Field Shadowgraph Images
In Figure 4, comparisons of the centerline slice with overlaid droplets are made to near field shadowgraph imagery. Instantaneous, time-averaged, and standard deviation of the shadowgraph data compared to the simulation show reasonable agreement in the penetration height in the very near-field region \( x/d_o < 15 \). The presence of the bow shock upstream of the plume is observed in the instantaneous shadowgraph image. The bow shock’s location upstream of the jet, curvature, and slope are in good agreement to the calculated results. When observing the time-averaged shadowgraph, the droplets appear to be over predicting the penetration height. However, the upper bound of the standard deviation shown in Figure 4 suggests that the Lagrangian droplets are within the uncertainty region of the spray height as determined by shadowgraph. In all images, the shadowgraph observes a much denser spray near the leeward side of the spray as compared to the simulated results.

Comparison in Plume Penetration Heights
Jet penetration height is an important figure of merit for simulating a jet in crossflow. Several correlations have been published describing the penetration characteristics of liquid jets in crossflows. For our aerated-liquid jet we compare to two different correlations. The first, developed by Lin et al., uses PDPA data with a threshold value of 0.0001 \( m^3/s/m^2 \) to define the penetration boundary of the jet [1]. The second uses shadowgraph imagery and considers the jet penetration to be defined by a 90\% transmittance in the imagery [13]. In Figure 5, penetration heights using both correlations are compared to the simulated crossflow.

Results are presented with and without a secondary break-up model.

Utilizing the flux averaged SMD at an \( x/d_o \) of 100 for the injector mean diameter forces the assumption that little to no break-up occurs between the injector face and one hundred injector diameters downstream. Results from both cases are presented to understand sensitivities to such an assumption. When the break-up model is included the initial penetration height is found to closely follow the correlation derived from shadowgraph imagery.

In contrast, the penetration height calculated without a break-up model largely follows the PDPA correlation. In both cases, a slight over-prediction compared to the PDPA and shadowgraph is observed past an \( x/d_o \) of 40. An increased mean droplet diameter at the injection location could be considered for the case with a break-up model as some level of break-up is expected for this flow field. Basing the injection properties solely on the PDPA data one hundred diameters downstream without consideration for break-up may be ill posed. Therefore, one could consider some type of correlation or modeling approach for initial droplet size specification at the injection location.

Comparison in Cross-Sectional Plume Structures
In Figure 6, qualitative comparisons are made between the simulated results to both laser-sheet and shadowgraph imaging. In the first row, time-averaged laser-sheet imaging is compared to cross-sectional slices of the simulated plume. The edge of the plume in the computed results is defined by an axial volume flux threshold value of 0.0001 \( m^3/s/m^2 \). The cross sectional areas are colored by droplet axial velocity. Similar comparisons are made in the second row, but here, the standard deviation of the laser-sheet imaging is used for comparison. Reasonable agreement is observed for the growth rate of the plume width between the simulation and experimental results. The growth of the penetration height in the near field of the spray \( x/d_o < 50 \) is in good agreement to the laser-sheet imaging, but is observed to over predict the penetration height in the farfield \( x/d_o \geq 50 \). The bottom images compare an averaged shadowgraph image to the Lagrangian droplet field. Shadowgraph again appears to predict a shallower penetration height as compared to the droplet field. We note that this case does include secondary break-up effects.

![Figure 5. Aerated-liquid jet penetration height comparison of PDPA [1], shadowgraph [13], and simulation with and without a secondary break-up model.](image-url)
In Figure 7, we consider the effects of secondary break-up with comparison to PDPA data at an $x/d_0$ of one hundred. Similar to Figure 5, penetration characteristics without the secondary break-up model are in closer agreement to the PDPA dataset. While we understand that this is a consequence of the selected mean droplet diameter at the injector location, we choose to consider the other measurements from PDPA with respect to the simulated results without a break-up model.

Cross sectional slices at an $x/d_0=100$ for the simulated results without a secondary break-up model are compared to PDPA results at the same axial location in Figure 8. Variables compared include velocity (Fig. 8, a and b), SMD (Fig. 8 c), volume flux (Fig. 8, d and e), and number density (Fig. 8 f). In general, the shape and distribution of the droplet velocities agree reasonably well with the experimental results. The axial velocity is slightly under predicted, but only minimally. The core region of the spray predicts a much smaller velocity as compared to the PDPA. In Figure 8c, SMD is found to be much larger in the core of the plume for the PDPA. Similarly, the computational method appears to over predict the volume fluxes and number density in the core region of the spray.

To better understand these large discrepancies we compare PDPA, simulation, and laser-sheet imaging in Figure 9. Laser-sheet imaging indicates a region of high scattering light intensity, which is closely related to the droplet number density, in the core of the plume. In contrast, PDPA only measures droplets in the top portion of the plume in a region where laser-sheet imaging provides little to no illumination. This suggests that both the PDPA and laser-sheet imaging may be missing a portion of the spray due to

Figure 6. Qualitative spray comparison between (first row) averaged laser-sheet imaging and simulated plume colored by axial droplet velocity, (second row) standard deviation of laser-sheet imaging and simulated plume at several $x/d_0$ cross sectional locations. Centerline Mach contours with overlaid droplet field are compared to shadowgraph imagery in the third row.
their biases. An arbitrary iso-line of the PDPA is extracted and overlaid on both CFD and laser-sheet imaging results. The regions of overlap for the two experimental data sets are minimal. This PDPA setup is known to be unable to process data within a given control volume where multiple droplets pass at a given instant at the same time. Therefore, PDPA will be biased towards larger droplets in less dense regions of the spray. Laser-sheet imaging applied to a spray measures light illumination due to interfacial light reflection and refraction and, therefore, will be biased towards regions of high interfacial density, or regions of high number density. This connection suggests that neither PDPA nor laser-sheet imaging can alone be used to model validation. If only one is used, the model specifications and development could easily become biased to one series of experiments. Here, the simulated results contain both attributes of the PDPA and laser-sheet imaging providing a baseline level of credibility to our model selection.

Figure 7. Cross sectional slice comparison at \( x/d_0=100 \) between PDPA and computational results with and without a secondary break-up model.

Figure 8. Cross sectional slice comparison at \( x/d_0=100 \) for (a) droplet u-velocity, (b) droplet v-velocity, (c) SMD, (d) volume flux in x-direction, (e) volume flux in y-direction, and (f) number density.

Summary and Conclusions
Simulations of an aerated-liquid jet into a Mach 1.94 crossflow were conducted utilizing a RANS framework coupled to a Lagrangian droplet tracking code. A simplified spherical cone was used to model the injector’s boundary condition. User specified spray angle (obtained from a previous x-ray image), mean droplet diameter (based on the present PDPA measurements), and selected standard deviation to the log-normal droplet size distribution with a simple
control volume analysis were shown to provide a representation of the injector’s exit properties.

The simulated jet’s results were compared to three measurements: PDPA, shadowgraph, and laser-sheet imaging. The effect of removing the secondary break-up model was considered. Sensitivities to the presence of a secondary break-up model with respect to penetration height were compared to both PDPA and shadowgraph correlations. The overall shape, width, and heights of the plume were found to be reasonable with respect to the laser-sheet imaging. Contrarily, the measures droplet SMD, droplet number density, and volume fluxes from PDPA suggests that there are uncertainties between the simulations and measurements specifically in the core region of the spray plume. It appears that both PDPA and laser-sheet diagnostics are biased towards different regions of the spray plume. Utilization of multiple datasets from different diagnostics for numerical simulation validation can potentially reduce uncertainties. By utilizing a holistic approach, one will not fall into a pitfall by assuming a dearth of droplets within the core region of the spray as suggested by PDPA.

Further considerations should be made to address the necessity for experimental data near the injector exit. A more thorough understanding of the injector’s exit condition can be beneficial to provide a boundary condition that does not require experimental data to drive its specifications. More validation of the present modeling approach should be carried out for more injection conditions with variations in liquid mass flow rate, GLR, nozzle geometry, and crossflow geometry.

![PDPA vs CFD and Laser-Sheet Imaging](image)

**Figure 9.** Comparison of PDPA, CFD, and laser-sheet imaging at the extracted plume location of $x/d_o=100$.

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**References**

7. Im, K.-S., Zhang, Z.-C., Cook, G., Lai, M.-C., and Chon, M.S., “Simulation of Liquid and Gas-Phase Characteristics of Aerated-Liquid Jets in
Quiescent and Crossflow Conditions,”
International Journal of Automotive Technology,