Three-dimensional Segment Analysis of Transient Liquid Jet Instability

D. Jarrahbashi* and W. A. Sirignano
Department of Mechanical and Aerospace Engineering
University of California, Irvine
Irvine, CA 92797 USA

Abstract

Primary atomization of a liquid jet injected into still air during the start-up period of injection at high Re and We numbers has been addressed in the present computational work. During start-up period, the velocity of the jet reaches to 200 m/s and very small-scale instabilities in the order of a few microns appear at the interface. The protrusions formed at the liquid jet interface as a result of Kelvin-Helmholtz (KH) instability are exposed to a high acceleration that leads to very small-scale Rayleigh-Taylor (RT) instability at their edges. The experimental size of the droplets that eventually detach from the liquid jet is very close to RT instability wavelengths. Sufficient resolution could be cumbersome; especially, for three-dimensional direct numerical simulation of transient jet instability. A new model has been developed to ease the resolution problem and capture the shortest unstable surface wavelengths. This model examines stream-wise segments of the jet during the transients instead of simulating the full liquid jet. By transforming the coordinate system from the laboratory frame to an accelerating frame fixed to the liquid a new term appears in the Navier-Stokes equations analogous to a body force. The value of the acceleration of the frame of reference applied in the equations of motion is obtained from an axisymmetric simulation of full transient jet performed previously. An initially quiescent cylindrical liquid jet is exposed to a high speed and high pressure air accelerating along its axis. Three-dimensional Navier-Stokes equations have been solved based on a finite-volume scheme on a Cartesian boundary-fitted-grid for liquid streams and adjacent gas. A level-set method has been applied for tracking the gas/liquid interface. The three-dimensional vorticity dynamics of the liquid jet describes the evolution of surface instabilities and formation of the ligaments that finally detach from the liquid due to capillary instabilities. The ranges of measured wavelengths of both KH and RT instabilities found for axisymmetric full jet and axisymmetric liquid-segment are comparable to those of three-dimensional liquid-segment model. The qualitative behavior of all kinds of jet instability is consistent with the experiments on a liquid jet exposed to fast gas stream blowing parallel to its axis. The three-dimensional liquid-segment approach can be useful as a predictor of droplet size. The axisymmetric liquid-segment approach also has very useful predictive value.

*Corresponding author: djarrahb@uci.edu
Introduction

Investigation of the behavior of the liquid fuel jet during the transient portion of injection, i.e., start-up and shut-down is crucial to understand the overall aspects of jet atomization and droplet size distribution. Enhancement of the quality of the fuel/air mixing process in a Diesel engine requires knowledge of the jet break-up characteristics and the size of the formed droplets during the start-up and very close to the injection nozzle. The liquid jet experiences a very high acceleration during the transient portion of the injection. The effects of this acceleration on jet break-up and formation and detachment of the ligaments and droplets must be emphasized.

Experimental studies of transient liquid jet [1, 2, 3, 4] provide limited information about the small-scale structures of the liquid jet. Atomization and evaporation of the liquid jet produces a dense fog around the jet that impedes the optical access to the jet. Experimental observation of Smallwood et al. [1] shows that near-field structures of the transient jet are noticeably different than its steady-state counterpart. However, the transient jet nearly resembles the steady jet at further positions downstream of the nozzle. Kim and Lee [2] depicted that, unlike the continuous sprays, the development of spray structure was a time-dependent process for transient jet. The measured Sauter Mean Diameter (SMD) was smaller for early stages of jet injection and gradually increased with time. High quality images from the near field of a transient liquid jet provided by ballistic imaging techniques by Linne et al. [3] showed that the periodic structures were smaller closer to the nozzle at early stages of injection. However, wavelengths increased to slightly greater than the orifice diameter at later stages of jet injection. Therefore, a broader study is required to capture the detailed information on the primary instability of the liquid transient jets.

Most of the numerical studies on transient liquid jet investigate the break-up lengths of the jet compared to the steady-state using the empirical constants [4]. Turner et al. [5] predicted the transient jet break-up length and its penetration into the gas by proposing a composite break-up model that was more consistent with the experiments compared to steady-state calculations. They also showed that the transient behavior of the jet plays an insignificant role in the overall break-up length of the jet. However, the effects of the acceleration that are crucial in the initial stripping of the droplets from the coherent jet needs consideration. Turner et al. [6] studied the effects of acceleration on the break-up lengths and break-up time for planar liquid jets by implementing a wave packet analysis on the disturbances initiated from the orifice. They showed that the unsteady effects of the jet are noticeable for high accelerations and high liquid to air density ratios, especially at early stages of injection. They also reported that for later times of injection when the velocity profile varied slowly with time, the overall characteristics of the unsteady jet, e.g. the break-up lengths and time were not affected significantly compared to that of the quasi-steady jet.

Three-dimensional simulation of primary atomization of turbulent liquid jets using Refined Level Set Grid (RLSG) by Herrmann [7, 8] exhibited a highly complex interfacial instability with large range of different droplet sizes. Capillary effects were shown to have a great effect on the topology changes at the interface where the local Weber number was small. Shinjo and Umemura [9] numerically investigated the three-dimensional physics of ligament and droplet formation from the interface of a liquid jet injected into still air. They concluded that the shear from the local vortices played an important role in the ligament formation. However, to our knowledge, the effects of high accelerations on jet instability have not been investigated thoroughly in the literature.

Wavelengths of instabilities and resulting dimensions of ligaments and droplets breaking from the stream will determine droplet-size distribution. The mechanisms for wave instabilities on the liquid-gas interface are capillary instability, Rayleigh-Taylor (RT) instability caused by local acceleration of the interface, Kelvin-Helmholtz (KH) instability caused by relative motion of the two phases parallel to the interface, and a synergism of the above mentioned mechanisms. Non-linear growth and distortion of these surface waves lead to protrusions of liquid into the surrounding gas; commonly named “fingers.” These protrusions are exposed to even higher accelerations normal to their interface that make them a good prey for the secondary RT instability associated with very short wavelengths comparable to the size of the droplets that detach from the jet core later.

This phenomenon has been experimentally observed by Marmottant and Villirmaux [10] for a small diameter liquid jet exposed to high-speed gas jet. They stated that the atomization process consisted of two steps. Firstly, the shear instability produces the primary KH wavelength, and secondly, smaller secondary RT instability wavelengths were generated on the wave crests resulted from the shear instability. Varga et al. [11] studied the disintegration of a liquid jet exposed to a fast stream gas flow and observed the same mechanism; formation of RT waves on top of the KH instabilities due to the high accelerations perpendicularly to the interface of the ligaments. They proposed a break-up model for the initial droplet size based on the same mechanism that breaks up liquid drops in high speed airstream originally investigated by Joseph et al. [12] based on the Viscous Potential Flow (VPF) analysis [13]. The range of droplet sizes predicted by Varga et al. was approximately proportional to one fifth of the


[9]

[11]

[12]

[13]

[10]
observed RT wavelengths. Therefore, quantitative descriptions of the nonlinear synergism of KH/RT instability for a transient liquid jet are a significant step in understanding the jet break-up. However, providing the sufficient resolution to capture small-scale structures of the transient jet could be cumbersome; especially, for three-dimensional direct numerical simulation of transient jet instability.

In our previous studies [14, 15], we created a new model for liquid-fuel injection breakup during start-up which incorporated the main physics involved in this phenomenon. Stream-wise segments of the jet exposed to an accelerating stream were examined and treated as ballistic slugs coming from the orifice. This reduction of the computational domain was designed to give the required resolution to characterize the physics through computations. These slugs were much longer than the jet diameter and the expected RT and KH wavelengths. The range of KH and RT wavelengths were proved to be consistent with the numerical simulation of a transient full jet, experiment, and linear instability theory. Axisymmetric Navier-Stokes equations were solved for both phases using finite volume method. A level-set method was applied to capture the topological changes of liquid/gas interface.

This paper addresses the development of the previous axisymmetric model to three-dimensions. The mechanisms responsible for breaking the ligaments into droplets, i.e. capillary necking for three-dimensionally-shaped fingers, are well defined in this three-dimensional model. The formation and development of the streamwise and transverse vortices of the liquid jet that leads to the formation of the three-dimensional ligaments will be investigated. Certain questions need to be answered: “What can be learned from the axisymmetric full-jet simulation and how does that correlate to the results obtained from axisymmetric liquid-segment method?” “What are the advantages of using liquid-segment method over the full-jet simulation, and finally”, “What do three-dimensional liquid-segment have in common with the axisymmetric models and what information does it add to our knowledge from the transient jet primary atomization?”

In the next section of this paper, the numerical method is discussed for both axisymmetric and three-dimensional simulation. The results are given in the following three sections: Firstly, a summary of the results obtained for axisymmetric full jet. Secondly, axisymmetric liquid-segment method will be provided. Thirdly, the three-dimensional liquid-segment model will be discussed.

Numerical Method

The Navier-Stokes and continuity equations which for an incompressible flow have a conservative form as (1) have been solved. The convection-diffusion problem has been discretized based on the finite volume method using the QUICK algorithm [16] and the Crank-Nicolson scheme for discretizing the unsteady term in the equations of motion. The coupling of continuity and momentum equations is done through the SIMPLE algorithm [17].

\[ \rho(\frac{\partial \bar{u}}{\partial t} + \bar{u} \cdot \nabla \bar{u}) = -\nabla p + \mu \nabla^2 \bar{u} + \bar{F}; \quad \nabla \cdot \bar{u} = 0 \]  

where \( u \) is the velocity field \( \rho \) and \( \mu \) are the density and viscosity of the fluid, respectively. \( p \) is the pressure field, and \( F \) is the body force applied to the fluid. The level-set method developed by Osher et al. [18] and [19] is used for tracking the liquid/gas interface. Level-set is defined as a distance function with zero value at the liquid/gas interface; positive values in the gas phase and negative values in the liquid phase. The level-set function is denoted by \( \theta \) and all the fluid properties in both phases in the Navier-Stokes equations can be defined based on its values and the equations could be solved for both phases simultaneously. The level-set function is also convected by the unknown velocity field based on the following equation:

\[ \frac{\partial \theta}{\partial t} + \bar{u} \cdot \nabla \theta = 0 \]  

In addition, the surface tension force applied on the interface is also defined based on the level-set function and curvature of the interface as is shown in the third term on right-hand side of Navier-Stokes equation as follows:

\[ \rho \frac{D\bar{u}}{Dt} = -\nabla p + \mu \nabla^2 \bar{u} - \sigma \kappa \delta(d) \bar{n} \]  

where \( \sigma \) is the surface tension coefficient, \( \delta \) is the delta function, \( d \) is the distance from the interface, \( \bar{n} \) and \( \kappa \) are the normal vector directing toward the gas phase and the curvature of the interface, respectively, defined as follows:

\[ \bar{n} = \frac{\nabla \theta}{|\nabla \theta|}; \quad \kappa = \nabla \cdot \bar{n} \]  

Continuity of both velocity and shear stress has been applied at the interface. For details of the numerical method, see [20, 21]. The computational domain and gridding system which consists of an orifice with 200 μm diameter, initially full of liquid and a gas chamber initially filled with quiescent gas is demonstrated in figure 1 (a). The fluid properties have been gathered in table 1. Re and We numbers have been de-
ined as follows: $Re = \rho u D/\mu$, $We = \rho u^2 D/\sigma$, where $\rho$, $u$, $\mu$, and $D$ are the maximum jet exit velocity, the liquid density, liquid viscosity, the surface tension coefficient, and the orifice diameter, respectively.

**Full Jet Axisymmetric Simulation**

The behavior of the liquid jet injected into air at 30 atm pressure during the early stages of start-up is shown in figure 2. A mushroom-shaped cap forms as the jet develops along the chamber, while the orifice pressure-drop and the jet exit velocity increase rapidly during the first stages of the start-up. The cap grows in volume and vortices at the interface roll back and entrain air into the rear side of the cap. The starting jet displays strong instabilities along the edges and moving front. As the jet develops along the chamber, the protruding “fingers” form and are drawn out of the jet and grow in the radial direction. The typical KH instabilities can be detected with average wavelength of 100 $\mu$m. On the other hand, since the liquid (heavier fluid) finger is accelerating into the gas (lighter fluid) during the start-up, these KH protrusions at the interface are susceptible to the secondary RT instabilities; thus, the RT instability appears at the rear side of the jet cap during the start-up as is shown in the magnified picture of figure 2. RT wavelengths are directed normal to the jet axis and have smaller wavelengths compared to KH wavelengths.

Figure 3 (a) demonstrates the development of both KH and RT wavelength at 100 $\mu$m after the start of injection. The vertical and horizontal tick marks indicate the KH, and RT wavelengths at the interface and back of the mushroom-shaped cap, respectively. The range of unstable KH and RT wavelengths during 100 $\mu$m from the start of injection has been demonstrated in figure 3 (b). The first 10 $\mu$m is associated with the development and roll-up of the jet cap; therefore, the interface has not been distorted due to instabilities at this stage. After about 10 $\mu$m the interface starts to be distorted due to shear instability and wavelengths in the range of 50 to 120 $\mu$m appear at the interface. At 20 $\mu$m, secondary RT instability wavelengths (10-30 $\mu$m) were detected at the back of the jet cap. We expect the RT instability on this side where the heavier fluid is accelerating into the lighter fluid. Simultaneously, KH waves continue to develop at the interface further. As the liquid jet develops with time, the primary KH wavelengths increase to more than 300 $\mu$m at 100 $\mu$m greater than the diameter of the orifice, i.e. 200 $\mu$m. The RT wavelengths associated with these longer KH waves also increase to 40 $\mu$m at 100 $\mu$m compared to 10 to 30 $\mu$m wavelengths observed earlier. This trend indicates that the RT secondary instability wavelength is non-linearly dependent on the primary KH wavelength. In other words, longer KH wavelengths produce longer RT wavelengths at their edge. This dependency has been experimentally observed by Varga et al. [11]. Therefore, the effects of acceleration on jet instability is firstly on producing shorter KH wavelength since the velocity difference between the liquid and gas is higher when the jet is accelerating into the liquid compared to the steady-state jet. Secondly, the KH protrusions are exposed to an acceleration exerted by the gas at the interface that is even higher than the acceleration of the liquid injected form the orifice.

Our simulations show that the local acceleration normal to the protrusions is an order of magnitude higher than that of the liquid at the orifice. The combination of these effects with same modification by the surface tension determines the KH and RT wavelengths. Surface tension has been observed experimentally and theoretically to have stabilizing effects on the shorter wavelengths [11]. Our numerical method confirms the same effect for the transient jet.

The RT instability dispersion relation and wavelength based on the classic linear instability analysis by Chandrasekhar [23] is as follows:

\[
\omega = \left[\frac{\mu (\rho_g - \rho_l)}{2 - \rho_l + \rho_g} a_n - k^3 \sigma \right]^{1/2}
\]

\[
\lambda_{RT} = 2\pi \frac{3\sigma}{\sqrt{(\rho_l - \rho_g)a_n}}
\]

where $\omega$ is the growth rate, $\lambda_{RT}$ is the RT instability wavelength, $k$ is the wavenumber, $\sigma$ is the surface tension coefficient, $\rho_l$ and $\rho_g$ are the density of the gas and liquid, respectively, and $a_n$ is the acceleration perpendicular to the liquid interface. Although this formulation neglects the effects of viscosity on jet instability, it is a straightforward way to predict the range of RT wavelengths directly from measuring the normal acceleration of the ligaments. This equation has been extensively used in many publications as a means to estimate the theoretical RT wavelengths compared to the numerical or experimental observations [5, 10, 11, 24, and 25].

The value of this normal acceleration has been obtained by measuring the change of the streamwise velocity at the crests of 10 samples of the observed protrusions for 1-µs intervals during 60 microseconds after the start of injection. This time period has been used since the liquid jet is experiencing the highest acceleration during the early stages of start-up associated with complicated and small-scale unstable structures on the liquid jet interface. The thickness of the interfacial protrusions, local normal acceleration, and RT wavelengths for a few selected ligaments at different injection times has been shown in table 2 for $Re$ and $We$ numbers equal to 16,000 and 230,000, respectively. Comparison of the
local computed RT wavelengths with the theoretical RT wavelength based on equation (5b) shows a reasonable agreement. The discrepancies stem from the fact that, as mentioned earlier, this formula does not take into account the effects of liquid viscosity that has stabilizing effects for shorter wavelengths. Therefore, the measured RT wavelength is slightly larger compared to the theory.

Our results discussed in [15] show that the upper limit of KH wavelength depends on the relative velocity between the liquid and gas. The liquid viscosity has stabilizing effects on the small-scale instabilities. Therefore, for higher liquid viscosity, RT waves at the lower end of their wavelength range are damped; however, larger KH wavelengths are not affected significantly. The most probable (fastest growing) RT wavelength depends on surface tension. Higher We number leads to smaller RT wavelengths on top of the primary KH protrusions.

**Axisymmetric Liquid-Segment Model**

The results obtained by full jet simulation have been used to develop a new model to capture the instabilities at the liquid/gas interface with better resolution and less computational resources. In this new model, a section of the jet whose fixed length is longer than the interesting wavelengths but still computationally manageable, e.g. 1-mm length for a 200-micron initial diameter of the liquid jet, has been considered during the start-up period of jet injection, see figure 1 (b). During the start-up, orifice exit velocity increases with time, which implies a stream-wise decreasing velocity through the jet due to the effects of drag forces acting on the liquid. As the jet emerges from the orifice, drag forces due to entry into the dense air cause a deceleration. Also, the dynamic protrusions from the jet interface are subject to a high acceleration that leads to the RT instability as discussed for full jet.

To consider the effects of this acceleration on the fluid motion, the frame of reference has been transferred from the laboratory frame to an accelerating frame fixed to the liquid. This transformation generates a new term $\rho V^2$ as a generalized body force per unit area analogous to gravity in the equations of motion as is shown in (6). Here, $V$ is the constant acceleration of the frame of reference equivalent to the acceleration of the liquid jet emerging from the orifice, averaged over 300 $\mu$s after the start of injection, i.e. start-up that was equal to 800,000 m/s$^2$ for the flow conditions shown in table 1.

$$\rho \frac{D\mathbf{U}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{U} - \sigma \kappa \& (d) \vec{n} - \rho V \vec{V} ; \nabla \cdot \mathbf{U} = 0 \quad (6)$$

The fluid section consists initially of two concentric cylinders; liquid is in the inner cylinder and the gas fills the surrounding outer cylinder. The diameters of the inner and outer cylinders are 200 and 800 $\mu$m, respectively, and the length of the liquid segment is one millimeter. The liquid section diameter is consistent with the jet-orifice diameter used in the full jet simulation. The total number of mesh points is 400,000 (1000 in $x$-direction and 400 in $r$-direction); a uniform mesh ($\Delta x = \Delta r = 1 \mu$m) has been used. The liquid is initially stationary and the gas flows over the interface from right to left with an initial value associated with the velocity of the liquid jet on the axis of symmetry obtained from a full jet analysis when the jet has penetrated about one millimeter into the gas. Therefore, initial disturbances with 100 $\mu$m wavelengths, consistent with the average KH wavelengths observed for full transient jet, have been applied at the interface of the section. Periodic conditions for pressure gradient at the right and left boundaries and symmetry boundary conditions at the bottom of the computational domain (axis of the jet) have been applied. In addition, the normal gradient of velocity is set to zero on the top (outer) boundary. The flow conditions are the same as the full transient jet and axisymmetric Navier-Stokes equations as shown in (6) have been solved. The level-set method has been applied for capturing the interface.

Figure 4 illustrates the development of the unstable wavelengths at the interface at two instants of time. The primary KH waves with wavelengths of 100 $\mu$m travel upstream relative to the liquid (left) while their amplitude increases and long ligaments (fingers) are drawn outward near the surface of the liquid. These ligaments turn and roll-up in the flow direction (right to left). Simultaneously, they turn into a very thin film with a blob of liquid at the end. This phenomenon has been reported for droplets accelerated by a constant force in a quiescent environment for larger accelerations [26] and in the numerical simulation of the liquid jet [9] and experiments with a liquid jet exposed to a high velocity stream of another fluid [10, 11]. In addition to the acceleration of the frame of reference, these ligaments are exposed to very high local accelerations normal to their interface that make them a good prey for small-scale RT instabilities (10-50 $\mu$m); these secondary instabilities appear at the edge of the ligaments formed by the primary instabilities at the interface. Therefore, the liquid-segment model repeats the same instability mechanisms observed for full transient jet.

The range of KH and RT wavelengths at the liquid/gas interface for the liquid-segment is shown in figure 5 from 10 to 80 $\mu$s after the start of simulation for the liquid-segment of length one millimeter with $Re$ and We numbers equal to 16,000, and 230,000, respectively. Initially, KH waves in the range of 70-120 $\mu$m appear at the interface. The wavelengths range extends
to larger values with time. Presumably, the growth rate for larger lengths is greater as predicted by linear theory. Then, the acceleration of the gas relative to the wave crests leads to a secondary RT instability. The smallest wavelengths on the spectrum designate the RT wavelengths and the longer wavelengths indicate the KH instability. We detected wavelengths as small as 10 µm at 20 µs, consistent with the full jet simulation shown in figure 3 (b).

Note that full transient jet and liquid-segment calculations cannot be exactly matched at a specific computational time due to the different nature of the analysis, i.e., spatial instability for full jet vs. temporal instability for liquid-segment. However, the liquid-segment qualitatively agrees with the full jet and predicts the same range of wavelengths observed in full jet simulations. For example, the primary KH waves become longer and the RT waves associated with them also increase in length as time elapses. This trend continues until the largest KH wavelength approach 300 µm and RT waves grow to about 35 µm. The RT instability should be studied together with KH instability which in turn is strongly dependent on the viscosity, density ratios, and the inertia of the two phases. The thickness, local normal acceleration, and RT wavelengths measured at the edge of a few selected ligaments at the interface of the liquid-segment have been gathered in table 3. The measured results show a good agreement with the predicted RT wavelength based on the linear instability theory as discussed for full-jet simulation.

**Three-dimensional Liquid-Segment Model**

The development of the three-dimensional liquid jet remains axisymmetric for early stages of injection. So, for this period, the axisymmetric liquid-segment model is capable of describing the physics of jet shear instability and RT secondary instability perpendicular to the ligament interface. However, three-dimensional vortex structures form at the interface later in time. Using a three-dimensional analysis of the liquid-segment (versus previous axisymmetric analysis) will allow better resolution of break-up mechanisms such as capillary necking for the fingers that result from the nonlinear KH and RT instabilities. Capillary action on the ligament is stabilizing in two dimensions; however, break-off of the ligaments by necking can only occur in three dimensions.

The computational domain consists of a Cartesian grid. The liquid-segment with a circular cross sectional area of one millimeter length and 200 µm diameter consistent with axisymmetric liquid-segment model is centered in the computational domain in the x-direction as figure 6 depicts. High-pressure air blows over the liquid segment that is initially stationary. The initial velocity profile has a hyperbolic tangent shape started from 70 m/s at the liquid/gas interface and increases to 100 m/s on the outer boundaries. The initial boundary layer thickness in the gas is 100 µm. The initial velocity of the liquid starts from zero on the centerline of the jet and exponentially increases to 70 m/s at the interface. Continuity of the velocity and shear stress has been applied across the interface and a pressure jump related to surface tension and local surface curvature has been considered. Navier-Stokes equations have been solved in three-dimensions and the level-set method has been used to capture the interface topological changes.

The size of the computational domain in y and z directions is 10 times that of the liquid jet diameter. More than five million grid points with five-micron uniform mesh-spacing has been used. Periodic boundary condition for all three components of velocity has been applied in the x-direction, zero normal gradients of velocity and pressure on the outer xz and xy planes have been applied. For the axisymmetric liquid-segment model discussed before, initial disturbances of wavelength equal to 100 µm were applied at the interface. For the three-dimensional model, initial disturbances consist of a series of sinusoidal surface waves producing axisymmetric vortex rings 100 µm apart, aligned in the x-direction with 10-µm initial amplitude. These vortex rings represent the initiation of primary shear or KH instability at the jet interface. The initial wavelength was chosen to be consistent with full-jet results.

Investigating the topological changes at the interface shows that the initial vortex rings remain axisymmetric 20 µs after the start of computations. The symmetry of the vortex rings is broken afterwards and secondary instabilities are developed in the streamwise direction in the braid region, i.e. between the vortex rings and ring regions similar to Bernal and Roshko’s vortical structures observed in three-dimensional mixing layers [27]. Figure 7 schematically shows the interaction of the primary and secondary vortex structures at the jet interface. The interaction of the streamwise vortex with the primary vortex rings leads to the distortion and stretch of the primary vortex rings with an angle with respect to the jet axis. In other words, the lobes of the distorted vortex rings make a cone-shaped zone in the streamwise direction. This phenomenon has been observed numerically for three-dimensional round jets subjected to streamwise and azimuthal perturbations [28]. The deviation of the flow from the axis of the jet to the lobes is referred to as the side jet phenomenon. According to Liepmann and Gharib [29], the streamwise vorticity is responsible for generation of three-dimensional structures and amplification of the air entrainment rate.

Figure 8 demonstrates the vorticity contours on the xy-plane at z equal to 150 µm for two instants of time for Re and We numbers equal to 1600 and 23,000, respectively. Both ring and streamwise vortices have been shown in this figure. At t=15 µs the ring vortices
spreading in the y-direction are stronger compared to the streamwise vortex. At t=25 µs, streamwise vortex is amplified in the braid region, i.e. between two consecutive vortex rings. The vortex rings spread more in the y-direction compared to the case at t=15 µs. The tip of the ring vortex acquires the maximum vorticity. The combination of these two types of vortices produces the cone-shaped behavior of the liquid flow as shown in figure 9. This figure demonstrates the development of the ligaments at the jet interface. The ligaments start to grow from the cone-shaped regions and from the lobes of the distorted vortex rings. The crest of this liquid protrusion then develops into a ligament and the length of the ligament increases with time while its cross-sectional area decreases closer to the tip of the ligament.

Another instability structure shown in this figure is the formation of ring-like or doughnut-shaped structures. These ring-like structures shown with white arrows will break up and produce two separate ligaments that grow in length later in time. The separated ring-like ligament has been shown with a black arrow. Shinjo and Umemura [9] found similar behavior of the formation of ligaments from the ring-like structures. In their analysis, the gas to liquid density ratio, gas to liquid viscosity ratio, \( Re \) and \( We \) numbers according to our definition for non-dimensional parameters based on the liquid properties discussed in the numerical method section were 0.04, 0.0068, 2954, and 28,266, respectively. The maximum jet velocity equal to 100 m/s and 100 µm diameter of the nozzle were used as the reference velocity and reference length in \( Re \) and \( We \) numbers.

Figure 10 schematically demonstrates the development of the ligaments from the ring-like structures. The cone-shaped liquid surface is sheared at the corners of the lobe where the maximum vortical motion occurs. The surface tension effects lead to the thinning of the hole on the lobes, i.e. the hole extends further in the liquid. The liquid then detaches due to capillary pinching. The detached liquid produces two ligaments that move away from the liquid jet core and stretch further into the gas. Finally, the capillary effects will break the ligaments into droplets.

Figure 11 depicts the development of the ligaments previously shown in figure 9 for a later time, i.e. 60 µs. The number and length of the ligaments have increased and small-scale wavelengths have been appeared on the ligaments. Formation of these instabilities is very similar to the situation discussed for axisymmetric full-jet and liquid-segment where the RT instability wavelengths were triggered at the edge of the protrusions from the primary shear instability, i.e. KH instability due to the high accelerations that these protrusions experience. Since these ligaments accelerate away from the liquid core, i.e. accelerating into the air the outer side is unstable; Consistent with the RT instability theory: the acceleration is destabilizing (stabilizing) when the heavier (lighter) fluid accelerates into the lighter (heavier) fluid [30]. The capillary waves would appear on all sides of the ligament; so, we conclude these are RT waves rather than capillary. The KH wavelengths observed in figure 11 varies between 100 to 150 µm and RT wavelengths lie between 50 to 70 µm. Figure 12 demonstrates the development of the instabilities and elongation and thinning of the ligaments at 70 µs. The break-off of the ligament due to surface tension should occur at the location of the thinner cross-sectional area of the ligament.

Figure 13 (a) schematically demonstrates the formation of the cone-shape liquid structures at the interface and development of the secondary RT instability. Primary KH instability determines the distance between the crests of these cones. As soon as the amplitude of the primary instability reaches a maximum value, the acceleration acting normal to the crests due to aerodynamic drag triggers the secondary RT instability with the waviness in the transverse direction. These RT protrusions are drawn out of the liquid and produce the ligaments that grow in lengths. Then a new RT mechanism corrugates the interface of the ligaments and produces small-scale RT wavelengths on the outer side of the ligaments as was discussed earlier. The cross-sectional area of the ligament decreases near its tip and droplets break-off from the liquid jet due to capillary effects. Figure 13 (b) shows the instability mechanism obtained from the numerical simulation for \( Re \) and \( We \) numbers equal to 1600 and 230,000, respectively, indicating the formation of the ligaments due to transverse RT instability as was schematically shown in figure 13 (a). The instability mechanism in Figure 13 (b) is qualitatively similar to the experiments of Marmottant and Villermaux [10]. In their co-flow experiment the velocity of the liquid and air were 0.6 m/s and 35 m/s, respectively. The gas to liquid density ratio, gas to liquid viscosity ratio, \( Re \) and \( We \) numbers were 0.00125, 0.016, 410, and 40, respectively. The diameter of the liquid jet used as the reference length was 7.8 mm.

Figure 14 shows the mechanism discussed in figure 13 and effects of surface tension on the overall shape of the jet, formation of the ligaments and a sample of the observed KH and RT instability wavelengths. The \( Re \) number is the same as that of figures 11 and 12; however, the surface tension coefficient is one tenth of the previous case, keeping the same values of other parameters, e.g. far-field velocity of the gas, liquid jet diameter, and liquid and gas density. The range of KH wavelengths is not affected significantly by lowering the surface tension since the main factor for determining the KH wavelengths is the relative velocity at the interface. However, the observed RT wavelengths for the case with lower surface tension, i.e. higher \( We \) number.
for the transverse RT instability on the crests from primary instability varies between 20 to 70 μm and on the ligaments is between 15-50 μm compared to 50 to 70 μm mentioned for lower We number case. This is consistent with the range of wavelengths observed in figure 5 for the axisymmetric liquid-segment method. Therefore, the range of measured wavelengths of both KH and RT has been correctly predicted by the axisymmetric model discussed before [15]. In conclusion, surface tension and the acceleration applied normal to the liquid protrusions control the small-scale RT instabilities.

Marmottant and Villermaux [10] argue that the capillary instability is not responsible for producing the transverse RT instability since the capillary time scale based on the primary KH wavelength is larger than the primary instability turnover time. Therefore, acceleration acting on the primary protrusions is responsible for the transverse RT instability. Moreover, they infer that as long as the ligament is attached to the liquid core and is still stretching, the effects of capillary instability are negligible and therefore, acceleration is the main factor to develop the RT instability on the ligaments as well as the crests of the primary KH instability. On the other hand, Shinjo and Umemura [9] believed that the formation of the small-scale waves on the ligaments is a result of the short-wave mode of the Rayleigh instability. They predicted wavelength of the order of approximately 3.6 times the diameter of the ligaments, independent of the surface tension. This is inconsistent with the experimental and theoretical analysis of Marmottant and Villermaux [10].

Based on our simulation, the acceleration acting on a ligament is of the order of $10^5$ m/s$^2$ or $10^3$ times the gravitational acceleration. Figure 14 showed that small-scale wavelengths are affected by the surface tension. The instability analysis by Chandrasekhar [23] can be used as a reference to get an estimate of the RT instability, including the effects of both surface tension and acceleration normal to the ligament. The RT wavelengths appeared on the outer side of the ligaments are consistent with RT instability theory discussed before. Therefore, it is unlikely that the development of the wavelengths on the edge of the ligaments is a result of the capillary instability although it causes the final pinch-off of the ligaments and formation of the droplets from the ligament tip.

It is unlikely that the aforementioned small wavelengths are KH wavelengths since this type of instability depends strongly on the relative velocity between the liquid and gas, i.e. shear. Based on KH linear instability analysis the most unstable KH wavelengths decreases with an increase in the relative velocity between the two phases. When the ligaments stretch in the gas the relative velocity between the liquid and the gas is negligible; however, the acceleration effects on these protrusions are high. So, if we assume that the stretched ligaments at the vicinity of the air are affected by KH instability, the wavelengths should be longer than what we have observed. In addition, the KH waves would appear on both side of the ligament; however, we observed small wavelengths on the outer side of the ligament.

Figure 15 shows the formation of a ligament by detachment from a ring-like structure for Re and We numbers equal to 1600 and 230,000, respectively. The mechanism is the same for the higher surface tension case discussed in figure 9. The ligament detaches from the ring at the location of minimum cross sectional area due to capillary forces. The black arrows show the location of the detachment. The tick marks at the inner side of the detached ligament demonstrate small-scale wavelengths at the inner side of the ligament. This ligament is accelerating toward the gas. Therefore, according to RT instability theory discussed before the outer side of the ligament should be unstable. One cannot deduce for certainty the formation of RT wavelengths here. Based on the simulations of Shinjo and Umemura [9] these waves are probably capillary waves. Marmottant and Villermaux [10] have not discussed the mechanism of ligament formation from the detachment of the liquid rings. Therefore, an in-depth study is needed to differentiate these two types of instability for the ring structures.

Comparing the results shown for axisymmetric full jet, axisymmetric and three-dimensional liquid-segment, the questions proposed in the introduction section can be answered. All three models repeat the same scenario for formation of the secondary RT instability wavelengths at the edge of the protrusions formed as a result of the KH or shear instability at the interface. The mechanism responsible for RT instability is the local relative acceleration of the liquid protrusions normal to their interface. The higher the relative velocity or lower the surface tension coefficient, the smaller the RT wavelengths for constant liquid to gas density ratio. The range of KH and RT wavelengths for the same flow conditions is similar for axisymmetric full-jet, liquid-segment, and three-dimensional liquid-segment models.

The liquid-segment model is helpful for simulating the jet instability farther from the orifice, i.e. when the jet has penetrated into the gas more than 10 orifice diameters. At this stage, the instabilities appear at the interface of the jet core as well as the head part. The formation of the mushroom-shaped cap and secondary instabilities at the back of the jet head can be well captured from the axisymmetric full jet simulations. Therefore, the combination of these two models provides substantial information about the primary instability both at the head part of the jet and the liquid-core protrusions that appear following the deformation of the jet head. Finally, the three-dimensional model explains the
three-dimensional physics of the ligament formation due to the interaction of the vortices, detachment from the ring-like structures, and as a result of the growth of the transverse RT instability protrusions. Other mechanisms that lead to RT instability are the same as described above for the axisymmetric models. In addition, the detachment of the ligaments into the droplets due to capillary instability that was missing in the axisymmetric model can be explained in three dimensions.

Summary and Conclusions

The transient behavior of a liquid jet injected into still air was investigated by solving multidimensional Navier-Stokes equations and applying level-set method to capture the topological changes at the liquid/gas interface from two different approaches. The development of the full axisymmetric jet injected into air at 30 atm pressure during the start-up process indicated two types of instabilities: Kelvin-Helmholz due to the shear between the two streams and Rayleigh-Taylor instability on top of the crests primarily formed due to the KH instability. The development of the jet initiated with the formation of a large mushroom-shaped cap that spread in the radial direction as a result of the deceleration of the jet due to the drag forces acting on the liquid. Shortly after the development of the mushroom-shaped cap, the long and thin liquid at the tip of the cap was exposed to a high acceleration acting normal to it that led to the formation of smaller RT instability wavelengths at the back of the jet cap.

Later, KH instabilities developed at the interface of the jet in addition to the jet head. These KH protrusions projected from the interface and elongated as ligaments. The same scenario of formation of RT instabilities was repeated for the protrusions appeared at the interface of the jet. Thus, RT instability can be considered as the secondary instability that is non-linearly dependent on the KH instability. The normal acceleration experienced by the ligaments was one order of magnitude larger than the acceleration of the liquid jet at the orifice exit. The wavelength of KH instability increased in length for later stages of the injection since the relative velocity of the liquid/gas at the interface decreased with time. RT instability wavelengths also increased as a result of the increase in KH wavelengths. The range of measured RT wavelengths was consistent with the linear instability theory.

The axisymmetric liquid-segment method was proposed as a means to provide the sufficient resolution for investigating the transient jet instabilities. A segment of the liquid jet of one millimeter length was exposed to a stream of dense air accelerating along the axis of the jet. In order to consider the effects of acceleration, the frame of reference was transferred from the laboratory frame to a frame of reference attached to the liquid. This transformation produced a body force in the equations of motion. The value of the average acceleration of the liquid was obtained from the full jet simulation for the same flow properties. The same mechanism of instability development, i.e. formation of the finger-shaped KH ligaments and small-scale RT wavelengths at the edge of these fingers was detected for liquid-segment method. The range of these wavelengths was consistent with the full-jet simulation.

The liquid-segment approach was next developed in three dimensions to capture the physics of the formation of the ligaments. A liquid-segment of the jet with the same diameter and length as the axisymmetric model was exposed to high density air blowing along the axis of the jet. Initial disturbances on the liquid interface consisted of axisymmetric sinusoidal waves at the interface with an initial wavelength of 100 μm. The axisymmetric vortex rings remained axisymmetric 20 μs after the start of computation after which the axisymmetry was broken due to the formation of the stream-wise vortices. The interaction of primary vortex rings and streamwise vorticity led to the distortion of the vortex rings into the lobes. A cone-shaped region of liquid then formed in the direction of the flow. The formation of the ligaments was initiated from the lobes of the distorted vortex rings. The ligaments started to grow in lengths and secondary RT instability was observed on the elongated ligaments.

Another mechanism observed in the numerical simulation was the formation of the ring-like structures, i.e. holes appeared at the interface. The ligaments detached from the ring at the location of minimum cross-sectional area and accelerated away from the jet core. Capillary instability was the responsible mechanism for the detachment of the ligament. In addition, the protrusions at the interface as a result of the transverse RT instability grew in lengths and formed the ligaments. A new mechanism of RT instability was repeated for these ligaments. RT wavelengths appeared at the outer side of the ligaments consistent with the RT instability theory. The range of KH and RT wavelengths were consistent with that of the axisymmetric liquid-segment model. Consequently, the three-dimensional liquid-segment approach can be useful as a predictor of droplet size. The axisymmetric liquid-segment approach also has very useful predictive value.

Acknowledgment

The authors gratefully acknowledge support from The U.S. Army Research Office through Grant No.W911NF-09-1-0208 with Dr. Ralph A. Anthenien Jr. as the Program Manager of Propulsion and Energetics.
References
Table 1. Fluid Properties.

<table>
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<tr>
<th>Fluid properties</th>
<th>Liquid</th>
<th>gas (air)</th>
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<tr>
<td>Viscosity (kg/m.s)</td>
<td>2.01 e-3</td>
<td>1.8 e-5</td>
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<tr>
<td>Density (kg/m³)</td>
<td>804</td>
<td>38.4 at 30 atm</td>
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<td>Surface tension coefficient (N/m)</td>
<td>0.028</td>
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<tr>
<td>Maximum jet velocity (m/s)</td>
<td>200</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 1. (a) Physical domain and orthogonal grid (flow from left to right.), (b) liquid-segment model.

Figure 2. Instability development at 30 µs after the start of injection, ($Re=16,000$, $We=230,000$, $ρ_ρ=0.048$.)
Figure 3. (a) Unstable structures at the liquid interface during start-up at 100 µs indicating KH and RT wavelengths (b) KH and RT wavelength spectrum from the numerical simulation during start-up vs. time, the error bars correspond to 5 µm (ρg/ρl= 0.048, Re = 16,000, We = 230,000.)

Table 2. RT wavelengths compared with theory for axisymmetric full jet, Re= 16,000, We=230,000.

<table>
<thead>
<tr>
<th>t (µs)</th>
<th>Thickness (µm)</th>
<th>a_s (m/s²)</th>
<th>λ_RT from computations (µm)</th>
<th>λ_{RT} = \frac{3\sigma}{(\rho_i - \rho_s)u_s}</th>
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<tr>
<td>26</td>
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<td>8.4e6</td>
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<td>35</td>
<td>2.7e6</td>
<td>40</td>
<td>38</td>
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Figure 4. Instabilities at the liquid/gas interface for liquid-segment model at two instants of time: $t = 15 \, \mu s$ (left) and $t = 30 \, \mu s$ (right), $Re = 16,000$, $We = 230,000$, $a = 800,000 \, m/s^2$.

Figure 5. KH and RT wavelength spectrum during start-up vs. time for the liquid-segment numerical simulation, the error bars correspond to $5 \, \mu m$ ($Re = 16,000$, $We = 230,000$).

Table 3. RT wavelengths compared with theory for the axisymmetric liquid-segment model, $Re=16,000$, $We=230,000$.

<table>
<thead>
<tr>
<th>$t$ (µs)</th>
<th>Thickness (µm)</th>
<th>$a_n$ (m/s²)</th>
<th>$\lambda_{RT}$ from computations (µm)</th>
<th>$\lambda_{RT} = 2\pi \sqrt{\frac{3\sigma}{(\rho_1 - \rho_2)a_n}}$</th>
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<tbody>
<tr>
<td>17</td>
<td>8</td>
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<tr>
<td>18</td>
<td>12</td>
<td>2.04e6</td>
<td>45</td>
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<td>19</td>
<td>11</td>
<td>4.07e6</td>
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Figure 6. Computational domain including the liquid-segment and initial disturbances at the interface and surrounding air that blows in the positive x-direction.

Figure 7. Vortical structures on the round liquid jet consisted of distorted vortex rings and secondary streamwise vortex.

Figure 8. Vorticity contours on the xy plane indicating ring vortices and formation of streamwise vortices: (left) \( t=15 \, \mu s \), (right) \( t=25 \, \mu s \) \( (Re = 1600, We = 23,000, \text{flow from right to left.}) \)
Figure 9. Development of the instabilities, formation of cone-shaped regions in the streamwise direction, $Re=1600$ and $We=23,000$. Ring-like structures shown with white arrows. Black arrow indicates the detachment of the ring. (top) $t=30 \, \mu s$ and (bottom) $t=40 \, \mu s$ (Flow from right to left.)

Figure 10. Schematic development of the ligaments from the liquid ring.

Figure 11. Development of the three-dimensional structures and formation of smaller RT wavelengths in the transverse direction and on the elongated ligaments. Flow from right to left ($Re=1600$ and $We=23,000$.)
Figure 12. Development of the three-dimensional structures and thinning of the elongated ligament. Black arrows show the thinning process of the ligament. Flow from right to left ($Re=1600$ and $We=23,000$.)

(a)

Figure 13. (a) Schematic of secondary RT instability in the transverse direction and formation of the ligaments (b) Similar behavior from the liquid-segment simulation. Flow from right to left ($Re=1600$ and $We=230,000$.)
Figure 14. Development of the three-dimensional structures and formation of smaller RT wavelengths on the elongated ligaments. Flow from right to left ($Re=1600$ and $We=230,000$.)

Figure 15. Detachment of a ligament from the ring-like structure. The time difference between the frames is 1 µs. Time increases from left to right. Black arrows show the detachment location and tick marks show the small-scale wavelengths. Flow from right to left ($Re=1600$ and $We=230,000$.)