Explaining the Planar Liquid Jet Atomization via Vortex Dynamics

A. Zandian\textsuperscript{1,*}, W.A. Sirignano\textsuperscript{1}, and F. Hussain\textsuperscript{2}
\textsuperscript{1}Department of Mechanical and Aerospace Engineering
University of California
Irvine, CA 92697 USA
\textsuperscript{2}Department of Mechanical Engineering
Texas Tech University
Lubbock, TX 79409, USA

Abstract
The 3D, temporal instabilities on a planar liquid jet are studied using DNS with level-set and volume-of-fluid surface tracking methods. The \( \lambda_2 \) method has been used to relate the vortex dynamics to the surface dynamics at different stages of the jet breakup, e.g. lobe formation, thinning and perforation, ligament formation, stretching, and tearing. The breakup character depends on the flow Ohnesorge number (\( Oh \)) and gas-to-liquid density ratio. At high Reynolds number (\( Re \)) and high \( Oh \), hairpin vortices form on the braid and overlap with the lobe hairpins, thinning the lobes, which puncture to form holes and bridges. The bridges break, creating one or more ligaments that stretch and break into droplets by capillary action. At low \( Oh \) and high \( Re \), lobe stretching and thinning is hindered due to the high surface tension and splitting of the primary Kelvin-Helmholtz (KH) vortices, inhibiting early hole formation. Corrugations form on the lobe edges, induced by the split vortices, and stretch to form ligaments. At low \( Re \), the breakup process moves from hole formation to direct stretching as \( Oh \) is decreased. The Kelvin-Helmholtz (KH) vortices depart from the liquid surface, with reduced influence on rolling and thinning of the lobes. As the vortices turn streamwise, they squeeze the lobes from both sides and shape them into thick ligaments. Streamwise vortex stretching and baroclinicity are the main causes of streamwise vorticity generation, resulting in three-dimensional instabilities at high and low density ratios, respectively. The gas-to-liquid viscosity ratio does not significantly affect the breakup process and time scales.

\textsuperscript{*}Corresponding Author: azandian@uci.edu
Introduction

Earlier computational works on the breakup of liquid streams at higher Weber number ($We$) and Reynolds number ($Re$) (i.e. in the atomization range) focused on the surface dynamics using either volume-of-fluid or level-set methods [1–3]. More recently, Jarrahbashi and Sirignano [4] and Jarrahbashi et al. [5] computed the temporal behavior of round jets and Zandian et al. [6] computed the temporal behavior of planar jets with additional data analysis that related the vorticity dynamics to the surface dynamics. Zandian et al. [6] presented several significant accomplishments: (i) three breakup mechanisms were identified and their zones of occurrence were specified on the gas-phase Weber number ($We_g$) versus liquid-phase Reynolds number ($Re_l$) map; (ii) the most important actions in each of the three breakup domains were explained; (iii) the effects of density ratio, viscosity ratio, and sheet thickness on the breakup domains were described; (iv) characteristic times for each of these breakup domains were correlated with key parameters; and (v) the same breakup domains were shown to apply for round jets and planar jets with a very similar $We_g$ versus $Re_l$ map.

Jarrahbalsi et al. [5] showed that important spray characteristics, e.g. droplet size and spray angle, differed in different ranges of $We$, $Re$, and density ratio. Therefore, further study of the breakup mechanisms is needed to fully understand the causes of these differences. Consequently, there are unresolved questions to be addressed in this paper. What are the details of the liquid dynamics in each breakup domain? What causes the difference in the breakup cascade? What are the roles of surface tension, liquid viscosity, and gas density (i.e. pressure)? How does the impact of streamwise vorticity (i.e. hairpin vortices) differ in the three breakup domains? What is the connection between the behaviors of a jet flow into like fluid (e.g. water into water or air into air) and liquid-jet flow into gas? The answers to the above questions would be crucial in understanding and relating the ligament and droplet size distribution in primary atomization of the liquid jets.

Vortex dynamics concepts can shed further light on surface deformation of a liquid jet in the primary atomization process - a cascade into smaller and smaller liquid structures. The Kelvin-Helmholtz (KH) instability at the liquid-gas interface promotes the growth of spanwise vorticity waves forming coherent vortices. These vortices evolve into hairpins with counter-rotating streamwise legs [7]. The streamwise and spanwise vortical waves combine to produce different surface structures, e.g. lobes, bridges, and ligaments, which eventually break up into droplets. The link between the vortex dynamics and surface dynamics in primary atomization is important, but rarely explored and poorly understood, and this study is an attempt to fill that gap.

There have been several studies of the jet instabilities from vortex dynamics perspective. Most of them however do not consider density and viscosity discontinuities. These studies have mainly focused on understanding and relating the vortex stretching [8], vortex tilting [9] and baroclinic effects [10] to the three-dimensional liquid jet instabilities. Experimental studies in this field [7, 9–15] have been followed and reproduced in more detail by numerical computations [1, 4, 5, 16–22].

In the first studies of the role of streamwise vorticity in round liquid jets flowing into a gas, Jarrahbashi and Sirignano [4] and Jarrahbashi et al. [5] showed how lobe and ligament formation mechanisms relate to streamwise vorticity generation. They also showed that a natural mode number of lobes exists for a given configuration and cannot be changed by weak forcing [4]; however, strong forcing can produce lobes of different mode numbers.

Empirical evidence [23] has long been available that spray character differs significantly for differing values of $Re$ and $We$. Jarrahbashi et al. [5] have shown that different breakup mechanisms result in differing spray angles and droplet-size distributions. Thus, we see that for control of spray character, it is very valuable to understand the cascade processes for each of the identified atomization domains. Control and optimization, although not addressed in this study, motivates the detailed exploration and the behavioral characterizations reported here.

Liquid jet breakup domains

Jarrahbashi et al. [5] found three distinct physical domains in round liquid jets, including hole formation and lobe stretching. The surface wave dynamics, vortex dynamics and their interactions were explained. The perforations were correlated with the fluid motion induced by the hairpin and helical vortices. They also found that the hole formation process is dominated by inertia rather than capillary forces, and the hole merging was related to the slower development of hairpin vortices and lobe shape.

Zandian et al. [6] identified three mechanisms for liquid sheet surface deformation and breakup, which were well categorized on a gas Weber number ($We_g$) versus liquid Reynolds number ($Re_l$) map; see Fig. 1. At high $Re_l$, the liquid sheet breakup
characteristics change based on a modified Ohnesorge number, \( \text{Oh}_m \equiv \sqrt{\text{We}_g/\text{Re}_l} \), as follows: (i) at high \( \text{Oh}_m \) and high \( \text{We}_g \), the lobes become thin and puncture, creating holes and bridges. Bridges break as perforations expand and create ligaments. Ligaments then stretch and break into droplets by capillary action. This domain is indicated as atomization domain II in Fig. 1, and its mechanism was called \( \text{LoHBrLiD} \), based on the cascade of structures seen in this domain (\( \text{Lo} \equiv \text{Lobe}, \text{H} \equiv \text{Hole}, \text{Br} \equiv \text{Bridge}, \text{Li} \equiv \text{Ligament}, \text{and} \ D \equiv \text{Droplet} \); (ii) at low \( \text{Oh}_m \) and high \( \text{Re}_l \), holes are not seen at early times; instead, many corrugations form on the lobe front edge and stretch into ligaments. This so called \( \text{LoCLiD} \) mechanism (\( C \equiv \text{Corrugation} \)) occurs in atomization domain III (see Fig. 1) and results in ligaments and droplets without having the hole and bridge formation steps. The third mechanism follows a \( \text{LoLiD} \) process and occurs at low \( \text{Re}_l \) and low \( \text{We}_g \) (atomization domain I in Fig. 1), but with some difference in details from the \( \text{LoCLiD} \) process. The main difference between the two ligament formation mechanisms at high and low \( \text{Re}_l \)'s is that at higher \( \text{Re}_l \) the lobes become corrugated before stretching into ligaments. Hence, each lobe may produce multiple ligaments, which are typically thinner and shorter than those in the lower \( \text{Re}_l \). At low \( \text{Re}_l \), on the other hand, because of the higher viscosity, the entire lobe stretches into one thick, usually long ligament. The structures seen in all these breakup mechanisms are sketched in Fig. 2; the gas flows from left to right, and time increases to the right.

There is also a transitional region in which both lobe/ligament stretching and hole-formation mechanisms are seen simultaneously. The transitional region at low \( \text{Re}_l \) follows a hyperbolic relation, i.e. \( \text{We}_g = A/\text{Re}_l \), shown by the dash-dotted line in Fig. 1; while at high \( \text{Re}_l \) limit, it follows a parabolic curve, i.e. \( \text{We}_g = B^2\text{Re}_l^2 \), shown by the dashed line in Fig. 1. The constant \( B \) is a critical \( \text{Oh}_m \) at high \( \text{Re}_l \), \( B \approx 0.021 \) [6].

**Objectives**

Our objectives for the planar jet are to (i) explain the mechanisms for surface deformation and breakup in the three domains introduced earlier using more sophisticated data analysis for the vortex dynamics (i.e. the \( \lambda_2 \) method); (ii) determine the importance of streamwise vorticity (i.e. hairpin vortices) in the breakup mechanisms; (iii) identify the generation mechanisms for streamwise vortices; and (iv) learn the differences in generation and impact of the spanwise and streamwise vorticity at low and high density ratios.

**Numerical Modeling**

The three-dimensional Navier-Stokes with level-set and volume-of-fluid surface tracking methods yield computational results for the liquid segment which captures the liquid-gas interface deformations with time. Details on the Navier-Stokes solution and surface tracking are presented by Zandian et al. [6].

**Flow Configuration**

The computational domain, shown in Fig. 1 of Zandian et al. [6], consists of a cube, which is discretized into uniform-sized cells. The liquid segment is a sheet of thickness \( h \) (\( h = 50 \mu m \) for the thin sheet and \( 200 \mu m \) for the thick sheet in this study), located at the center of the box. The liquid segment is surrounded by the gas zones on top and bottom. The gas moves in the positive \( x \)- (streamwise) direction, with a constant velocity \( (U = 100 \text{ m/s}) \) at the top and bottom boundaries, and its velocity diminishes to the interface velocity with a hyperbolic tangent profile. The velocity decays exponentially to zero at the center of the liquid sheet. For more detailed description of the initial conditions see Zandian et al. [24].
The liquid/gas interface is initially perturbed symmetrically on both sides with a sinusoidal profile and predefined wavelength and amplitude. Both streamwise ($x$-direction) and spanwise ($y$-direction) perturbations are considered in this study. Periodic boundary condition for all components of velocity as well as the level-set/VoF variable is imposed on the four sides of the computational domain.

The most important dimensionless groups in this study are the Reynolds number ($Re$), the Weber number ($We$), and the gas-to-liquid density ratio ($\hat{\rho}$) and viscosity ratio ($\hat{\mu}$), as defined below. The initial wavelength-to-sheet-thickness ratio ($\Lambda$) is also an important parameter that defines the relative length of the initial perturbations.

\begin{align}
Re &= \frac{\rho_l U h}{\mu_l}, \quad We = \frac{\rho_l U^2 h}{\sigma}, \\
\hat{\rho} &= \frac{\rho_g}{\rho_l}, \quad \hat{\mu} = \frac{\mu_g}{\mu_l}, \quad \Lambda = \frac{\lambda}{h}.
\end{align}

The sheet thickness $h$ and the velocity of the far field gas $U$ are considered as the characteristic length and velocity. The subscripts $l$ and $g$ refer to the liquid and gas, respectively.

**Data analysis**

Our goal is to study the vorticity dynamics as well as the liquid surface dynamics in order to understand breakup mechanisms at different flow conditions. To this end, $\lambda_2$ criterion is used to define a vortex. An objective definition of a vortex should permit the use of vortex dynamics concepts to identify coherent structures (CS), to explain formation and evolutionary dynamics of CS, and to explore the role of CS in turbulence phenomena. Jeong and Hussain [25] define a vortex core as a connected region with two negative eigenvalues of $S^2 + \Omega^2$: where, $S$ and $\Omega$ are the symmetric and anti-symmetric components of $\nabla u$; i.e. $S_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ and $\Omega_{ij} = \frac{1}{2}(u_{i,j} - u_{j,i})$. If $\lambda_1, \lambda_2$, and $\lambda_3$, are the eigenvalues such that $\lambda_1 \geq \lambda_2 \geq \lambda_3$, this definition is equivalent to the requirement that $\lambda_2 < 0$ within the vortex core, since $\lambda_3$ is always negative because the sum of the normal viscous stresses is zero. This definition is proven to meet the requirements for existence of a vortex core in different flow conditions [25].

**Results and discussion**

In this section, the vorticity dynamics of each of the breakup mechanisms are analyzed to explain the hole formation, the corrugation formation and the lobe/ligament stretching at different Reynolds and Weber numbers. For this purpose, one case is picked from each domain, shown in Fig. 1, and its vorticity dynamics are studied based on the $\lambda_2$ criterion of Jeong and Hussain [25]. The sequential deformation of the liquid surface following the vortices’ evolution are sketched to describe each process and explain various liquid structures.
Figure 3. Schematic of the LoHBrLiD mechanism at four consecutive times. The liquid/gas interface is shown in blue, and the KH vortex in black. The red and black lines are the hairpin vortices near the trough and crest of the KH wave, respectively. The solid or dashed lines show where the hairpins are stretched upstream and inward, or downstream and outward, respectively. The gas flows from left to right.

Hole and bridge formations (LoHBrLiD mechanism)

The LoHBrLiD mechanism occurs in atomization domain II at medium $Re_l$ and high $We_g$, as shown in Fig. 1. The lobes form and thin on the primary KH wave crests. The middle section of the lobes (the braid), where the highest strain occurs, thins faster and thus perforates, creating a hole and a bridge on the lobe rim. Bridges become thinner as the holes expand. Finally, the bridges break and create one or two ligaments depending on the breakup location. The ligaments stretch and eventually break into droplets under capillary action.

The role of vortices in the LoHBrLiD breakup mechanism is summarized schematically in Fig. 3. This figure shows the liquid surface and also the qualitative location of the nearby vortices at four consecutive times. At an early time $t_1$, hairpin vortices form on the braids where the maximum strain rate occurs [9]. The hairpins closer to the streamwise KH crest, shown in black lines, are stretched towards the downstream KH vortex, and the hairpins near the streamwise trough, shown in red lines, are stretched upstream due to the induced motion of the upstream roller. The hairpins that are stretched downstream are rolled over the KH vortex tube and are illustrated by solid lines, while the hairpins that are stretched upstream are pulled under the KH vortex tube. These sections of the hairpins are sketched...
Later at $t_2$, the KH vortices deflect more under the influence of the hairpin vortex filaments. The KH vortex pulls the lobes over itself, and the KH roller lies underneath the surface of the lobe at later times (bottom images of Fig. 3). Pulling of the upstream and downstream hairpins from the outer and inner sides of the interface by the KH roller causes these two hairpins to align spanwise and overlap - one layer (black hairpins) locating on the outer surface of the lobe, i.e. on the streamwise wave crest, and the other layer (red hairpins) on the inner side of the lobe. As shown in the illustrative sketches of Fig. 4 and also described by Jarrahbashi et al. [5], the liquid sheet between a pair of these overlapping hairpins becomes thinner. Figure 4(a) schematically depicts two overlapping hairpin vortices in the liquid-gas interface region - one originating from the lobe crest and stretching downstream (shown by the slender black tube), and the other originating from the braid and stretching upstream (shown by the red tube). The KH vortex is shown by the thicker gray tube in this figure. Figure 4(b) shows a cross-sectional view of the vortex structure along with the liquid sheet located between the two hairpin vortices on the $A$-plane of Fig. 4(a). The induced velocity of the hairpin vortices (see the qualitative streamlines shown by the black and red arrows in Fig. 4b) pushes the top surface of the liquid lobe downward and the bottom surface upward, causing the liquid lobe to become thinner in the middle and thus vulnerable to puncture at that region. These overlapping regions have been marked in Fig. 3 at $t_3$. Hence, the hairpin overlapping causes the lobe that fills the gap between these two hairpin groups to become thinner and vulnerable to puncture at that location.

Whether the liquid sheet subject to these conditions punctures or not depends on other flow conditions, particularly the surface tension. At high $We_g$ (high $Oh_m$), the hole formation prevails, and we see the holes forming at $t_4$ at the predicted locations.

As these overlapping hairpin filaments continue to stretch, the holes also stretch and expand, creating even larger holes and thinner bridges. If $We_g$ is not large enough, the liquid sheet in the overlapping region can recover instead. In this case, hole formation is inhibited, and the lobes stretch directly, but more slowly, into ligaments via LoLiD or LoCLI D mechanisms (domains I and III), as will be discussed in the next sections.

**Corrugation formation at high $Re_l$ (LoCLI D mechanism)**

The LoCLI D mechanism occurs in domain III at high $Re_l$ and low $We_g$ (low $Oh_m$), as indicated in Fig. 1. The lobes form similar to the previous case, but do not stretch as much. Corrugations form on the lobes’ front edge and stretch to create ligaments. Multiple ligaments are formed per lobe, typically shorter and thinner compared to the ligaments seen in domain II. Eventually, the ligaments detach from the liquid jet and break up into droplets by capillary action. These droplets are consequently smaller.
The role of vortices on the liquid surface deformation at high $Re_l$ and low $We_g$ is summarized schematically in Fig. 5. At early times $t_1$, the spanwise vortices on the braid deflect due to the induced motion of the neighboring KH rollers in both the upstream and downstream directions - creating the hairpin vortex structures with a spanwise perturbations wavelength. The deflected hairpin filaments form the lobes as they are stretched by the KH roller. So far, the process is similar to the $LoHBrLiD$ mechanism.

At high $Re_l$, the inertia effects dominate the viscous forces. Consequently, the higher velocity of the gas phase compared to the liquid phase causes the KH roller to split into two eddies at $t_2$, as shown in Fig. 5. The low liquid viscosity does not allow sufficient resistance to keep the KH vortex bound near the interface; hence, the outer part of the KH roller, which resides in the fast-moving gas layer, separates from the part of the KH vortex that is inside the surface of the lower speed liquid.

As demonstrated in Fig. 5, the part of the KH vortex that resides in the faster moving gas, outside the liquid, advects faster than the slow-moving eddy in the liquid. The slow-moving eddy however advects with the interface velocity remaining stationary relative to the liquid surface. This vortex separation has two significant effects. (i) The slow-moving eddy downstream of the KH wave is
Figure 6. 3D Schematics showing the overlapping of the crest hairpin (black slender tube) and the trough hairpin (red tube) resulting in formation of lobe corrugations (a); A is the plane in which (b) is drawn; cross-sectional view of the A-plane showing the corrugation formation and thinning of the gas lobe due to the hairpin overlapping (b). The vortex schematics are meant to be periodic in x- and y-directions.

not strong enough to curl the KH wave and pull the lobe downstream over itself. Consequently, the outer hairpin filaments on the lobe do not overlap with the inner braid hairpins as in the LoHBrLiD domain, and hole formation at early times is inhibited. (ii) The fast-moving eddy gets closer to the downstream hairpins as it moves away from the upstream hairpins near the trough. The hairpin filaments become less orderly due to the successive change in the distance between the hairpins and the fast-moving vortex, as follows: as the fast-moving vortex passes over the trough hairpin (the red hairpin), it pulls the trough hairpin in the downstream direction and creates a new bend on the hairpin, as shown in Fig. 5 at t_2. Similarly, the crest hairpin (the black hairpin) is pulled in the upstream direction by the fast-moving vortex tube, causing the hairpin vortices to undergo more undulations with smaller local wavelengths. The streamwise stretching direction on different parts of the hairpins are indicated by the black and red arrows in Fig. 5. The upstream turns and bends on the hairpins also prevent further downstream stretching of the lobes. Consequently, the lobes are less stretched and more blunt; compare t_2 in Fig. 5 with t_3 in Fig. 3. Notice that the split vortex tubes in Fig. 5 are thinner at t_2 than at t_1.

When the fast-moving eddy passes over the crest hairpin (black hairpin) at t_3, it creates yet another turn in the hairpin vortex, as shown in Fig. 5. The liquid surface approximately follows the hairpin structures with some delay at this high ReL range. Because of these shorter hairpin wavelengths, corrugations with length scales comparable to the hairpin wavelengths form on the front-most edge of the lobes, as shown in Fig. 5 at t_3. Both experimental observations [9, 15] and numerical computations [21, 22] have shown that the number of corrugations (lobes) increases with increasing the jet Reynolds number.

Upon creation of a stronger eddy downstream of the KH waves at t_4 - after amalgamation of the fast- and slow-moving eddies - the new KH roller (now a thicker tube) has enough strength to stretch the hairpin vortices. The hairpins on the outer and inner sides of the lobe overlap as illustrated in Fig. 5 at t_4. In this figure, the dashed-lines represent the hairpins stretching upstream and pulled under the liquid lobes, i.e. inner surface of the gas lobe, while the solid lines denote parts of the hairpins that are stretched downstream on the inner side of the liquid lobe; i.e outer surface of the gas lobe.

The illustrative sketches of Fig. 6 show the corrugated hairpin structures and their position with respect to the lobe in the LoCLiD domain (corresponding to t_4 in Fig. 5). The black tube represents the hairpins on the lobe crest and the red tube represents the hairpins on the streamwise trough. The two hairpin layers - after getting corrugated due to the pull from the two halves of the split KH vortex in the opposite directions (see t_2 and t_3 in Fig. 5) - overlap under the liquid lobe, as shown in Fig. 6(a). The liquid lobe front edge gets corrugated with comparable length scales to the hairpin undulations wavelength, following the movement of the fluid elements induced by the corrugated hairpins; see Fig. 6(a). The layer of the crest hairpins (black
tubes) are located underneath the liquid lobe (on top of the gas layer), and the layer of the trough hairpins (red tubes) are located on top of the interface at the trough; see Fig. 6(b). The induced flow creates undulations on both the bottom surface of the lobe and the trough surface. The gap filled by the gas layer gets closed, i.e. the lobe collapses on the jet core, as the bottom surface of the liquid lobe descends and the trough surface ascends due to induced flow by the overlapped hairpins; see the qualitative streamlines in Fig. 6(b).

As the counter-rotating pairs of hairpins stretch, the lobe corrugations stretch with them and form thin ligaments (see Fig. 5). The ligaments stretch downstream and break up into droplets as they undergo capillary instabilities. In the meantime, the eddies diffuse into the gas phase and cascade into smaller vortical structures as the turbulence kicks in. The outward diffusion of the eddies spreads the droplets in the normal direction, helps the expansion of the liquid sheet, and enhances the two-phase mixing.

**Lobe and ligament stretching at low Re_l (LoLiD mechanism)**

At low Re_l and low We_g (atomization domain I in Fig. 1), the surface tension force does not allow the lobes to perforate easily. The liquid viscosity is also fairly high and prevents corrugation formation on the lobe front edge. Consequently, the entire lobe stretches slowly into a thick and long ligament, which eventually breaks into large droplets.

Similar to the previous cases, the vortex field starts with a large KH roller downstream of the KH wave, hairpin filaments on the braid, and a much stronger hairpin filament on the KH wave crest. Later, the entire KH roller departs from the liquid surface and moves downstream into the gas zone. Since the gas phase has higher velocity compared to the liquid phase, the vortices that are more distant from the liquid surface advect faster with respect to the interface. Hence, the KH roller gains higher velocity as it moves away from the interface, while the rest of the vortices (the hairpin filaments) are almost stationary with respect to the interface.

While the KH roller reaches the neighboring downstream crest hairpin filament, the braid hairpins overlap with the crest hairpins constraining the lobe sheet in between. So far, the vortex dynamics manifests the conditions required for both hole formation, i.e. hairpin overlapping on two sides of the lobe, and corrugation formation; i.e. constant pull in alternating directions from a fast-moving eddy. However, none of these structures are seen on the lobe. The reason for inhibition of the hole formation lies in the high surface tension. In such a low We_g, the inertia and viscous forces do not have enough strength to overcome the surface tension force to thin and stretch the lobe; hence, the lobe perforation is inhibited. Also, because of the high liquid viscosity at such low Re_l, the liquid surface deformation is much slower. Hence, the corrugation formation on the lobe edges does not occur as quickly as the higher Re_l cases, and small scale corrugations are dampened by the viscous and surface tension forces. Thus, the whole lobe has enough time to slowly stretch into a thick ligament. Moreover, the KH roller is also farther away from the interface in this case compared to the LoCLiD mechanism, which means that it has a much weaker influence on the hairpin filaments, resulting in fewer bends and smaller amplitudes on the hairpins.

The schematics of the vortex structures in the LoLiD mechanism of domain I are illustrated in Fig. 7. The KH vortex has a higher undulation in this domain compared to the other two domains and is also farther away from the interface in the gas zone (compare Fig. 7 with Figs. 4 and 6). Because of the high strain rate at the braid, the hairpin vortices become streamwise near the braid region in both spanwise crest and trough. Two pairs of counter-rotating hairpins, one on the lobe crest (shown by the black tube), and the other on the trough (shown by the red tube) stretch and wrap around the KH vortex; see Fig. 7(a). These hairpins are periodic in both spanwise (y) and streamwise (x) directions; i.e. the tubes that emerge from the figure at the bottom corner or the left side of the domain, re-enter from the top corner or the right side of the 3D sketch shown in Fig. 7(a). As shown in the cross-sectional view of the A-plane passing through the lobe in Fig. 7(b), both the black and the red hairpins are located slightly above and on the sides of the lobe at this moment. While the flow induced by the KH vortex creates a streamwise flow on the two sides of the lobe, the gas flow induced by these two counter-rotating hairpins (shown by the curly arrows is Fig. 7b) generates a spanwise flow towards the lobe. Consequently, the lobe is both squeezed in the spanwise direction - via the hairpins effects - and stretched in the streamwise direction - by the induced flow of the KH vortex. The gas flow also lifts the lobe in the z-direction.

Since the streamwise vortices induce a gas flow in the spanwise direction towards the lobe, the lobe shape gets transformed into a ligament as the strong shear near the lobe sides deforms the liquid surface. Ligament creation is strongly correlated with its local velocity field, and is induced by local shear as in-
Figure 7. 3D Schematics showing the vortex structures in the LoLiD mechanism of domain I (a), \( A \) is the plane in which (b) is drawn; cross-sectional view of the \( A \)-plane, showing the spanwise squeezing of the lobe by the hairpin vortices (b). The vortex schematics are meant to be periodic in \( x \)- and \( y \)-directions.

Figure 8. Schematics of lobe thinning in the normal direction, i.e. \( LoHBrLiD \) (a), and lobe thinning in the spanwise direction, i.e. \( LoLiD \) (b). The red arrows indicate the direction of thinning.

In summary, whether the lobe thins in the normal direction and perforates, or thins in the spanwise direction and forms a ligament depends on the orientation of the vortices in the vicinity of the lobe. The spanwise vortices result in formation of holes and spanwise bridges, while streamwise vortices result in spanwise lobe compression and streamwise ligaments stretching.

Streamwise vorticity generation

The streamwise vorticity \( (\omega_x) \) is crucial in initiation of the three-dimensional instability on liquid jets. \( \omega_x \) generation via vortex stretching and vortex tilting, i.e. strain-vorticity interactions, and baroclinic effects are studied in this section for a low density ratio of 0.05 and a high density ratio of 0.5. We compare the contributions of the different terms in the vorticity equation to \( \omega_x \) generation to understand the role of density ratio in the liquid-jet breakup.
The complete form of the vorticity equation is
\[
\frac{D\vec{\omega}}{Dt} = (\vec{\omega} \cdot \nabla) \vec{v} - \vec{\omega} (\nabla \cdot \vec{v}) + \nabla \times \left( \frac{\nabla \cdot \mathbf{T}}{\rho} \right) + \frac{1}{\rho^2} \nabla \rho \times \nabla p + \nabla \times \vec{F}_\sigma, \tag{2}
\]
where \(\vec{v}\) and \(\vec{\omega}\) are the velocity and vorticity vectors, respectively. \(\mathbf{T}\) is the viscous stress tensor, and \(\vec{F}_\sigma\) is the surface tension force. Since the fluids are incompressible in this study, the second term on the right hand side is zero. The surface tension term (third term on the right-hand-side) have negligible contributions to vorticity generation; thus, the rate of change of \(\omega_x\) is approximately
\[
\frac{D\omega_x}{Dt} = \omega_x \frac{\partial u}{\partial x} + \omega_y \frac{\partial u}{\partial y} + \omega_z \frac{\partial u}{\partial z} + \frac{1}{\rho^2} \left[ \frac{\partial \rho}{\partial y} \frac{\partial \rho}{\partial z} - \frac{\partial \rho}{\partial z} \frac{\partial \rho}{\partial y} \right], \tag{3}
\]
where \(\omega_x, \omega_y, \omega_z\), and \(u\) denote the streamwise, spanwise, and cross-stream (normal) vorticities, and streamwise velocity, respectively. The terms on the right-hand-side denote streamwise stretching, spanwise tilting, and cross-stream (normal) vorticities and streamwise velocity, respectively. The terms on the right-hand-side denote streamwise stretching, spanwise tilting, and cross-stream (normal) vorticities and streamwise velocity, respectively. Density gradient is normal to the liquid interface; i.e. approximately in the \(z\) direction. The spanwise density gradient, i.e. \(\partial \rho/\partial y\), is negligible compared to \(\partial \rho/\partial z\), since the sheet cross-section remains fairly rectangular for early instability development. Yet, this baroclinic effect can deform the interface in the spanwise direction.

In the cases studied in this section, no initial perturbation is imposed on the liquid surface. Except for numerical errors which for our purpose correspond to small random physical disturbances, all terms in the \(\omega_x\) generation equation (Eq. 3) are initially zero. Namely, the first and the third terms are zero because there is no vorticity components in the \(x\) and \(z\)-directions initially, and the second term is zero since the streamwise velocity is uniform in the spanwise direction. The baroclinic terms are identically zero since density and pressure gradients in the spanwise direction. The baroclinic terms are identically zero since density and pressure gradients in the spanwise direction. The baroclinic terms are identically zero since density and pressure gradients in the spanwise direction. The baroclinic terms are identically zero since density and pressure gradients in the spanwise direction. The baroclinic terms are identically zero since density and pressure gradients in the spanwise direction.

Since the streamwise \((\omega_x)\) and normal vorticities \((\omega_z)\) cannot be generated, but can be enhanced, the main source of \(\omega_x\) generation at early times is either the streamwise vorticity tilting or the baroclinic torque, which become non-zero as a result of small perturbations of \(u\) and \(p\) in the spanwise direction, respectively. This interpretation is consistent with the results of Jarrahbashi and Sirignano [4] in round jets at early times, where for a wide range of density ratios, the baroclinic torque and the azimuthal vortex tilting terms were dominant for the first 5 \(\mu s\) of their computations; however, they might be overtaken later by other terms. Baroclinicity becomes more pronounced at lower density ratios, since the density gradient across the interface is higher.

The gradients have been calculated and averaged along the computational interface thickness that equals three mesh points in the \(z\) and tangential directions. The terms in Eq. 3 are:

- Streamwise vortex stretching: \(\omega_x \frac{\partial u}{\partial x}\)
- Spanwise vortex tilting: \(\omega_y \frac{\partial u}{\partial y}\)
• Normal vortex tilting: $\omega_z \frac{\partial u}{\partial z}$

• Baroclinic vorticity generation:

$$\frac{1}{\rho} \left[ \frac{\partial \rho}{\partial y} \frac{\partial p}{\partial z} - \frac{\partial \rho}{\partial z} \frac{\partial p}{\partial y} \right]$$

Two different density ratios have been analyzed in this section. The non-dimensional characteristics of these two cases are: $Re_l = 2500$, $We_l = 14,400$, $\hat{\mu} = 0.0066$, and $\hat{\rho} = 0.05$ and $0.5$. The sheet thickness is $h = 50 \mu m$.

Figure 9 shows the contribution of each term in the generation of $\omega_x$ for the high and low density ratios, in the first $20 \mu s$. Baroclinicity (circles) is the most important factor at low density ratio. However, at high density ratio, baroclinicity is the least significant. Baroclinicity is only slightly larger than the streamwise stretching (squares) in the beginning of the computations for high density ratio, but it is outrun by this term at about $13 \mu s$ and remains the lowest of all terms thence. The baroclinic vorticity generation term is an order of magnitude smaller than the vortex stretching and tilting terms at the end of the computations.

In both low and high density ratios, the spanwise and normal tilting seem to be more important than the streamwise stretching for the first $20 \mu s$. The spanwise tilting is high because the vortex lines are essentially spanwise first, then are gradually tilted in the streamwise direction. The normal tilting is also high since the velocity gradient is much higher in the normal direction ($\partial u/\partial z$), in the beginning of the computations. The streamwise stretching however, has the highest growth rate and almost reaches the magnitude of vortex tilting at about $20 \mu s$. Later on, as $\omega_x$ grows, the vortex stretching becomes more significant. These results are consistent with the findings of Jarrahbash and Sirignano [4] for round liquid jets. As described by them and also evident in our figures, the vortex tilting terms are the largest at early times; however, new findings show some cancellations, discussed below.

Figure 10 shows the contours of the four $\omega_x$ generating terms at $13 \mu s$, on a $y$-plane of the $\hat{\rho} = 0.05$ case. The spanwise and normal vortex tilting terms (Fig. 10b,c) are stronger than the streamwise stretching, but with opposite signs. As demonstrated in Fig. 9, the two vortex tilting terms are also nearly equal and hence nearly cancel each other early on. Based on this, our earlier conclusion (and also that of Jarrahbash and Sirignano [4]) should be modified: the spanwise and normal vortex tilting terms, even though the largest among the $\omega_x$ generating terms, are not the most important in $\omega_x$ generation, since they nearly cancel each other. Thus, the streamwise vortex stretching and baroclinic effects are the most important in generation of $\omega_x$, at high and low density ratios, respectively.

Figure 10(a) also confirms that the vortex stretching originates from the braids first, as the strain due to the adjacent primary vortical structures is highest at the saddle (braid) and the ribs are aligned along the diverging separatrix [26]. Most of the colored spots in Fig. 10(a) are on the braids and not the wave crests. This is consistent with the experimental observations of earlier researchers [7, 9, 15] for uniform-density flows. The location and direction of the stretch can also be seen in Fig. 11, which shows the fluctuation velocity vectors relative to the average KH vortex velocity on a blown-up section of the liquid jet at $13 \mu s$. It is evident that the saddles with the highest strain rate are on the braids between two adjacent vortices, where the fluctuation velocity vectors depart in the opposite directions. The stretch direction at the saddle point is shown by the green arrows in Fig. 11. The saddle points are
in the gas phase, close to the interface. The streamwise vortex stretching is highest at the saddle points (see Fig. 10a), where the flow is primarily discrete ribs [26]. The fluid elements are stretched along the interface, i.e. along the diverging separatrix shown by the green arrows, and compressed normal to the interface at the saddle points. The center of the spanwise vortices (rolls) are at the crest of the interface waves, as denoted by the vector field and the vorticity contours. Interestingly, the vorticity peak coincides with the interface at the crests, but not at the troughs.

The stretching and tilting terms are centered at the interface (see Fig. 10a–c), but the baroclinic torque term $\frac{1}{\rho^2} \nabla \rho \times \nabla \rho$ is always larger in the gas phase (see Fig. 10d). Baroclinicity, being proportional to $1/\rho^2$, is two orders of magnitude larger in the gas phase compared to the liquid phase (for $\hat{\rho} = 0.05$). As density ratio increases, the difference between the gas and liquid densities decreases; thus, core of the baroclinicity contours get closer to the liquid interface. This is seen in the baroclinicity contours of $\hat{\rho} = 0.5$ in Fig. 12. Since the density ratio is an order of magnitude higher than that of Fig. 10(d), the local density in the gas zone is much higher, hence the baroclinicity in the gas is lower and closer to its value in the liquid. Thus, the contours are closer to the interface (compare Figs. 12 and 10d). This contributes to the $\omega_x$ peak being closer to the interface and growing larger compared to the low density ratios, hence creating and stretching more lobes at higher density ratios. Also, the peak of baroclinic torque is an order of magnitude smaller in Fig. 12 compared to Fig. 10(d), since the density gradient normal to the interface is lower at higher density ratios.

In order to understand how fast the liquid sheet deforms and manifests 3D instabilities, the magnitudes of the vorticity components are examined through time. The 3D instabilities are directly related to the magnitudes of $\omega_x$ and $\omega_z$ against $\omega_y$, which exists from the beginning when the flow is still 2D. As mentioned by the earlier researchers [4, 5, 24], the streamwise vorticity is the main cause of the three-dimensional instabilities.

The absolute value of each vorticity component has been averaged over the entire liquid/gas interface, plotted in Fig. 13 for low and high density ratios. The spanwise vorticity $\omega_y$ (KH vortex) is the only component that exists initially. In both cases, $\omega_y$ grows for a certain time, about 15 $\mu$s, and then onward keeps more or less the same order of magnitude. The spanwise vorticity is larger for lower density ratio. $\omega_x$ and $\omega_z$ grow very slowly up to 10 $\mu$s, after which, there is a sudden increase in their growth rate. In both cases, $\omega_x$ and $\omega_z$ are of the same order of magnitude, which indicates that initially spanwise vortex filaments are lifted in the normal direction and tilted in the streamwise direction at almost equal rates. The growth rate of $\omega_x$ is higher at higher density ratios. $\omega_x$ reaches the same order of magnitude as $\omega_y$ at $t = 20 \mu$s, for the high density ratio. For the lower density ratio, however, the growth is slower. Hence, three-dimensionality manifests sooner at higher gas densities. The growth rate of $\omega_x$ is reduced by decreasing the density ratio. For $\hat{\rho} = 0.05$, the magnitude of $\omega_x$ and $\omega_z$ are still half of $\omega_y$ at 20 $\mu$s. Thus, $\omega_y$ is still dominant and 2D
deformations build up while the streamwise vorticity grows. $\omega_x$ growth has consequent impacts on the surface dynamics. In order to understand this, the liquid surface has been compared at two instances for both low and high density ratios in Fig. 14.

The higher $\omega_x$ growth rate at high density ratio causes the liquid surface to undergo 3D instabilities much faster, and there are more lobes seen at high $\hat{\rho}$ than at low $\hat{\rho}$. At 15 $\mu$s, the surface of the sheet with $\hat{\rho} = 0.05$ is still roughly two-dimensional, while the high density-ratio case manifests more 3D deformations, and lobes are apparent on top of the primary KH waves. On the other hand, the higher $\omega_y$ compared to $\omega_x$ at low $\hat{\rho}$ causes the liquid sheet to become antisymmetric much faster (compare the top images of Fig. 14).

The difference in the vorticity dynamics in the two cases has significant effects on the characteristics of the jet instabilities. As can be seen at $t = 18$ $\mu$s (Fig. 14), the low $\hat{\rho}$ case can be characterized by roll-up of the KH waves, which creates more spanwise-aligned liquid structures and fewer stretched lobes; the entire sheet thins faster, and the liquid sheet breaks sooner. On the other hand, at high $\hat{\rho}$, the liquid structures orient streamwise more and manifest more lobes. The lobes are more stretched and thinned due to the larger $\omega_x$ and are more prone to perforation. Hence, the hole-formation mechanism is expected to prevail over a larger area in the parameter space of $W_e l$ versus $Re_l$, at higher density ratios. This is consistent with the zones in Fig. 1.

The top and bottom liquid surfaces tend towards an antisymmetric mode, whether we start with a flat surface or symmetric perturbations. The antisymmetric behavior is eventually favored since a planar jet is more unstable to the antisymmetric mode than the symmetric mode in the parameter range of practical interest. The transformation towards antisymmetry occurs sooner as density ratio is lowered.

Conclusions

The present study has focused mainly on the vortex dynamics of planar liquid jets. A vortex has been defined using the $\lambda_2$ criterion. The relation between the surface dynamics and the vortex dynamics is sought to explain the physics of different breakup mechanisms that occur in primary atomization, by conducting DNS with level-set and volume-of-fluid surface tracking methods.

The vortex dynamics are able to explain the hairpins formation. The interaction between the hairpin vortices and the KH vortex explains the perforation of the lobes at moderate $Re_l$ and high $W_e l$, which is attributed to the overlapping of a pair of hairpin vortices on top and bottom of the lobe. The formation of corrugations on the lobe front edge at high $Re_l$ is also explained by the structure of the hairpins and also the splitting of the KH vortex. At low $Re_l$ and low $W_e l$, on the other hand, the lobe perforation and corrugation formation are inhibited due to the high surface tension and viscous forces, which dampen the small scale corrugations and resist against hole formation. The hairpin vortices stretch in the normal direction while wrapping around the KH vortex. The induced gas flow squeezes the lobe from the sides and forms a thick
and long ligament. In summary, the vortex dynamics analysis helps explain various breakup mechanisms at different flow conditions.

Baroclinicity is the most important factor in generation of the streamwise vortices and manifestation of three-dimensional instabilities at low density ratios. At higher density ratios, the streamwise vortices are mostly rendered by streamwise vortex stretching. The streamwise vorticity growth is higher at higher density ratios, resulting in a sooner appearance of three-dimensional instabilities. As density ratio is reduced, fewer lobes with less undulation form; hence, hole formation prevails more at higher density ratios. The relation between vortex dynamics and surface dynamics aids prediction of liquid-structure formations at different flow conditions and different stages of the primary atomization. This is very important in prediction and control of the ligaments and droplets size distribution in liquid jet atomization.

References


