A Three-Dimensional Numerical Study of the Breakup Length of Liquid Sheets

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Abstract
A three-dimensional study of the primary breakup of a liquid sheet is performed. A VOF-based solver is employed to solve the governing equations. Young's method is used to reconstruct the liquid-gas interface at each time step. Linear stability theory is applied to implement the required boundary condition at the liquid-gas interface. The effect of fluid properties and flow parameters on the breakup length is studied via non-dimensional numbers, i.e. Weber number, Ohnesorge number, and gas to liquid density ratio. In addition to the formation of span-wise ligaments associated with two-dimensional studies, stream-wise ligaments are captured using the three-dimensional model. Formation of stream-wise ligaments is due to the generation of counter-rotating stream-wise vortices. It is demonstrated that the liquid surface tension tends to stabilize the liquid sheet by decreasing the strength of vortices while the density of the surrounding gas enhances the breakup by intensifying stream-wise vorticities. Additionally, it is demonstrated that the presence of the free edge would result in the enhancement of the breakup.

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Introduction

Liquid sheets are used in many industrial processes, including the combustion in jet engines, internal combustion engines, icing phenomena on the wings of aircrafts, heat exchangers, ink-jet printers, coating, and painting. In all these applications, liquid sheets break into smaller ligaments and furthermore, to fine droplets. The final diameter and velocity of the produced droplets are greatly affected by the mechanisms dominating the breakup process.

Primary breakup is defined as the disintegration of liquid sheets into ligaments. As schematically shown in Figure 1, instabilities generated on the surfaces of liquid sheets can be categorized into two distinct groups; sinusoidal (anti-symmetric) and dilatational (symmetric), as indicated in the work of Senecal et al.[1] and, Li and Tankin [2].

![Figure 1. Two types of instabilities, (a) symmetric, (b) anti-symmetric](image)

Li and Tankin [2] have shown that at small values of gas to liquid density ratios, ρ_g/ρ_l<<1, the anti-symmetric mode dominates, and this kind of disturbances would grow and make the liquid sheet break into smaller ligaments. Since the gas to liquid density ratios considered in this work is in the order of 10^{-2} to 10^{-3}, only anti-symmetric disturbances are discussed in this paper. In addition to ρ_g/ρ_l, two other non-dimensional numbers governing the flow field in sheet breakup problems are Weber number (Wel=ρ_lU^2h/σ) and Ohnesorge number (Oh=μ/(ρ_lh)^0.5), where h is half of the sheet thickness, U is the sheet velocity, and ρ, μ, and σ represent density, viscosity and surface tension, respectively. Subscript l denotes liquid properties.

The initial studies on the primary breakup of liquid sheets were conducted by Hagerty and Shea [3]. The aerodynamic forces acting on the liquid-gas interface were introduced as the major source of the sheet breakup. The surface tension force was identified as a force which tends to stabilize the liquid sheet. The effect of viscosity was not considered in their study. Dombrowski and John [4], however, included the effect of viscosity. A linear stability analysis was performed in order to identify the most unstable instability growing on the surfaces of the sheet. Their results have been verified by the experimental results of Mansour and Chigier [5] and Carvalho et al [6].

Most of the theoretical studies on the primary breakup of liquid sheets can be categorized into linear and nonlinear stability analyses. These analyses can be done either temporally, to find the breakup time of the sheet, or spatially, to study the breakup length of the liquid sheets. Li and Tankin [2] and, Senecal et al. [1] performed a two-dimensional temporal stability analysis while Li [7] applied a spatial linear stability analysis to find the breakup length of the liquid sheet. Mehring and Sirignano [8] and, Kim and Sirignano [9] performed three-dimensional temporal and spatial stability analyses to study the breakup of liquid sheets. While these methods implement accurate boundary conditions at the free surface, they do not track the liquid-gas interface sharply since there is a discontinuity in the density of the liquid and gas. Additionally, the linear stability theory neglects some terms of the governing equations due to linearization.

A vortex line analysis was introduced for sheet breakup problems by Inoue [10], who studied disintegration of a three-dimensional liquid sheet. It was demonstrated that, generally, there are two types of ligaments; span-wise and stream-wise ligaments, depending on the orientation of the generated ligaments with respect to the flow field. Span-wise ligaments are captured by two-dimensional analyses, while three dimensional studies are capable of capturing both types of ligaments. It was reported that the stream-wise vortex lines are responsible for the formation of stream-wise ligaments. These stream-wise vortices are generated by the deformation of initially span-wise vortex lines. The results are in agreement with the later experimental work of Stapper et al. [11].

Several numerical schemes have been introduced to track the interface between two fluids such as 'marker methods' by Glimm et al. [12], Tryggvason and Unverdi [13], and Tryggvason [14], 'level set methods' by Osher and Sethian [15] and Sussman et al. [16], and 'Volume of Fluid (VOF) methods' by Hirt and Nichols [17] and Gueyffier et al. [18]. These methods have been applied to model the sheet breakup such as that in the work of Herrmann [19], in which a level set method is employed to model the primary breakup of liquid sheets.

Among the present numerical methods in two-phase flows, VOF solvers have been acknowledged as shape preserving methods suitable for flows with large distortions, Kothe, and Mjolsness [20].
However, mesh dependency has been identified as the major drawback of VOF methods rising from geometrical algorithms mainly used to reconstruct the liquid-gas interface, Raessi et al. [21].

The goal of this work is to simulate three-dimensional primary breakup of liquid sheets considering the effects of gas to liquid density ratio and liquid surface tension. This work is the extension of the previous work of Movassat and Dolatabadi [22] in which the breakup length of the liquid sheet was studied employing a two-dimensional simulation. A VOF solver has been employed to solve the governing equations for the liquid phase and to capture the interface between the liquid and gas. The gas-liquid interface boundary condition is applied using linear stability analysis.

Methodology
Consider a liquid sheet moving with an initial velocity of \( U \) and an undisturbed thickness of \( 2h \). The governing equations for the liquid phase are mass and momentum conservation equations which are stated as,

\[
\nabla \dot{V} = 0
\]

\[
\frac{\partial \dot{V}}{\partial t} + \nabla \cdot (\dot{V} \dot{V}) = -\frac{1}{\rho_l} \nabla p + \nu_l \left( \nabla \cdot \left( \nabla \dot{V} \right) \right) + \frac{1}{\rho_l} \dot{F}_b
\]

(1)

where \( \dot{V} \) is the velocity vector, \( p \) is pressure, \( \nu_l \) and \( \rho_l \) are the kinetic viscosity and density of liquid, respectively. \( \dot{F}_b \) represents body forces. A three-dimensional VOF solver developed by Bussmann et al. [23] is employed to solve governing equations. The solver is basically an extension of the two-dimensional RIPPLE code, [20]. In VOF methods, a scalar field called volume fraction, \( f \), is used to capture the interface between the liquid and gas. \( f \) is defined as,

\[
\begin{align*}
    f & = 0 \quad \text{no liquid in the cell} \\
    f & = 1 \quad \text{cell filled with liquid}
\end{align*}
\]

With this definition, cells with \( 0 < f < 1 \) are at the liquid-gas interface. The definition of \( f \) and the reconstruction of the interface are shown in Figure 2. In VOF algorithms, the volume fraction is advected by the flow field following the equation,

\[
\frac{\partial f}{\partial t} + \left( \dot{V} \cdot \nabla \right) f = 0
\]

(2)

Equations (1) and (2) are discretized on a uniform square mesh using the Marker and Cell scheme, Welch et al. [24], in which the velocities are defined at cell faces whereas the pressure and volume fraction are defined at cell centers. Youngs' method, Youngs [25], is used to reconstruct the interface between the liquid and gas. Surface tension force is applied as a body force using the Continuum Surface Force (CSF) method proposed by Brackbill et al [26].

Boundary conditions required to solve governing equations are shown in Figure 3. The boundary condition in the y-direction would be explained when results are explained. Liquid-gas interface boundary conditions are applied using linear stability theory.

![Figure 2. Definition of volume fraction](image)

![Figure 3. (a) Domain boundary condition (b) Interface boundary condition](image)
Spatial Linear Stability Theory

The linear stability theory assumes that there are infinite small disturbances with different wavelengths, frequencies, and growth rates traveling on the liquid sheet surfaces [1]. The location of the disturbed upper and lower interfaces is stated as,

\[ z = \pm h + \eta \]  \hspace{1cm} (3)

where \( \eta \) tracks the liquid interface. The equation of the disturbance can be written as,

\[ \eta = \eta_0 \exp(-k_x x) \cos(k_x x - \omega t) \]  \hspace{1cm} (4)

where \( \eta_0 \) is the initial amplitude, \( \omega \) is the wave frequency, \( k_x \) is the wave number, and \( k_i \) is the growth rate.

Linearized governing equations are solved implementing appropriate boundary conditions to find the mathematical relation between the wavelengths and corresponding growth rates. This relation is called the dispersion equation, [1]. The wave with the highest growth rate is identified as the most unstable disturbance which causes the liquid sheet to breakup.

The main flow is in the \( x \)-direction with the velocity \( U \). It is assumed that the flow variables are perturbed with small disturbances so that each variable is composed of two parts; the main and the disturbed parts. The disturbed variables are \( u' \), \( w' \), and \( p' \) for \( x \)-velocity, \( z \)-velocity, and pressure, respectively. Replacing the main and disturbed variables into the governing equations (i.e. equations (1) and (2)), and neglecting higher order terms containing disturbed variables leads to the linearized governing equations for the liquid phase,

\[
\begin{align*}
\frac{\partial u'}{\partial t} + U \frac{\partial u'}{\partial x} &= -\frac{1}{\rho} \frac{\partial p'}{\partial x} + \nu \left( \frac{\partial^2 u'}{\partial x^2} + \frac{\partial^2 u'}{\partial z^2} \right) \\
\frac{\partial w'}{\partial t} + U \frac{\partial w'}{\partial x} &= -\frac{1}{\rho} \frac{\partial p'}{\partial z} + \nu \left( \frac{\partial^2 w'}{\partial x^2} + \frac{\partial^2 w'}{\partial z^2} \right)
\end{align*}
\]  \hspace{1cm} (5)

Boundary conditions required to solve the linearized governing equations are stated as,

\[
\begin{align*}
&\frac{\partial \eta}{\partial t} = 0 \\
&\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} = 0
\end{align*}
\]  \hspace{1cm} (6)

\[
\Delta p + 2 \mu_i \frac{\partial w}{\partial z} = \sigma \frac{\partial^2 \eta}{\partial x^2}
\]

The resulting dispersion equation for an inviscid case is [7],

\[ k_i h = \left( k_i h \right) \times \left( \frac{\rho_s / \rho_l - k_i h / We_l}{\tanh(k_i h)} \right)^{0.5} \]  \hspace{1cm} (7)

Derivative of the equation (7) is used to find the highest growth rate, \( k_{i,\text{max}} \), by solving \( dk_i / dk_r = 0 \). The value corresponding to the highest growth rate is employed to implement the liquid-gas interface vertical velocities, shown in Figure 3 (b), which is required to solve equations numerically.

\[ w = \left( \frac{\partial \eta}{\partial t} \right)_{k_{i,\text{max}}} \]  \hspace{1cm} (8)

Results

First, the formation of span-wise ligaments is demonstrated based on the two-dimensional simulations. These results have been discussed extensively in [22]. Then three-dimensional simulations are presented illustrating the formation of stream-wise ligaments. It should be mentioned that in order to implement the interface boundary condition, the results of inviscid dispersion equation are used and the effect of the liquid viscosity is included by changing this property in the flow solver.

For two-dimensional simulations, grid size is selected to provide initially 8 computational cells per sheet thickness with \( \Delta x = \Delta z \). The domain length in the \( x \)-direction is 6 times the wavelength corresponding to the maximum growth rate, \( \lambda_{\text{max}} \), to ensure that the sheet breaks before leaving the computational domain.

Figure 4 illustrates the evolution of a liquid sheet in space. As the sheet develops, instabilities start to grow (Figure 4 (b)) resulting in thickening and shrinking of the sheet (Figure 4 (c)). Finally at a distance, \( L \), defined as the breakup length the sheet breaks into smaller ligaments (Figure 4 (d)).
The numerical results are presented in terms of non-dimensional numbers in Table 1. In addition to $We$, $Oh$, and $\rho g/\rho l$, a non-dimensional breakup length, $L^*$, is defined as $L^* = L/2h$. The three cases presented in Table 1 have various inlet velocities, surface tensions, and viscosities while sharing the same $We$ and $Oh$. As it is shown in Table 1, as long as the Weber and Ohnesorge numbers are the same, the variation in the calculated $L^*$ is less than 3%. This clearly shows that the simulation results of the breakup phenomena are only a function of $We$, $Oh$, and $\rho g/\rho l$.

For three-dimensional simulations, the domain is extended in the span-direction, $y$-direction. Figure 5 illustrates the deformation and breakup of a liquid sheet moving in the $x$-direction. The boundary condition in the span-direction is set to periodic. The liquid sheet is disturbed in the $y$-direction with a wavelength equal to that of the most dominant wave in the flow direction, [8]. Figures 5 (b) and (c) show the volume fraction of the liquid in stream- and span-direction planes represented in Figure 5 (a). In addition to span-wise ligaments shown in Figure 5 (b), which were captured in two-dimensional analysis, stream-wise ligaments are captured, as demonstrated in Figure 5 (c). The generation of stream-wise ligaments is due to the three-dimensional effects.
Table 1. Table 1: Dependency of non-dimensional breakup length on non-dimensional parameters for $\rho_g/\rho_l = 1/1000$

<table>
<thead>
<tr>
<th>Case</th>
<th>$U$ (m/s)</th>
<th>$h$ (m)</th>
<th>$\sigma$ (N/m)</th>
<th>$\mu$ (kg/ms)</th>
<th>$We_l$</th>
<th>$Oh$</th>
<th>$L^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7.74</td>
<td>$250 \times 10^{-6}$</td>
<td>$30 \times 10^{-2}$</td>
<td>$87 \times 10^{-3}$</td>
<td>500</td>
<td>1.0</td>
<td>21.2</td>
</tr>
<tr>
<td>2</td>
<td>9.49</td>
<td>$250 \times 10^{-6}$</td>
<td>$45 \times 10^{-2}$</td>
<td>$106 \times 10^{-3}$</td>
<td>500</td>
<td>1.0</td>
<td>21.8</td>
</tr>
<tr>
<td>3</td>
<td>10.95</td>
<td>$250 \times 10^{-6}$</td>
<td>$60 \times 10^{-2}$</td>
<td>$122 \times 10^{-3}$</td>
<td>500</td>
<td>1.0</td>
<td>21.6</td>
</tr>
</tbody>
</table>

Figure 6. Velocity vectors at cross section of the liquid sheet, (a) $L = \bar{L}/4$, (b) $L = \bar{L}/2$, (c) $L = \bar{L}$

Figure 7 demonstrates the effect of the gas to liquid density ratio on the strength of stream-wise vorticities at a cross section of the liquid sheet prior to its breakup. Increasing the gas to liquid density ratio leads to more intense vortices due to higher values of velocities and smaller wavelengths predicted by linear stability analysis.

Figure 8 illustrates the variation of the intensity of stream-wise vortices with Weber number. As Weber number increases, the magnitude of the velocities is increased. As well, higher Weber numbers result in smaller dominant wavelengths making more intense vortices.

Figure 9 illustrates the velocity vectors at three cross sections of a liquid sheet which is not initially disturbed in the span-direction with the free edge at the right side. As the sheet evolves in space,
some instabilities are induced at the free edge, Figure 9 (b). These instabilities as well as three-dimensional effects result in the formation of stream-wise vortices, Figure 9 (c).

![Figure 9: Velocity vector at the cross section of liquid sheet with free edge for $\rho_g/\rho_l = 1/700$, $Oh = 1$, and $We_i = 500$.](image)

To investigate the effect of free edge on an initially disturbed liquid sheet, Figure 10 illustrates the stream-wise vortices at cross sections of liquid sheets with different lengths in the span direction; 2.5, 3.5, and 4.5 wavelengths in the span direction. In all the cases in addition to the initial disturbance and three-dimensional effects, the free edge, which is on the right side, intensifies the stream-wise vortices.

![Figure 10: Stream-wise vorticity for $\rho_g/\rho_l = 1/700$, $Oh = 1$, and $We_i = 400$. (a) 2.5 wavelength, (b) 3.5 wavelength, (c) 3.5 wavelength](image)

**Conclusion**

Three-dimensional studies of the primary breakup of liquid sheets are conducted in order to capture span-wise and stream-wise ligaments. A VOF based code is used to solve the governing equations for the liquid phase and to capture and reconstruct the interface between the liquid and the surrounding gas. Since the interaction between the gas and liquid is the major source of the breakup, the interface boundary condition is applied using the linear stability analysis.

The effect of the gas to liquid density ratio and Weber number on the strength of stream-wise vortices is investigated. It is shown that by increasing the gas to liquid density ratio and the Weber number, the strength of vortices is increased, demonstrating the destabilizing effect of the surrounding gas and the stabilizing effect of the liquid surface tension.

Additionally, the effect of the free edge on the breakup is studied, demonstrating the enhancement of the breakup due to the instabilities induced by the free edge.

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**References**