Detailed Numerical Simulation of Liquid Jet in Cross Flow Atomization: Impact of Nozzle Geometry and Boundary Condition

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Abstract
The atomization of a liquid jet by a high speed cross-flowing gas has many applications such as gas turbines and augmentors. The mechanisms by which the liquid jet initially breaks up, however, are not well understood. Experimental studies suggest the dependence of spray properties on operating conditions and nozzle geometry. Detailed numerical simulations can offer better understanding of the underlying physical mechanisms that lead to the breakup of the injected liquid jet. In this work, we present detailed numerical simulation results of turbulent liquid jets injected into turbulent gaseous cross flows for different injector geometries and operating conditions. We employ a finite volume, balanced force fractional step flow solver to solve the Navier-Stokes equations coupled to a Refined Level Set Grid method to follow the phase interface. To enable the simulation of atomization of high density ratio fluids, we ensure discrete consistency between the solution of the conservative momentum equation and the level set based continuity equation by employing the Rescaled Conservative Momentum method. We analyze the impact of injector geometry and inflow jet boundary condition on different jet properties including jet penetration and compare the results to those obtained experimentally by [1].

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Introduction

The atomization of turbulent liquid jets injected into fast moving, subsonic gaseous crossflows is an important application for example in gas turbines, ramjets, and augmentors. Breakup mechanism influences the efficient mixing of the fuel/air mixture, and as a result the combustion efficiency and pollutant formation. Liquid jet breakup in a crossflow is a highly complex process, that has been extensively studied experimentally over the past decades. Different type of instabilities grow along the liquid surface and stretch ligaments around the periphery of the liquid jet. These ligaments are terminated when drops are stripped from their ends. The breakup is influenced by different parameters such as aerodynamic forces, turbulence in the crossflow and liquid jet, geometry of the injection nozzle. It was found that the occurrence of cavitation inside the nozzle significantly influences the breakup of the liquid into droplets [2], [3]. Experimental results also show correlation between statistics such as liquid jet penetration and trajectory, Sauter mean diameter of drops and physical variables [4], [5].

Detailed numerical simulation, on the other hand can offer a better understanding of the underlying physical mechanisms that lead to the initial breakup of the injected liquid jet, since one can access and explore the entire domain of simulation. Although atomization of jet in crossflow has been widely studied numerically in the past few years, but required resolution, tracking the interface, surface tension and phase interface is a discontinuity makes it a challenging approach specially when density ratios are high.

The outline of this paper is the following: after summarizing the governing equations, the numerical method employed to solve them for multiphase flow problems with high density ratios are explained. Finally simulation results of the primary atomization of liquid jet (q=6.6, We=330, Re=14,000) with different liquid inflow boundary conditions injected into a turbulent gaseous crossflow (Re=570,000) are analyzed and compared to experimental results.

Governing equations

The equations governing the motion of an unsteady, incompressible, immiscible, two-fluid system are the Navier-Stokes equations in conservative form,

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot (\mu (\nabla u + \nabla^T u)) + \rho g + T_\sigma, \quad (1)
\]

or in non-conservative form,

\[
\frac{\partial u}{\partial t} + u \cdot \nabla u = -\frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \cdot (\mu (\nabla u + \nabla^T u)) + g + \frac{1}{\rho} T_\sigma \quad (2)
\]

where \( \mathbf{u} \) is the velocity, \( \rho \) the density, \( p \) the pressure, \( \mu \) the dynamic viscosity, \( g \) the gravitational acceleration, and \( T_\sigma \) the surface tension force which is non-zero only at the location of the phase interface \( x_f \),

\[
T_\sigma(\mathbf{x}) = \sigma \kappa \delta(\mathbf{x} - x_f) \mathbf{n}, \quad (3)
\]

with \( \sigma \) the assumed constant surface tension coefficient, \( \kappa \) the local mean surface curvature, \( \mathbf{n} \) the local surface normal, and \( \delta \) the delta-function. In addition, conservation of mass results in the continuity equation,

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \quad (4)
\]

The phase interface location \( x_f \) between the two fluids is described by a level set scalar \( G \), with

\[
G(x_f, t) = 0 \quad (5)
\]

at the interface, \( G(x, t) > 0 \) in fluid 1, and \( G(x, t) < 0 \) in fluid 2. Differentiating (5) with respect to time yields the level set equation,

\[
\frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = 0 \quad (6)
\]

For numerical accuracy of geometric properties of the phase interface it is advantageous, although not necessary, to define the level set scalar away from the interface to be a signed distance function,

\[
|\nabla G| = 1 \quad (7)
\]

Assuming \( \rho \) and \( \mu \) constant within each fluid, density and viscosity at any point \( \mathbf{x} \) can be calculated from

\[
\rho(\mathbf{x}) = H(G) \rho_1 + (1 - H(G)) \rho_2 \quad (8)
\]

\[
\mu(\mathbf{x}) = H(G) \mu_1 + (1 - H(G)) \mu_2 \quad (9)
\]

where indices 1 and 2 denote values in fluid 1, respectively 2, and \( H \) is the Heaviside function. Finally, the interface normal vector \( \mathbf{n} \) and the interface curvature \( \kappa \) can be expressed in terms of the level set scalar as

\[
\mathbf{n} = \frac{\nabla G}{|\nabla G|}, \quad \kappa = \nabla \cdot \mathbf{n} \quad (10)
\]
Numerical Method

The Navier-Stokes equations are solved using a fractional step method [6] on unstructured collocated meshes. In order to ensure discrete consistency between the solution of the conservative momentum equation and the level set based continuity equation Consistent Rescaled Momentum Transport method[7] is used.

Computational Domain and Operating Conditions

Detailed numerical simulation of jet in crossflow atomization with high density ratio was performed for different cases based on the experimental study by Brown & McDonell [1]. Table 1 summarizes the operating conditions and resulting characteristic numbers.

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Table 1. Operating conditions and characteristic numbers [1].

Figure 1 depicts the computational domain and the used boundary conditions as well as a zoom into the near-injector region to show the mesh detail used in the simulations. The chosen computational domain is (-25D...50D X 0...25D X -10D...10D) is smaller than the channel used in the experiment (-77D...127D X 0...54D X -27D...27D) where D is nondimensional diameter of the jet exit. However, simulations using the full experimental channel geometry were conducted to verify that the reduced computational domain does not impact the reported results [8].

The injector geometry used in the experiments consists of a long initial pipe section of diameter 7.49mm, followed by an 138° angled taper section, followed by a short pipe section of diameter D with $L/D = 4$, whose exit is mounted flush with the lower channel wall.

The flow solver grid consists of hexahedra of edge length D/4, which are isotropically refined in layers near the injector and lower channel walls, such that the spatial region where the phase interface is tracked is completely filled with equidistant grid cells of the minimum cell size $\Delta x = D/32$ for the coarse mesh and $\Delta x = D/64$ for the fine mesh. Note that, the G-grid is a factor 2 finer than the flow solver grid in order to enhance numerical accuracy of the interface tracking scheme. At $t = 0$, the liquid jet is initialized in the computational domain by a small cylindrical section of length D capped by a half-sphere, protruding into the crossflow channel. For more detail see [8].

The inflow gas is assumed fully developed and a channel flow velocity distribution is assigned to it. In order to investigate the impact of the nozzle geometry and turbulence in the velocity of the liquid inflow different jet in crossflow simulations was performed using the following jet inflow velocity profiles:

To account for its effect in the atomization simulations, detailed single phase Large Eddy Simulations (LES) of the pre-taper pipe, the taper, the post-taper pipe, and the cross flow channel in the vicinity of the injector exit were performed using a dynamic Smagorinsky model. The channel section was included in these simulations to capture the effect of the cross flow on the injector exit plane velocity distribution. Inflow boundary conditions for the pre-taper pipe were taken from a pre-computed LES pipe flow simulation database at the appropriate Reynolds number. The injector exit plane velocity distributions were then stored as a time sequence in a database to be used in the subsequent two-phase
atomization simulations.

The inflow database described in the above section was averaged over the time in order to neglect the effect of turbulence in the velocity of the liquid inflow. This averaged velocity profile is used for all the timesteps of the two-phase simulation of the atomization.

**Figure 2.** Instantaneous injector exit plane velocity distributions in axial direction form: database including nozzle geometry (left-top) [8], averaged database including nozzle geometry (right-top) and turbulent pipe flow database (bottom). Gas crossflow is from left to right.

In order to neglect the effect of the cross flow, LES pipe flow simulation with the appropriate Reynolds number is performed for a single pipe with the diameter of the post-taper pipe of the actual nozzle to generate the database. Figure 2 shows the Instantaneous injector exit plane velocity distributions in axial direction all three velocity profiles used as jet inflow boundary condition. Figure 2 shows three mentioned jet inflow velocity distributions.

**Including nozzle geometry directly:**

In order to investigate the effect of replacing the nozzle geometry with a database at the exit plane of the injector, two-phase atomization simulation was performed using fully developed turbulent pipe flow as inflow boundary condition for the pre-taper pipe.

**Results and Discussion**

We first performed simulations with density ratio $r=100$, keeping all other nondimensional parameters in table 1 the same. Figure 3 shows a snapshot of the simulation using the data base including nozzle geometry and its average on top of each other. Instabilities generated right after the nozzle exit and their grow rate along the jet penetration are comparable from both simulations, which suggests that at this resolution the turbulence in the injected jet does not have significant impact on the generation of instabilities.

**Figure 3.** Snapshot of the simulation with density ratio 100, using the data base including nozzle geometry (blue) and its average (green) at time=30.0.

Figure 4 shows a snapshot of the simulation using the data base including nozzle geometry and pipe flow data base on top of each other. In the simulation using pipe flow data base, liquid jet penetrates more in the cross flow gas since the jet inflow boundary condition does not include the effect of the cross flow gas.

Figure 5 shows different averaged normal cross sections of the jet for different distances from the bottom wall. Liquid column in the simulation using the pipe flow data base is more deformed and separation of ligaments and drops from the sides of the liquid column occurs faster comparing to corresponding results from the simulation using data base including nozzle geometry. This can be due to the higher drag forces acting on the jet that penetrate faster and higher in the cross flow gas which is from the simulation with pipe flow data base.
Figure 4. Snapshot of the simulation with density ratio 100, using the data base including nozzle geometry (blue) and its average (green) at time=30.0.

Figure 5. Averaged normal cross sections of the jet for different distances from the bottom wall: y/D=0.5(a), y/D=1.5(b), y/D=2.5(c).

Another important parameter in the atomization of the liquid jet in cross flow is jet penetration correlation. Mean leading edge can be used to determine the jet penetration of the simulations. In order to calculate the mean leading edge, Volume of Fluid (VOF) scalar is averaged over time and different probability isolines is fitted to it (figure 6). In our simulations probability isoline of VOF=0.5 is used to calculate the mean leading edge of the jet.

Figure 6. Averaged Volume of Fluid (left) and probability isoline (right).

The comparison between the experimental jet penetration correlation of Wu et al [9], and jet penetration from our simulations (figure 7) shows that in our simulations liquid jet bends faster than experimental studies. One potential reason can be the difference between the density ratios. Experimental studies are usually performed at the ambient pressure and high density ratio between gas and liquid, while in numerical simulations it is preferable to apply the boundary conditions similar to operating conditions of those devices that atomization occurs in, which means low pressure and high density ratio.

Figure 7. Comparison between jet penetration from numerical simulations with density ratio r=100 and experimental correlations.
In order to investigate the effect of density ratio on the jet penetration another simulation was performed with the same density ratio of the experiment ($r=816$). Comparison between the experimental jet penetration and jet penetration from the simulation with high density ratio (figure 8) suggests that density ratio has an important impact on the jet penetration and results from simulations with high density ratio is significantly closer to the experiment.

Figure 8. Comparison between jet penetration from numerical simulations with high density ratio and experimental correlations.

Conclusions

Detailed numerical simulation of liquid jets injected into turbulent gaseous cross flows for different liquid jet inflow velocity profiles was performed using a Consistent Rescaled Momentum Transport method. Three different jet inflow velocity profiles were applied to investigate the impact of turbulence in the inflow jet velocity and the effect of the cross flow on the on the incoming jet velocity profile. Results suggest that at the grid resolution that simulations were performed turbulence in the in the inflow jet velocity profile does not have a significant impact on the instabilities that grow on the surface of the liquid column and lead to the breakup of the jet. Results also show that impact of the cross flow gaseous on the velocity profile of the inflow jet effects the results of the simulation including the penetration of the liquid jet in the cross flow gas. Comparison between the jet penetration for simulations with different density ratios indicates changing the density ratio changes the jet penetration and using the same density ratio as experiment makes the results of the simulation more comparable to the experimental penetration correlations.

References


