Doctoral Thesis

The experimental analysis and simulation of the breakup of a liquid filament jetting from a rotary laminar spray nozzle

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The spray processing of simple- and multiple emulsion structures under laminar conditions at subcritical Reynolds and Weber numbers preserves the internal disperse structure of the emulsions being sprayed. Rotary laminar spraying leads to liquid filament disintegration in a Rayleigh-Plateau breakup regime. The combination of rotary spraying and Rayleigh-Plateau breakup leads to a narrow spray drop-size distribution and subcritical spraying of emulsion structures whereby encapsulation of functional components within these emulsion structures is maintained.

The work herein performs an in-depth analysis on the liquid jet breakup behavior of one such rotary laminar spray system. In particular, high-speed videography was used to analyze the properties of the liquid filament near the nozzle exit. The results lead to the development of a simplified rotational model, which accurately describes the dominant forces acting on the liquid filament under the prescribed operating conditions.

This doctoral thesis then connects experiment results, which measure spray drop formation under Rayleigh-Plateau breakup conditions in a rotary system, to an axisymmetric CFD model. The comparison of results shows that the two-dimensional axisymmetric CFD model is a good predictor of laminar rotary spray breakup.
The experimental analysis and simulation of the breakup of a liquid filament jetting from a rotary laminar spray nozzle

A dissertation submitted to attain the degree of

DOCTOR OF SCIENCES of ETH ZURICH

(Dr. sc. ETH Zurich)

presented by

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Prof. Dr. Kathleen A. Feigl, Co-Examiner

2016
In loving memory of my Godparents,
Richard and Sandra Ristow
Facilities for the work described were provided by the Laboratory of Food Process Engineering (FPE); Institute of Food, Nutrition and Health (IFNH); Department of Health Sciences and Technology (DHEST) at the Swiss Federal Institute of Technology, Zurich (ETHZ) from September 2011 to June 2016. The project work was in collaboration with the Dept. of Mathematical Sciences at Michigan Technological University (MTU). Funding for my research was provided by the EU 7th Framework Programme through the Marie Curie Initial Training Network for powder technologies (PowTech_ITN) under REA grant agreement no. 264722.

My greatest appreciation goes out to my supervisor Professor Dr.-Ing. Erich J. Windhab for giving me the opportunity for a PhD. It was your creative insight that steered my project in an interesting and new direction. It was your optimism and positive outlook that helped me turn what I thought were sour grapes into a fine wine. It was your flexibility that made it possible for me to reap the benefits of Switzerland and home. For this I am grateful.

I would like to express my deepest gratitude to my co-examiners and research Götti & Gotti, Professor Franz Tanner and Professor Kathleen Feigl, who through the years have been my mentors and advisors. I am grateful for the countless hours, ideas, dinners and excursions that you have provided me along the way. It was your recommendations that brought me into this research and your guidance that brought me through.

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To my beloved VT coworkers both past and present, during the hard times of my research, I stayed because you have been family to me. My heart goes out to each and every one of you. A special thank you to Anna Emslander for all the work in
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# Notation

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<th>Unit</th>
<th>Meaning</th>
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<td>m</td>
<td>nozzle orifice radius</td>
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<td>filament diameter</td>
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<td>m</td>
<td>diameter of spherical drop</td>
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<td>diameter of nozzle</td>
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<td>viscous and surface tension forces</td>
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<td>( V_{\text{drop}} )</td>
<td>m(^3)</td>
<td>volume of a drop</td>
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<td>m/s</td>
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## Notation

### Greek Letters

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<td>angle of incidence</td>
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<td>offset angle</td>
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<td>$\gamma$</td>
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<td>$\lambda_{opt}$</td>
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### Indices

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<td>$I$</td>
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<td>$l$</td>
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Notation

Dimensionless Numbers

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<td>Froude number</td>
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<td>Ohnesorge number</td>
</tr>
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<td>Rb</td>
<td>Rossby number</td>
</tr>
<tr>
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<td>gas-Reynolds number</td>
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<tr>
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</tr>
<tr>
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<td>Weber number</td>
</tr>
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<td>critical Weber number</td>
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<tr>
<td>We_{gas}</td>
<td>gas-Weber number</td>
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Abbreviations

- BIM: boundary integral method
- CDF: cumulative distribution function
- CFD: Computational Fluid Dynamics
- DHEST: Department of Health Sciences and Technology
- ESR: early stage researcher
- ETHZ: Swiss Federal Institute of Technology, Zurich
- FC: functional component
- FOV: field of view
- FPE: Laboratory of Food Process Engineering
- FV: finite volume
- IFNH: Institute of Food, Nutrition and Health
- LSM: level set method
- MTU: Michigan Technological University
- OpenFOAM: Open Source Field Operation and Manipulation
- PDF: probability density function
- PSA: particle size analyzer
<table>
<thead>
<tr>
<th>Symbol</th>
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<tr>
<td>RRBN</td>
<td>Rotary Rayleigh Breakup Nozzle</td>
</tr>
<tr>
<td>VoF</td>
<td>volume of fluid</td>
</tr>
<tr>
<td>mTAB</td>
<td>modified Taylor analogy breakup</td>
</tr>
<tr>
<td>O/W/O</td>
<td>oil-in-water-in-oil</td>
</tr>
<tr>
<td>W/O/W</td>
<td>water-in-oil-in-water</td>
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Summary

Previous studies show that spray processing of emulsion and multiple emulsion structures using a pressure driven rotary spray nozzle, which is operated under laminar conditions at subcritical Reynolds and Weber numbers preserves the internal disperse structure of the emulsions being sprayed. At subcritical operation, the liquid filament jetting from the spray nozzle undergoes jet disintegration in a Rayleigh breakup regime. The drops produced from Rayleigh filament breakup are characterized by having diameters that are larger than those resulting from wind-induced jet disintegration or atomization.

The study herein uses high-speed videography measurements near the nozzle of the pressure driven Rotary Rayleigh Breakup Nozzle (RRBN) to analyze in detail the behavior of a liquid filament jetting from the nozzle of the rotary device. Using image superposition of multiple video frames of the liquid filament as a basis for analysis, it was determined that the Rayleigh-Plateau disturbances traveling on the surface of the liquid filament could act as a tracer in determining fluid velocity within the filament. The analysis showed that inertia plays the most significant role in determining the arc-shape of the liquid filament; whereas viscosity, surface tension and wind resistance were significantly less important.

A mathematical model describing the arc-shape of a liquid filament was developed in the rotating frame of reference in terms of Coriolis, centrifugal, viscous and surface tension forces. When viscosity, surface tension and wind resistance are neglected, the model simplifies and the arc-shape of the liquid jet is determined entirely by the characteristic Rossby number. The model showed close agreement with near-nozzle and remote-nozzle videography of the liquid filament, thereby validating that viscosity, surface tension and wind resistance could be neglected in this analysis. Moreover, the techniques described in this analysis can be used for improving measurements of rotational speed and fluid velocity without the need for tracer particles.

In a second study the operating conditions for nozzle exit velocity and rotational speed of the RRBN were varied and high-speed videography measurements were taken downstream after the Rayleigh breakup of the liquid filament. Since the sampling capabilities of the spray particle size analyzer (PSA) were limited due to the rotation of the device, drop detection and particle tracking techniques were developed herein to identify unique drops and their trajectories from the high-speed videos in order to measure the size of the detected spray drops. The resulting drop size measurements
were found to be in agreement with the liquid filament breakup theory of Rayleigh and Weber, which predicts the drop size of 2.6 times the nozzle diameter based on the material properties of the liquid. The cumulative distribution functions (CDFs) and plots of the median drop diameter show that the RRBN produces spray drops that are smaller in diameter than those from a non rotational device that operates in a Rayleigh breakup regime. Furthermore, span measurements demonstrate that the drop sizes are narrowly distributed. The CDF, median drop diameter and span were compared for the various operating conditions of the RRBN. The comparisons show that drop diameters decrease with rotational speed. Based on median drop diameter and span, an optimum rotational speed of 2000 rpm to 3000 rpm could be recommended, which yields a median drop diameter of approximately 2.0 times the nozzle diameter and a narrow drop-size distribution. The comparisons also show that drop diameter is generally unaffected by nozzle exit velocity, which agrees with the Rayleigh and Weber theory.

An axisymmetric CFD model was developed for comparison of liquid filament breakup behavior to the results from the RRBN experiments. The model was solved using the OpenFOAM two-phase finite volume (FV) volume of fluid (VoF) solver with an additional centrifugal force contribution to the momentum equation. The simulation results were post-processed using a computational tool developed herein, which identified drops based on the phase fraction of liquid in the simulation results. The tool then calculated drop size, centroid and velocity of the identified drops.

Limiting behavior of the filament diameter at pinch-off and breakup length were determined as a function of rotational speed using the drop centroid and velocity at pinch-off. The limiting behavior of the filament diameter at pinch-off showed a strong correlation to the diameter of resulting drops as a function of rotational speed. The limiting behavior of the filament diameter also explained why the breakup length versus rotational speed showed a limit of 60 times the nozzle diameter.

Based on the material properties of the fluid being simulated, Rayleigh theory predicts the drop diameter to be 1.9 times the diameter of the nozzle for an unstretched liquid filament. The simulations produced drops with diameters that were 1.3 times the nozzle diameter after filament stretching, which was in agreement with Rayleigh breakup theory. The simulation drop diameter results were compared to measured drop diameters as a function of rotational speed. There was good agreement between the two results. Is it recommended to further improve the simulation model to account for reduction in stretching forces, which occurs due to the bending of the liquid filament. Moreover, it is recommended to explore alternatives to the two-phase FV VoF that would improve stability when simulating high viscosity ratios.

Based on the material properties of the fluid being simulated, Rayleigh theory predicts the drop diameter resulting from the breakup of an unstretched liquid filament.
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ameters that were 1.3 times the nozzle diameter after filament stretching, which was in agreement with Rayleigh breakup theory. The simulation drop diameter results were compared to measured drop diameters as a function of rotational speed. There was good agreement between the two results. It is recommended to further improve the simulation model to account for reduction in stretching forces, which occurs due to the bending of the liquid filament. Moreover, it is recommended to explore alternatives to the two-phase FV VoF that would improve stability when simulating high viscosity ratios.
Zusammenfassung


In dieser Arbeit dienten Hochgeschwindigkeitskameraaufnahmen nahe der rotierenden Rayleigh-Zerfall Zerstäuberdüse (RRBN) zur detaillierten Analyse des austretenden Flüssigkeitsstrahls. Basierend auf der Bildüberlagerung mehrerer Videoaufnahmen konnte gezeigt werden, dass eine auf der Oberfläche des Flüssigkeitsstrahls erkennbare Rayleigh-Plateau Instabilität als Geschwindigkeitsindikator dienen kann. Dabei spielten Trägheitseffekte im Gegensatz zu Viskosität, Oberflächenspannung und Luftwiderstand eine entscheidende Rolle für die Bildung des bogenförmigen Sprühstrahls.

Unter Berücksichtigung der Coriolis-, Zentrifugal- und Zugkräfte wurde ein mathematisches Modell entwickelt, welches die bogenförmige Ausprägung des Flüssigkeitsstrahls beschreibt. Dieses Modell konnte durch Vernachlässigung von Viskosität, Oberflächenspannung und Luftwiderstand vereinfacht werden, was eine Charakterisierung der bogenförmigen Flüssigkeitsstrahlausprägung durch die Rossby-Zahl erlaubt. Das Modell zeigt eine gute Übereinstimmung in Nah- und Fernbereich der Düse, was wiederum bestätigt, dass Viskosität, Oberflächenspannung und Luftwiderstand vernachlässigt werden können. Zusätzlich kann die entwickelte Videoanalyse dazu beitragen, die Messung der Rotations- und Flüssigkeitsgeschwindigkeit ohne den Einsatz von Markerpartikeln zu verbessern.

Zusammenfassung


Die Rayleigh-Theorie sagt basierend auf den Materialeigenschaften der simulierten Flüssigkeit voraus, dass der Tropfendurchmesser resultierend vom Aufbruch eines undeformierten Flüssigkeitsstrahls 1.9-mal so gross ist wie der Düsendurchmesser. Bei zentrifugaler Deformation des Flüssigkeitsstrahls lieferte die Simulation Tropfen mit einem Durchmesser von Faktor 1.3 des Düsendurchmessers, was wiederum mit der Rayleigh Tropfenzerfallstheorie für das gedehnte Flüssigkeitsfilament übereinstimmt.
Zusammenfassung

1 Introduction

Multiple emulsions are able to encapsulate both hydrophilic and lipophilic functional components (FCs) making them useful in industries such as the food and pharmaceutical industries. In both the food and pharmaceutical industries encapsulation allows for controlled release of the FCs to maximize desired benefits. The intended time of release of FCs can occur at any time beginning with mixing and up to, and including, digestion. The FCs can range from nutrients and medical doses, which would have a controlled release during digestion, to flavors and aromas, which would have a controlled release during mixing and processing or in the oral cavity.

A key disadvantage with emulsions, and even more so, with multiple emulsions is that they are thermodynamically unstable and generally require surfactants and emulsifiers to prevent separation and loss of FC encapsulation. The addition of surfactants and emulsifiers can be inhibitive to the desired processing and release characteristics of the emulsions. Furthermore, the available surfactants and emulsifiers are greatly restricted in products to be consumed.

Spray processing of multiple emulsions to produce powders offers several advantages. The emulsions need only remain stable until the powderization process is completed. This allows for a reduction in the amount stabilizers needed to retain the emulsion structure. In addition, the powder form of an emulsion reduces instabilities caused by FCs diffusion as well as increases shelf life and storage stability.

Unfortunately, multiple emulsion structures are sensitive to mechanical processes. This presents an optimization challenge for spray processing of multiple emulsion structures. The challenge is to target nondestructive spray methods, while producing spray particles that meet a prescribed set of requirements, such as size range and size distribution.

The PhD thesis work of Dubey (Dubey, 2013) under the supervision of Prof. E.J. Windhab led to the development of the pressure driven Rotary Rayleigh Breakup Nozzle (RRBN), which met these challenges. In particular, his work showed that the emulsion structure was preserved at increased rotational speeds (see Fig. 1.1), while throughput and the spray drop-size distribution could be tuned by adjusting feed pressure and rotational speed. However, a detailed study was still needed to characterize the effects of the operating conditions of the device on the liquid filament behavior, resulting drop diameters and drop-size distribution of the sprayed liquid.
1 Introduction

Dispersed phase size distribution resulting from rotary spraying

Figure 1.1: The effect of spraying on the dispersed phase drop size, source (Dubey, 2013). The pre-spray curve (open-diamonds) illustrates the drop size of the dispersed phase without spraying. The remaining curves demonstrate that the majority of the structure loss comes from nozzle effects and not the rotation.
The work in this PhD thesis focuses on quantifying the behavior of the jetted liquid and resulting spray drops as a response to the operation of the RRBN. In particular, there are three areas of study in this thesis:

1. High-speed videography was used to study the liquid filament near the nozzle and in the region where the filament transitions to drops.
2. Drop sizes were calculated using high-speed video and compared to operating conditions of the RRBN.
3. Using Computational Fluid Dynamics (CFD) the Rayleigh breakup of liquid filaments was simulated in a centrifugal force field and compared with measured data.

1.1 Chapter descriptions

Chapter 2 provides a background and literature review on fundamentals of liquid jet disintegration under Rayleigh breakup conditions. In addition, it provides a review of CFD methods for solving two-phase flow problems, in particular finite volume (FV) methods for spatial discretization coupled with the volume of fluid (VoF) method or the level set method (LSM) for interface capturing.

The main results of this thesis are described in Chapters 3, 4 and 5. They address the three areas of study highlighted above.

Chapter 3 consists of a detailed analysis of the liquid filament, which is jetted from the RRBN. A mathematical model was developed, which describes the arc-shape of a liquid filament as it exits a rotary sprayer. This chapter describes the techniques used to analyze high-speed videography and the results of comparing the measurements with the model.

Chapter 4 discusses the use of high-speed videography to determine the size of spray drops resulting from Rayleigh breakup of a liquid filament jetting from the RRBN. In particular, this chapter develops a methodology for analyzing drop diameters from high-speed video. The results of these data are related to the operating conditions of the RRBN.

The simulation of liquid filament breakup of a jet in a centrifugal force field is described in Chapter 5. This chapter discusses the simulation conditions and the CFD model. The simulation results include the size of resulting spray drops, the breakup length of the filament and the velocity at breakup. These data were compared to results of Chapter 4, which validate the model.
2 Background

Double emulsions can be water-in-oil-in-water (W/O/W) or oil-in-water-in-oil (O/W/O). In the case of W/O/W, the inner droplet is composed of water, which is dispersed in an oil globule, which is then dispersed in a continuous phase of water. Similarly an O/W/O is oil dispersed in water, which is dispersed in a continuous oil phase. The compartmental structure of double emulsions allows them to encapsulate both hydrophilic and lipophilic FCs, making them useful in such industries as the food and pharmaceutical industries (Bibette, 2007; Dubey et al., 2010; Pays et al., 2002). In these industries encapsulation allows for controlled release of the FCs to maximize desired benefits. The intended time of release of FCs can occur at any time beginning with mixing and up to, and including, digestion. The FCs can range from nutrients and drugs, which would have a controlled release during digestion, to flavors and aromas, which would have a controlled release during preparation and/or in the consumer’s mouth.

Double emulsions are inherently unstable. This presents a major challenge when utilizing them as a vehicle to encapsulate FCs. The mechanisms driving the instabilities in double emulsions are coalescence and compositional ripening, which ultimately lead to a premature release of encapsulated FCs (Florence and Whitehill, 1985; Pays et al., 2001). Coalescence can cause a rupture in the globule wall, which leads to a release of the inner phase into the continuous phase. Whereas compositional ripening describes diffusion and/or permeation of the FCs across the globule layer.

Spray processing of multiple emulsions to produce powders offers several advantages. The emulsions need only remain stable until powder processing is completed, after which the powder form of an emulsion reduces instabilities caused by coalescence and compositional ripening as well as increasing shelf life and storage stability. This also allows for a reduction in the amount of stabilizers needed to retain the emulsion structure.

Unfortunately, multiple emulsion structures are sensitive to mechanical processes (Muguet et al., 2001). This presents an optimization challenge for spray processing of multiple emulsion structures targeting nondestructive spray methods, while producing spray particles that meet prescribed sets of requirements, such as size range and size distribution. In their experiments Dubey et al. (Dubey et al., 2010, 2011) sprayed W/O/W emulsions using a prilling process under Rayleigh breakup
conditions to produce powders, which retain the double emulsion structure as shown in Fig. 2.1.

![Picture of a solid W/O/W particle produced by prilling](image_url)  
**Figure 2.1:** Picture of a solid W/O/W particle produced by prilling, taken from Dubey et al. (Dubey et al., 2010).

Dubey’s experimental work shows good results, however there exists a need for an analytical tool set that can help determine optimal operational parameters from a prescribed set of material properties. This literature review discusses the theory developed around the spraying of liquid jets to form droplets in a Rayleigh breakup regime. The review further discusses numerical techniques for the simulation of multiphase flows, which is needed to address the complex fluid structures of double emulsions and the liquid-gas interactions of the spray system.

### 2.1 Jet breakup

In powder production the spraying of a liquid, whether it be a homogeneous mixture or an emulsion, relies heavily on the principle of jet breakup to form droplets. These droplets undergo a phase change either by drying or by freezing in order to produce the powder. A major component of this thesis is a detailed study of the breakup behavior of emulsion jets and the resulting drop size distribution.

A liquid jet, or filament, experiences disturbances when exiting a nozzle. These disturbances can be induced by pressure or velocity fluctuations within the jet or on the jet surface, and also by variations in fluid properties of the jet due to minute differences in temperature, viscosity or surface tension (Ashgriz and Yarin, 2011). While some of these disturbances will dampen, others will grow over time, leading to instabilities within the liquid filament and eventually cause the jet to undergo breakup.
2 Background

2.1.1 Basic equations

The analysis of filament breakup requires frequent use of fundamental equations including the mass and momentum conservation equations. For an incompressible, Newtonian flow these can be written as (Ashgriz and Yarin, 2011)

\[ \nabla \cdot \mathbf{u}_\alpha = 0 \]
\[ \frac{\partial \mathbf{u}_\alpha}{\partial t} + \mathbf{u}_\alpha \cdot \nabla \mathbf{u}_\alpha = - \frac{\nabla P_\alpha}{\rho_\alpha} + \nu_\alpha \nabla^2 \mathbf{u}_\alpha + \mathbf{g} + \frac{\mathbf{F}}{\rho_\alpha}, \]

where \( \mathbf{u} \) is the velocity vector, \( P \) is the pressure, \( \rho \) is the density, \( \nu \) is the kinematic viscosity, \( \mathbf{g} \) is gravity as a vector, and \( \mathbf{F} \) represents external forces or source terms. The subscript \( \alpha \in \{\ell, g\} \) denotes the phase of the reference species with \( \ell \) and \( g \) representing liquid and gas phases respectively. For brevity, dropping the subscript implies the liquid phase.

Additionally several dimensionless numbers are frequently utilized to relate filament breakup results to operational parameters,

\[ \text{Re} = \frac{\rho w r_0}{\eta}, \quad \text{We} = \frac{\rho w^2 r_0}{\gamma}, \quad \text{Bo} = \frac{\rho g r_0^2}{\gamma}, \quad \text{Oh} = \frac{\sqrt{\text{We}}}{\text{Re}} = \frac{\eta}{\sqrt{\rho \gamma r_0}}, \]

where \( \eta \) is dynamic viscosity, \( w \) represents the mean jet velocity, \( r_0 \) is the jet radius at the nozzle, and \( \gamma \) represents the surface tension. The dimensionless numbers defined in Eq. (2.2) are the Reynolds, Weber, Bond, and Ohnesorge numbers respectively. The Reynolds number is the ratio of inertial forces to viscous forces, the Weber number is the ratio of inertial forces to surface tension forces, and the Bond number represents the ratio of gravitational forces to surface tension forces. The Ohnesorge number is a combination of Reynolds number and Weber number, which relates viscous forces to inertial and surface tension forces. Similarly expressions for the gas-Reynolds number (\( \text{Re}_{\text{gas}} \)) and the gas-Weber number (\( \text{We}_{\text{gas}} \)) are defined with a characteristic velocity in place of jet velocity and characteristic length in place of jet radius.

2.1.2 Rayleigh’s stability analysis of inviscid jets

Rayleigh was the first to perform an in-depth analysis of the instabilities of liquid jets (Rayleigh, 1878). Building on the experimental work from Plateau, Rayleigh argued that the driving factor causing jet breakup was not from capillary force alone as Plateau concluded, but from small displacements on the surface of the jet, without which, the jet would remain in equilibrium no matter how unstable.
In his analysis he assumed the filament and the resulting jet breakup were axisymmetric, the fluid was inviscid, and the influence of surrounding gas was negligible. Without loss of generality, stationary flow was assumed by using a Galilean reference. He considered an initial disturbance having some wavelength $\lambda$ in the axial direction $z$ that changes in time. At some arbitrary time, the perturbed radius of the jet is modeled by
\[ \tilde{r} = r_0 + a \cos (\kappa z), \] (2.3)
where $\kappa = 2\pi/\lambda$ is the wave number and $r_0$ is the unperturbed radius of the jet. From this he determined that potential energy due to capillary forces, i.e., surface energy, increases when $r_0\kappa > 1$ or $\lambda < 2\pi r_0$. Thus for a disturbance to grow and not decay it is a necessary condition that $0 < r_0\kappa < 1$. This result supports the axisymmetric assumption, since asymmetrical disturbances will eventually decay. He further theorized that the wavelength, $\lambda_{\text{opt}}$, corresponding to the fastest growing disturbance will determine the breakup length of the jet, furthermore, he determined the value to be
\[ \lambda_{\text{opt}} = 9.02r_0, \] (2.4)
which leads to spherical droplets with diameter $d_{\text{drop}} = 1.89d_0$, where $d_0 = 2r_0$.

### 2.1.3 Weber’s analysis of viscous jets

Building off the work of Rayleigh, Weber (Weber, 1931) was able to calculate filament breakup for viscous fluids. Weber applied the method of small perturbations to laminar flows and assumed axisymmetric perturbations $\delta$ of the form
\[ \delta = \delta_0 e^{qt} \cos \bar{\kappa} \frac{z}{r_0}, \] (2.5)
where $\bar{\kappa}$ is the normalized wave number $\bar{\kappa} = 2\pi r_0/\lambda$, $t$ is time, and $q$ is the growth rate of the instability. He calculated the wavelength, $\lambda_{\text{opt}}$, and growth rate, $q_{\text{opt}}$, corresponding to the fastest growing instability, yielding:
\[ \lambda_{\text{opt}} = 2\pi r_0 \left(2 + \sqrt{\frac{18\eta^2}{\gamma \rho r_0}}\right)^{0.5}, \] (2.6)
\[ q_{\text{opt}} = \left(\frac{8r_0^3 \rho}{\gamma} + \frac{6\eta r_0}{\gamma}\right)^{-1}. \] (2.7)

From Eq. (2.6), the resulting spherical droplet diameter is
\[ d_{\text{drop}} = 1.89d_0 \sqrt{1 + 3 \text{Oh}}, \] (2.8)
which for inviscid flows reduces to Rayleigh’s calculation of the droplet diameter. Furthermore, the time required for the fastest growing disturbance to grow critically to size \( r_0 \) is \( t_{\text{crit}} = \ln \left( \frac{r_0}{\delta_0} \right) / q_{\text{opt}} \). Therefore he was able to calculate the breakup length of the jet \( L = wt_{\text{crit}} = \ln \left( \frac{r_0}{\delta_0} \right) w \left( \sqrt{\frac{8r_0^3 \rho}{\gamma}} + 6\eta r_0 \gamma \right) \). This can be written in terms of dimensionless numbers as:

\[
\frac{L}{d_0} = \ln \left( \frac{r_0}{\delta_0} \right) \left( \sqrt{2} \text{We} + 3 \frac{\text{We}}{\text{Re}} \right),
\]

where he took \( \ln \left( \frac{r_0}{\delta_0} \right) = 12 \). From his analysis Weber was able to conclude that increasing the viscosity will cause an increase in droplet size and breakup length. Furthermore, when the inertial effects of the surrounding gas are negligible, an increase in jet velocity will not affect the droplet size, but will increase the breakup length. However, once the inertial effects of the gas can no longer be neglected, the surrounding gas enhances the growth rate of disturbances in the jet, causing an earlier breakup of the jet (Reitz and Bracco, 1986).

The work of both Rayleigh and Weber as well as other classical analysis are reviewed in detail by Eggers (Eggers, 1997) and by Ashgriz & Yarin (Ashgriz and Yarin, 2011).

### 2.1.4 Breakup regimes

The characteristics of four different breakup regimes were described by Ohnesorge (Ohnesorge, 1936). The regimes he described are as follows:

1. Slow drop formation direct from the nozzle without jet formation, i.e., dripping
2. Axisymmetric cylindrical jet formation with jet breakup first analyzed by Rayleigh (see section 2.1.2)
3. Jet formation having a “cork-screw” pattern with jet breakup described by Weber-Hänlein as cited by Ohnesorge
4. Jet atomization

From experiments Ohnesorge was able to determine breakup regimes primarily in terms of viscosity, surface tension, density, jet diameter and velocity, yielding a plot of Oh versus Re that well describes the boundaries of the different breakup regimes. Miesse later correlated breakup regime data and presented his results in a similar form to Ohnesorge as shown in Fig. 2.2, while Torda included gas density effects (both are cited by Reitz & Bracco (Reitz and Bracco, 1986), who published a review of this topic). Also included in their review was an extension to Torda’s work that
mapped the density ratio $\rho_g/\rho_l$ on a third scale, as well as a detailed description of the jet breakup mechanisms dominant in each breakup regime.

![Figure 2.2: Summary of jet breakup regimes as described by Ohnesorge, Miesse and Torda, taken from Reitz & Bracco (Reitz and Bracco, 1986).](image)

2.1.5 Spatial/Temporal Models

Unlike his predecessors, Keller et al. (Keller et al., 1973), assumed disturbances were not limited to temporal growth, but could also grow spatially. He applied this theory to liquid jets in air. Wallwork & Decent et al. (Wallwork et al., 2002) determined the trajectory of a liquid inviscid jet emanating from a rotary nozzle using asymptotic methods. The resulting equations of motion were scaled in terms of non-dimensional velocity, pressure, jet radius, arc length of the jet and time scale, as well as Weber number and Rossby number\(^1\). Afterward the jet trajectory equations were solved numerically and the resulting trajectory stability was analyzed using a linear approach applying Keller’s assumptions to determine breakup length in terms of arc length. The results were compared against experiments, showing reasonably good agreement. The authors suggested that this method is applicable both to gravity driven jets under non-rotational conditions as well as jets under both influence of gravity and rotation. However, they went on to suggest that a non-linear analysis is necessary to get a more comprehensive understanding of droplet formation from a rotary jet.

\(^1\)Rossby number represents the ratio of inertial forces to rotational forces.
Wong et al. (Wong et al., 2004) performed laboratory experiments to measure breakup dynamics and drop size distributions from rotary jets i.e., jets resulting from rotary spraying. In their investigations they consider spiraling jets in a Rayleigh breakup regime, where influences of wind and internal flow can be considered negligible. From their experiments they describe four phenomenological modes of breakup \( \{M_1, M_2, M_3, M_4\} \), which detail the behavior of droplet production and resulting droplets. Briefly these modes are described here:

- \( M_1 \to \) Rapid formation of droplets after nozzle, which is caused by jet breakup with minimal satellite droplet formation.
- \( M_2 \to \) Primary droplets are formed due to jet breakup with satellite droplets forming from liquid fragments leftover from primary breakup.
- \( M_3 \to \) Long axisymmetric wavelengths form causing droplets 2-5 times the jet diameter to form with satellite droplets formed as in \( M_2 \).
- \( M_4 \to \) Nonlinear breakup behavior and a reverse bend at the end of the jet are observed. The end of the jet eventually shatters into small droplets and the jet recoils.

The breakup modes were then plotted in a diagram of Ohnesorge number versus Weber number as shown in Fig. 2.3. In further analysis Wong concluded that the breakup mode is strongly driven by dynamic viscosity and jet velocity, information well represented in Fig. 2.3. Additionally, he concluded that operation in the \( M_1 \) and \( M_4 \) modes produced uni-modal distributions and in all modes of breakup drop size was decreased by increasing rotational speed (decreasing the Rossby number). Wong compared his experimental results with the analysis theory of Wallwork & Decent et al. (Wallwork et al., 2002) and concluded that linear analysis was not sufficient to predict accurately breakup length and that a nonlinear model is necessary.

Following the work of Wong et al., Partridge et al. (Partridge et al., 2005) performed similar experiments at the pilot scale. Părău et al. (Părău et al., 2007) developed a viscous nonlinear model extending the theory from Wallwork & Decent and used the experimental results from Partridge to validate this model. They were able to show that breakup length increases with viscosity and rotation rate. Primary droplet and satellite drop sizes were in agreement for some cases. Decent et al. (Decent et al., 2009) continued development on the Wallwork model using a linear viscous model. The article addresses some of the assumptions in the model developed by Părău that were necessary in order to develop a nonlinear model. In their analysis Decent et al. were able to predict primary and satellite drop formation and size. These results were validated with experiments.

Uddin et al. (Uddin et al., 2008) analyzed the effect of surfactants on the jet breakup behavior of a rotary liquid jet in gas breakup based on the theoretical work of Wallwork (Wallwork et al., 2002) and Părău (Părău et al., 2007). These results show a
2 Background

Figure 2.3: The four breakup modes \{M1, M2, M3, M4\} mapped using Ohnesorge number versus Weber number as characterized by Wong et al. (Wong et al., 2004).

dampened trajectory when the concentration of surfactant is increased. Furthermore, an increase in surfactant caused a delay in rupture of the jet allowing for a longer jet length. This led to the conclusion that primary droplets tended to increase in size, but only when the wave numbers of the rapid growing disturbances were small. On the other hand, satellite droplets always decreased in size with the use of surfactants.

2.1.6 Laminar rotary spraying

Targeting a high throughput atomizer, which is able to produce droplets having a narrow drop size distribution, Walzel developed a laminar rotary atomizer (LAMROT) (Walzel, 1994). This design is discussed by Schröder & Walzel (Schröder and Walzel, 1998). The authors discuss key advantages to laminar rotary atomization including Rayleigh type breakup with a narrow monodisperse drop size distribution, drop sizes smaller than the nozzle diameter, resistance to plugging, and high throughput. Design parameters for optimal operation were also discussed such as flow conditions to maintain a Rayleigh type breakup and component sizing. The resulting design had a throughput of 0.8 m$^3$/h and was able to produce droplets with a volumetric mean diameter, $d_{50,3}$, in the range of $250\eta m < d_{50,3} < 450\eta m$ at a fluid viscosity of 0.1Pa·s.
Mescher & Walzel (Mescher and Walzel, 2010) carried out experiments to directly compare capillary breakup behavior of a filament stretching under gravity versus a filament stretching in a rotary environment. In the experimental setup, the filament, which was stretched under gravity, was subject to similar gas crossflow conditions as the jet in a rotating environment would be. Moreover, the rotational speed was fixed such that the filament in the rotating environment experienced one g of centrifugal acceleration at the nozzle and a relative gas crossflow velocity could be adjusted using a co-rotational layer. The resulting jet breakup length and drop sizes were measured and their non-dimensional analogues were compared. Their results showed that the two systems exhibit similar behavior, however rotary spraying has a tendency to produce shorter breakup lengths and slightly larger droplet sizes at low (relative) gas velocities.

Mescher et al. (Mescher et al., 2012) experimentally determined the effect that gas velocity in a crossflow has on breakup behavior and the drop size distribution. These experiments demonstrated only minor influences due to inclination angle and nozzle diameter on the breakup lengths and drop size. The mean drop size was found to increase at higher crossflow velocities, furthermore, there was a strong influence on drop size distribution from the gas-Weber number. At low gas-Weber numbers an increase caused a wider drop size distribution; and at higher gas-Weber numbers the breakup regime was altered, which caused a much wider drop size distribution. These results were intended to be applied directly to design optimization of laminar rotary atomization conditions.

2.1.7 Other related work

Kitamura et al. (Kitamura et al., 1985) considered the jet breakup of fluids with emulsion structures. In his experiment he measured the breakup length and droplet size of a kerosene-water emulsion, which had a disperse phase of less than 50 wt%, in order to determine if the emulsion structure has a direct effect on breakup length and drop size. He held the disperse phase relatively dilute in order to have fluids that exhibited Newtonian flow behavior. He concluded from his experiments that the emulsion structure has no significant effects on breakup length or droplet size when compared to homogeneous liquids and are in agreement with predictions from stability analysis.

Kitamura & Takahashi (Kitamura and Takahashi, 1976) took Weber’s analysis further by performing a stability analysis on the breakup of liquid jets in the presence of a gas flow acting normal to the liquid jet. From their analysis an increase in gas-Weber numbers, $We_{gas}$, causes an increase in the critical (fastest growing) wave number and its related growth rate. The increased value of the critical wave number implies smaller resulting droplets and the faster rate of growth results in a shorter
2 Background

jet breakup length. They supported their analysis with experiments, leading to the same conclusions.

Cheong & Howes (Cheong and Howes, 2004) utilized a one-dimensional numerical model developed by Eggers & Dupont (1994), as cited, to analyze the effects of gravity stretching on jet breakup behavior. They adapted the model to directly utilize gravity, which is then adjusted to determine jet breakup behavior. The results of the calculations were compared to experimental values to determine optimum disturbance frequencies. Their simulations showed strong agreement with measurement. They concluded that gravity decreases the optimum disturbance wave number thus increasing wavelength both numerically and in experiment.

2.2 Material interfaces in Computational Fluid Dynamics

In CFD special consideration must be taken when handling multiphase problems. In particular the material interface between the two or more phases presents a challenge. For example, the simulation of a liquid jet in air requires fluid equations to describe both the liquid and the air behaviors, while a another set of equations is needed to address the behavior at the interface (Jasak and Tukovic, 2006). Three particular problems arise when addressing a material interface; first is how to represent the interface mathematically, second is how to handle its evolution in time, and third is how boundary conditions are imposed on the interface (Hirt and Nichols, 1981). Two of the most popular approaches for addressing these problems are interface capturing and interface tracking.

The interface capturing approach treats the multiphase problem as a single fluid with varying material properties, so that the interface is handled implicitly. In the interface capturing approach the mesh does not deform to the interface, thus these methods inherently adapt to changes in topology such as coalescence, breakup, and mesh refinement (Sethian, 1985). Two common interface capturing methods are the VoF method and the LSM, which are discussed below.

The interface tracking approach explicitly handles the interface, so that each phase and the interface are handled separately. This is typically done by a deforming the mesh at at the interface. A common interface tracking method is the boundary integral method (BIM), which is not discussed in this review.
2 Background

2.2.1 Volume of fluid method

In the simplest case, the VoF method addresses a two-phase problem on an Eulerian mesh by using an indicator variable to describe the phase of the fluid occupying each mesh element. For example in a water-air problem we let $\alpha$ represent the phase with $\alpha = 0$ representing a mesh element that contains only air and $\alpha = 1$ is an element containing only water. The interface lies in any mesh elements that have an $\alpha$ value $0 < \alpha < 1$. In fact the value of $\alpha$ corresponds directly to the volume fraction of water contained by the mesh element. Hirt (Hirt and Nichols, 1981) describes details of this method, addressing how the method handles time evolution and imposition of boundary conditions.

A key advantage of VoF methods is that mass is conserved automatically by construction (Sethian, 1985). James (James and Lowengrub, 2004) was able to adapt the VoF method to include surfactants on the interface, where again mass was conserved. Rudman (Rudman, 1998) demonstrates that VoF type methods well handle multiphase problems with large density differences among the phases making it ideal for liquid in air multiphase problems, such as jet breakup simulations.

2.2.2 Level set method

In contrast to VoF, the LSM uses a level set function, where the level set function $\phi$ at position $x$ and time $t$ is described by $\phi(x, t) > 0$ if $x$ is in fluid 1, $\phi(x, t) = 0$ if $x$ is on the interface, and $\phi(x, t) < 0$ if $x$ is in fluid 2 (Feigl, 2011). One common selection for the level set function uses the distance from the interface as the magnitude of the function and the sign, i.e. $\pm$, is determined by the fluid. This ensures that the gradient vectors across the interface are continuous, which is not imposed by the VoF method.

The theory is developed rigorously by Osher et al. in (Osher and Sethian, 1988), who designed the method to track the propagating interface by using the zero-contour of the level set function. This allows for a precisely defined boundary, which is smoothed in the VoF method. Although the LSM does not inherently conserve mass in its calculations, van der Pijl et al. (van der Pijl et al., 2005) achieved this by borrowing from VoF the concept of tracking volume fraction in the mesh to conserve mass. Furthermore, Osher et al. (Osher and Sethian, 1988) noted that LSM algorithms can be devised to satisfy the entropy condition.
2.2.3 Multiphase simulation in OpenFOAM

For the purpose of analyzing jet breakup behavior, both for prediction of laboratory experiments and further insight into breakup mechanisms and sensitivity, CFD is to be used through a large scope of this project. In particular, the finite volume based Open Source Field Operation and Manipulation (OpenFOAM) will be used. It is an open source CFD software package and C++ toolbox containing a number of two-phase and multiphase fluid solvers (OpenFOAM Foundation, 2011a,b). InterFoam, a two-phase solver in OpenFOAM, and variants thereof use the VoF method in numerically solving two-phase flows. Shu (Shu et al., 2007) has also developed a LSM for OpenFOAM, however, there remains some limitations such as conservation of mass is not enforced.

2.2.4 Spurious currents in multiphase simulations

Conservation of mass and momentum, Eq. (2.1), must hold in each phase and at the interface of the two-phase problem. The reshaping of the interface causes the interfacial tension to change, and therefore has to be accounted for in the momentum equation. Interface compression methods address this by using a transport equation to model the change in momentum. A detailed review of interface compression methods and other multiphase methods is given by (Wörner, 2012).

The VoF method uses the volume fraction, \( \alpha \), of the mesh cells to locate the interface. The motion of the interface is captured using the transport equation:

\[
\frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \nabla \alpha = 0. \tag{2.10}
\]

The contribution of the interfacial tension to the momentum equation is given as follows:

\[
\mathbf{F}_s = \gamma \kappa \delta_s \mathbf{n} = -\gamma \nabla \cdot \left( \frac{\nabla \alpha}{|\nabla \alpha|} \right) |\nabla \alpha|, \tag{2.11}
\]

where \( \mathbf{F}_s \) is the interfacial tension force vector, \( \gamma \) is the interfacial tension, \( \kappa \) is the mean curvature at the interface, \( \mathbf{n} \) is the normal vector of the interface and \( \delta_s \) is the Dirac delta function, which is 1 at the interface and 0 otherwise.

Spurious currents arise from inaccuracies in the calculation of Eq. 2.11, which lead to errors in the momentum equation (Pan et al., 2015). As a consequence of spurious currents, a two-phase simulation in which the viscosity of one phase is much larger than the other, can yield unrealistically high velocities in the low viscous phase. That is, since momentum is not conserved due to spurious currents, additional momentum is sourced into the low viscous phase causing local velocities near the interface to
become unrealistically high. For simulations that employ adaptive time-stepping, the high velocities force the time-step to be reduced in order to maintain low Courant numbers.

Deshpande (Deshpande et al., 2012) names two primary sources for spurious currents: inaccurate calculation of the curvature and the lack of a discrete force balance between the pressure gradient and the surface tension.

The OpenFOAM two-phase solver, interFoam uses the VoF method for interface compression. It is therefore subject to spurious currents. Several approaches have been tried or suggested when spurious currents become problematic:

- The pressure, viscosity and density experience a jump discontinuity at the interface. Ménard (Ménard et al., 2007) used a ghost fluid method (GFM) to reduce spurious currents in the velocity field compared to the continuum surface force (CSF) method. This was included in the coupled level set volume of fluid (CLS-VOF) approach and showed good results.
- The analysis of (Deshpande et al., 2012), showed that mesh refinement leads to more problems. Therefore a possible approach is to locally and temporarily coarsen the mesh to allow velocities to stabilize.
- Wardle (Wardle and Weller, 2013) suggested using the multiphaseEulerFoam solver, which is a multiphase CFD solver for segregated flows. The two phases are solved separately and the momentum is transferred across the interface using a drag force.
- The analysis of (Galusinski and Vigneaux, 2008) showed there are two time scales that must be addressed concerning spurious currents. One time scale is based on density and the other based on viscosity. This was verified by (Deshpande et al., 2012). This suggests that a local time stepping (LTS) method be incorporated into the model to reduce the time steps where spurious currents are a problem.

The occurrence of spurious currents in capillary flows is known to be a potential problem. Addressing this issue in the interFoam solver is an important step in accurately modeling the breakup of liquid filament jets.
3 Filament arc-shape in rotary spraying

3.1 Introduction

The difficulty of spray processing emulsions arises from their sensitivity to fluid mechanical stress, which under standard spray conditions causes the emulsive structure to break down. This in turn causes loss of encapsulation of functional components that drive the need for the emulsive structures in the first place Dubey and Windhab (2013); Dubey et al. (2011); Jafari et al. (2008); Munoz-Ibanez et al. (2015); Rodriguez-Huezo et al. (2004); Soottitantawat et al. (2005).

Rotary spraying of liquids under laminar conditions is one method for handling shear sensitive materials. This spray regime is a jetting regime characterized by low Reynolds and Weber numbers, in which the liquid jet breaks up due to Plateau—Rayleigh instability Ohnesorge (1936); Reitz and Bracco (1986) or what we will refer to as Rayleigh breakup, that is liquid filament breakup due primarily to the effect of surface tension. By maintaining low Reynolds and Weber numbers, the shear stress remains low, thus reducing loss of encapsulation due to nozzle and spraying effects Dubey (2013). Furthermore, the coupling of rotary spraying with Rayleigh breakup of the liquid jet produces droplets having a narrow drop-size distribution with the added benefit that the filament stretching causes filament diameter to reduce, therefore reducing droplet size Schröder and Walzel (1998); Walzel (2010).

Measurements of Rayleigh breakup in rotational systems were taken by Kitamura et al. Kitamura et al. (1977) using a stroboscope and camera. Measurements carried out by Wong et al. Wong et al. (2004) used a high-speed camera. They characterized experiment conditions using the dimensionless Weber (We), Reynolds (Re) and Rossby (Rb) numbers as follows: \(0.5 < \text{We} < 25, 1 < \text{Re} < 1000\) and \(0.2 < \text{Rb} < 4.0\). Partridge et al. Partridge et al. (2005) measured Rayleigh breakup on a pilot scale rotary sprayer with \(1 < \text{We} < 275, 1 < \text{Re} < 1000\) and \(0.13 < \text{Rb} < 4.4\). Gramlich and Piesche Gramlich and Piesche (2012) used a rotating cup sprayer to study Rayleigh breakup behavior with \(5 < \text{We} < 100\) and \(0.001 < \text{Ro} < 10\), where Ro is the rotational number.
A common approach for analyzing the Rayleigh breakup behavior of a liquid filament into droplets is to approximate the liquid filament as an axisymmetric jet, since the curvature of the filament arc is large in comparison to the radius of the filament Ashgriz and Yarin (2011). The axisymmetric jet is then analyzed according to Rayleigh breakup theory Rayleigh (1879); Weber (1931), which has been discussed rigorously by Eggers and Villermaux Eggers and Villermaux (2008), Chandrasekhar Chandrasekhar (2013) and Lefebvre Lefebvre (1989) as well as others. This approach has been employed by a number of authors, including Gramlich and Piesche Gramlich and Piesche (2012), Decent et al. Decent et al. (2002, 2009), Wallwork et al. Wallwork et al. (2002) and Părău et al. Părău et al. (2007) to analyze Rayleigh breakup behavior of liquid filaments formed by rotary spraying under laminar conditions.

Approximating the liquid filament as an axisymmetric jet requires a set of equations defining the trajectory of the liquid filament coupled with conservation of mass and momentum. In particular, the fluid velocity, pressure and filament radius are defined as a function of material properties, boundary conditions and position. In the analysis of Gramlich and Piesche Gramlich and Piesche (2012), Mescher Mescher (2012) and Părău et al. Părău et al. (2007), the formulation is set up in a Lagrangian framework, which after simplifying results in a system of equations in a Frenet-Serret frame of reference containing a tangential component, a principle normal component and a binormal component, the last of which may be zero.

This chapter addresses only the arc-shape and trajectory of the liquid filament, which is jetting from rotary sprayer under laminar conditions. Rather than coupling the conservation equations directly into the model of the fluid trajectory, a force balance is applied to an arbitrary fluid element in a rotating frame of reference. The resulting equations of motion, when translated to an inertial frame of reference, result in a Cartesian formulation of position and velocity for all points along the trajectory.

The goal herein is to establish the performance of this simplified model under experimental conditions. The model was verified using high-speed video capture of an oil-in-water emulsion liquid filament jetting from a laminar rotary sprayer. Image analysis of the liquid filament trajectories shows that the assumptions made in the model are valid under the experimental conditions considered here. Moreover, the arc-shape of the trajectories compares well with those predicted by the model.

### 3.2 Mathematical model

A liquid filament with an initial nozzle speed $w_0$ exits the nozzle of a rotary sprayer with radius of the rotor $r_0$ and constant angular speed $\omega$ as shown in Fig. 3.1. The
shape of the filament curve is determined primarily by a force balance among inertial forces, viscous forces, surface tension, gravity, and wind resistance.

In analyzing the shape of the curve formed by the filament, we assume that the liquid filament behaves as a chain of minuscule liquid segments, where intra-particle forces within the liquid segments do not significantly affect the shape of the curve. In this chain adjacent fluid segments are coupled together by viscous and surface tension forces, which act in the axial direction of the fluid segments. Thus, viscous and surface tension forces are grouped together as the tension vector, denoted by $\mathbf{T}$, which by convention points in the negative tangential direction of the liquid filament.

The analysis is performed in a rotating frame of reference with origin $O$. In the rotating frame of reference centrifugal force and Coriolis force accelerate each filament segment and the remaining force balance remains unchanged. The resulting trajectory of the filament segment is defined as a function of time, $t$, by the position vector $\mathbf{r}(t)$ with arc length $s(t)$ and velocity vector $\mathbf{w}(t)$.

We assume that inertial forces are significantly greater than the force due to gravity, that is, $w_0^2/r_0 \gg g$, where $g$ denotes the acceleration due to gravity. Therefore, the remaining force balance and fluid motion are restricted to the $xy$-plane. The position vector then becomes $\mathbf{r}(t) = (x(t), y(t), 0)^\top$ and the velocity vector becomes $\mathbf{w}(t) = (u(t), v(t), 0)^\top$. Likewise, we assume that wind resistance plays a small role in determining the trajectory. Then the force balance at an arbitrary point, $P$, on the trajectory determines the acceleration $\mathbf{w}'(t)$ of a segment with length $\delta s$ and per
unit length density, $\rho_s$, as follows:

$$\rho_s \delta s \mathbf{w}'(t) = -\rho_s \delta s \mathbf{\omega} \times (\mathbf{\omega} \times \mathbf{r}(t)) - 2\rho_s \delta s \mathbf{\omega} \times \mathbf{w}(t) + \mathbf{T}.$$  \hspace{1cm} (3.1)

The magnitude of the tension depends on the position along the trajectory, which is implicitly defined in terms of time. Furthermore, the tension force vector is parallel with but acting opposite to the velocity. Therefore rewriting Eq. (3.1) in component form, dividing by segment mass, and writing in dimensionless terms results in the parametric form as follows:

$$\ddot{X}(T) = \frac{X(T)}{Rb^2} + \frac{2}{Rb} \dot{Y}(T) - F(T)\dot{X}(T)$$

$$\ddot{Y}(T) = \frac{Y(T)}{Rb^2} - \frac{2}{Rb} \dot{X}(T) - F(T)\dot{Y}(T),$$ \hspace{1cm} (3.2)

where $F(T)$ represents a scaling of the tension forces and the overhead dot represents the derivative $\frac{d}{dT}$. The equation uses the scaling:

$$X = \frac{x}{r_0}, Y = \frac{y}{r_0}, T = \frac{t}{w_0}, \text{Rb} = \frac{w_0}{r_0\omega},$$

where $\text{Rb}$ is the Rossby characteristic number, which represents the ratio of inertial forces to Coriolis force. The dimensionless terms for the arc length, position vector and velocity vector follow from the scaling, which results in:

$$S(T) = \frac{s(t)}{r_0}$$

$$\mathbf{R}(T) = \frac{\mathbf{r}(t)}{r_0} = (X(T), Y(T))^\top$$

$$\mathbf{W}(T) = \frac{\mathbf{w}(t)}{w_0} = (U(T), V(T))^\top,$$

where $U(T)$ and $V(T)$ are the dimensionless velocity components in the x-direction and y-direction, respectively. Since the fluid motion is nonzero only in the xy-plane, the zero-valued $z$-component of all vectors has been omitted in the remainder of the chapter for notational convenience.

Equation (3.2) is an initial value problem with $\mathbf{R}(0) = (\cos \theta, \sin \theta)^\top$ and $\mathbf{W}(0) = (\cos \theta, \sin \theta)^\top$, where the phase angle, $\theta$, represents the angular position of the nozzle exit. After relaxing the tension term, the initial value problem has the closed form solution:

$$X(T) = \frac{T}{Rb} \sin \left(\frac{T}{Rb} - \theta\right) + (T + 1) \cos \left(\frac{T}{Rb} - \theta\right)$$

$$Y(T) = \frac{T}{Rb} \cos \left(\frac{T}{Rb} - \theta\right) - (T + 1) \sin \left(\frac{T}{Rb} - \theta\right),$$ \hspace{1cm} (3.3)
which defines the trajectory of a filament segment in a rotating frame of reference.

In Eq. (3.3) the tension term has been neglected, which implies that the arbitrary filament segment is not bound to adjacent segments as required by a tension encompassing model. Therefore the trajectory defines the equation of motion of a particle exiting the nozzle at time $T = 0$. Furthermore, the particle trajectory in a rotating frame of reference is equivalent to the liquid filament arc-shape in an inertial frame of reference.

The magnitude of the position vector, $R(T)$, represents the radial position of a fluid particle in the rotating frame of reference. Likewise the magnitude of the velocity vector, $W(T)$, represents the speed of a fluid particle. It follows from Eq. (3.3) that $R(T)$ and $W(T)$ are calculated as follows:

$$
R(T) = \sqrt{(T + 1)^2 + \left(\frac{T}{R_b}\right)^2}, \\
W(T) = \sqrt{\left(\frac{T}{R_b}\right)^2 + 1^2 + \left(\frac{T}{R_b}\right)^2}.
$$

Note that both $R(T)$ and $W(T)$ are independent of the initial nozzle angular position.

### 3.2.1 Relation to inertial frame of reference

Using orthogonal transformations, Eq. (3.3) can be rewritten in terms of rotation matrices as follows:

$$
\mathbf{R}(T) = \text{rot} \left( -\frac{T}{R_b} \right) \text{rot}(\theta) \left( T + 1, \frac{T}{R_b} \right)^\top,
$$

where $\text{rot}(\cdot)$ is the two dimensional rotation matrix defined by

$$
\text{rot}(\cdot) = 
\begin{pmatrix}
\cos(\cdot) & -\sin(\cdot) \\
\sin(\cdot) & \cos(\cdot)
\end{pmatrix}.
$$

The form of Eq. (3.5) implies that the solution to the initial value problem with initial conditions $\mathbf{R}(0) = (\cos \theta, \sin \theta)^\top$ and $\mathbf{W}(0) = (\cos \theta, \sin \theta)^\top$ is simply a rotation of the solution to the initial value problem with initial conditions $\mathbf{R}(0) = (1, 0)^\top$ and $\mathbf{W}(0) = (1, 0)^\top$. Moreover, the rotation $\text{rot} \left( -\frac{T}{R_b} \right)$ takes the inertial frame of reference into the rotating frame of reference. Therefore, we can calculate the position of a fluid particle in the inertial frame of reference as follows:

$$
\mathbf{R}_I(T) = \text{rot}(\theta) \left( T + 1, \frac{T}{R_b} \right)^\top,
$$

where the subscript $I$ is to denote the inertial frame of reference.
The inertial velocity vector, \( \mathbf{W}_I(T) \), is defined as the derivative of \( \mathbf{R}_I(T) \), which is linear in \( T \). As a result the inertial velocity vector is independent of \( T \) so that \( \mathbf{W}_I(T) = \mathbf{W}_I \), which yields:

\[
\mathbf{W}_I = \text{rot}(\theta) \left( 1, \frac{1}{\text{Rb}} \right)^\top.
\] (3.7)

Eq. (3.7) implies that the inertial velocity of a fluid particle maintains a constant magnitude, \( W_I = \sqrt{1 + 1/\text{Rb}^2} \). Furthermore, the direction of travel is determined entirely by the nozzle angular position and the Rossby characteristic number. This results in a direction given by the angle \( \theta + \beta_0 \), where \( \beta_0 = \arctan(1/\text{Rb}) \).

Furthermore, the position of a fluid particle in the rotating frame of reference can be written in terms of its inertial position as follows:

\[
\mathbf{R}(T) = \text{rot} \left( -\frac{T}{\text{Rb}} \right) \mathbf{R}_I(T).
\] (3.8)

The relation between the inertial frame of reference and the rotational frame of reference is summarized in Fig. 3.2.
3.2.2 Comparison to a Frenet-Serret frame of reference

The Frenet-Serret frame of reference defines a vector space in terms of the tangential direction, principle normal direction and binormal direction and is useful for describing a particle trajectory or a curve in terms of its tangential velocity, curvature and torsion. If the curve remains in a two-dimensional plane, as is assumed in this analysis, then the torsion term is zero and the Frenet-Serret frame of reference requires two equations, one to describe tangential motion and one to describe motion in the principle normal direction, in order to sufficiently describe a trajectory.

Gramlich and Piesche (2012) develop the differential equations defining the liquid jet trajectory in a Frenet-Serret frame of reference resulting in the tangential equation and the normal equation. In these equations $\kappa$ is the curvature of the trajectory and $\alpha$ is the angle of incidence of a line extending from the center of rotation to the filament, as described therein and shown in Fig. 3.2.

In order to compare the equations in the Frenet-Serret frame of reference to our model, we write the rotational number, $\text{Ro} = \frac{1}{Rb^2} \frac{a_0}{r_0}$, in terms of the Rossby number, where $a_0$ is the initial filament radius. Moreover, the $\sin \alpha$ relates to $R$, $S$, $T$ and $W$ as follows:

$$\sin \alpha = \frac{dR}{dS} = \frac{1}{W} \frac{dR}{dT}.$$  

By neglecting viscous forces, surface tension forces and wind resistance, the tangential equation simplifies to

$$W \frac{dW}{dS} - \frac{R}{Rb^2} \frac{dR}{dS} = 0.$$  

After applying the boundary values: $S = 0$, $R = 1$, $W = 1$, the equation further reduces to

$$W^2 - \frac{R^2}{Rb^2} = 1 - \frac{1}{Rb^2}. \quad (3.9)$$  

Likewise, the normal equation reduces to

$$W^2 \kappa + \frac{R}{Rb^2} \cos \alpha - \frac{2W}{Rb} = 0. \quad (3.10)$$

The results of the inertial trajectory formulation, Eq. (3.3), are substituted into the above tangential and normal equations to show that they are equivalent solutions.
3 Filament arc-shape in rotary spraying

After substitution into Eq. (3.9), the tangential equation becomes

$$W^2 - \frac{R^2}{Rb^2} = \left( \dot{X}^2 + \dot{Y}^2 \right) - \frac{X^2 + Y^2}{Rb^2}$$

$$= \left( 1 + \frac{2T}{Rb^2} + \frac{T^2}{Rb^4} + \frac{T^2}{Rb^4} \right) - \left( \frac{1}{Rb^2} + \frac{2T}{Rb^2} + \frac{T^2}{Rb^2} + \frac{T^2}{Rb^4} \right)$$

$$\equiv 1 - \frac{1}{Rb^2}.$$

The normal equation requires that we first resolve $\kappa$ and $\cos \alpha$, which after simplification yields:

$$W^3 \kappa = |\dot{X}\dot{Y} - \dot{Y}\dot{X}|, \quad WR \cos \alpha = |\dot{X}Y - \dot{Y}X|.$$

The former simplification results from the calculation of curvature, where the derivatives of $X(T)$ and $Y(T)$ are with respect to $T$. The latter simplification uses the relationship $\sin \alpha = \frac{1}{W} \frac{dR}{dT}$, so that $WR \sin \alpha = R \frac{dR}{dT}$.

Multiplying Eq. (3.10) by $RbW$ and substituting Eq. (3.3) into it yields:

$$RbW^3 \kappa + \frac{WR}{Rb} \cos \alpha - 2W^2$$

$$= Rb \left| \dot{X}\dot{Y} - \dot{Y}\dot{X} \right| + \frac{1}{Rb} \left| \dot{X}Y - \dot{Y}X \right| - 2W^2$$

$$= \left( 2 + \frac{2T}{Rb^2} + \frac{T^2}{Rb^2} + \frac{T^2}{Rb^4} \right) + \left( \frac{2T}{Rb^2} + \frac{T^2}{Rb^2} + \frac{T^2}{Rb^4} \right)$$

$$- 2 \left( 1 + \frac{2T}{Rb^2} + \frac{T^2}{Rb^2} + \frac{T^2}{Rb^4} \right)$$

$$\equiv 0.$$

3.3 Experimental details

The measurement test-stand was set up according to Fig. 3.3. The emulsion used was a 30%wt oil-in-water (O/W) single emulsion with the dispersed phase composed of sunflower oil. The continuous phase was composed of 89.3%wt water and 8.9%wt Polyethylene glycol. The surfactant tween-20 was included in the continuous phase at 1.8%wt before mixing. The mean drop size of the dispersed phase was 11 $\mu$m.

The zero shear viscosity of the fluid, $\eta_0$, was measured to be 0.06 Pa.s. Although the fluid was shear-thinning, the shear rates in the experiments remained in the zero shear rate regime. Therefore, the fluid was treated as Newtonian. The surface tension, $\gamma$, was estimated to be 0.04 N/m. This value was the result of the surface tension measurement of a similar 40%wt O/W emulsion, in which the continuous and dispersed phases were identical except for the greater mass fraction of the dispersed phase. The fluid density, $\rho$, was calculated based on mass ratios to be 980 kg/m$^3$. 

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Further details of the experiment setup including preparation of the O/W emulsion can be found in Dubey Dubey (2013).

The rotary spray nozzle was configured with two spray nozzles mounted opposite each other on the rotor, each with an orifice diameter of 0.3 mm. The diameter of the rotor measured as the distance from nozzle exit to opposite nozzle exit was 68.55 mm, thus the corresponding radius, $r_0$, is 34.28 mm.

A high-speed camera, Memrecam fx RX-6, was secured to a 3-axis platform and positioned normal to the plane formed by rotary spraying. The camera was focused so that the liquid filament was captured in the camera field of view. The field of view was illuminated from the front using eight 100 watt xenon bulbs, which provided sufficient lighting for the high rate of image capture. An initial video capture of a millimeter scale was taken with a frame rate of 5000 frames per second (fr/s), which corresponds to an image size of 512 pixels wide $\times$ 500 pixels high. The resulting image was used to determine the size of an individual pixel to be 56.2 $\mu$m $\times$ 56.2 $\mu$m.

The data from two experiment conditions are presented here. The first set of conditions was a near-nozzle measurement, labeled RA08, in which the high-speed camera was positioned, such that the nozzle was visible within the camera field of view. Under these conditions the high-speed camera recorded at a frame rate of 5000 fr/s, yielding an image field of view of 512 pixels $\times$ 500 pixels high. The rotational speed of the motor was adjusted to approximately 1000 rpm in the counterclockwise direction with respect to the camera. The actual rotational speed was later determined.
Table 3.1: Geometry and material properties for high-speed video capture of a liquid filament exiting a rotary spray nozzle (top). Experiment specific conditions for near-nozzle (RA08) and remote-nozzle (RA20) measurements (bottom).

<table>
<thead>
<tr>
<th>Experimental conditions</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rotor radius to nozzle exit, $r_0$ (mm)</td>
<td>34.3</td>
</tr>
<tr>
<td>Nozzle orifice diameter, $2a_0$ (mm)</td>
<td>0.3</td>
</tr>
<tr>
<td>Pixel size ($\mu$m/px)</td>
<td>56.2</td>
</tr>
<tr>
<td>Dimensionless pixel size (px$^{-1}$)</td>
<td>$1.64 \times 10^{-3}$</td>
</tr>
<tr>
<td>Zero shear viscosity, $\eta_0$ (Pa s)</td>
<td>0.06</td>
</tr>
<tr>
<td>Surface tension, $\gamma$ (N/m)</td>
<td>0.04</td>
</tr>
<tr>
<td>Liquid density, $\rho$ (kg/m$^3$)</td>
<td>980</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RA08</th>
<th>RA20</th>
</tr>
</thead>
<tbody>
<tr>
<td>5000</td>
<td>6000</td>
</tr>
<tr>
<td>1026</td>
<td>1026</td>
</tr>
<tr>
<td>2.0</td>
<td>4.0</td>
</tr>
<tr>
<td>2.5</td>
<td>4.5</td>
</tr>
<tr>
<td>3.68</td>
<td>3.68</td>
</tr>
</tbody>
</table>

using high-speed video capture of several revolutions of the rotary spray nozzle. The average time measured for one complete revolution of nozzle resulted in a rotational speed of 1026 rpm, which corresponds to an angular speed of $\omega = 107.4$ rad/s. The supply pump was adjusted, such that a pressure of 2.0 bar was maintained at the inlet of the rotary sprayer while rotating. An inline flow meter was used to determine the average flow rate of 21 mL/min, which computes to an estimated mean fluid velocity, $\bar{w}_0$, of 2.5 m/s exiting radially at the nozzle exit.

The second set of conditions was a remote-nozzle measurement, labeled RA20, in which the nozzle position was not visible within the high-speed camera field of view. The procedure for controlling the experiment conditions was the same as with the near-nozzle measurement. The high-speed camera recorded at a frame rate of 6000 fr/s, yielding an image field of view of 512 pixels $\times$ 384 pixels high. The rotational speed was adjusted to 1000 rpm and later measured to be 1026 rpm. The supply pump was adjusted, so that a pressure of 4.0 bar was maintained at the inlet. The flow rate measured 38 mL/min, resulting in an estimated mean nozzle exit velocity of 4.5 m/s.

The experimental conditions are summarized in Table 3.1.
3.4 Results and discussion

3.4.1 Near-nozzle analysis of the liquid filament

The near-nozzle measurements, labeled RA08 in Table 3.1, resulted in the video capture of 38 consecutive frames displaying the liquid filament. An image composed by superimposing these 38 consecutive frames of video capture of the counterclockwise rotating nozzle is shown Fig. 3.4. The composite image is ordered, such that the rightmost liquid jet represents the liquid jet captured in the first video frame and each adjacent liquid jet corresponds to the next video frame. The image has been scaled to a non-dimensional length scale using the pixel scaling of $1.64\times10^{-3}$ px$^{-1}$.

In observing the composite image, the development of Rayleigh disturbances and eventual Rayleigh breakup are highly visible. Rayleigh disturbance can be recognized...
Figure 3.5: Near-nozzle composite image, where the white lines in the image trace visible Rayleigh disturbances by an optical trough traveling from lower right to upper left in the image, where the optical trough is the result of a thinning of the light-gray liquid filament allowing the dark background to become more visually dominant.

The composite image enables one to visually trace the Rayleigh disturbances backward to the start of their formation, as shown by the white lines in Fig. 3.5. Tracing several disturbances back to their formation leads to three important observations: (i) the Rayleigh disturbances are propagating in a line across the composite image, (ii) the formation of Rayleigh disturbances can be recognized a short distance after nozzle exit, and (iii) the lines formed by tracing Rayleigh disturbances fan out from right to left.

According to Keller Keller et al. (1973), Rayleigh disturbances travel with the fluid at the same speed as the fluid. Hence they provide a tracking mechanism for measuring fluid velocity. Consequently, a Rayleigh disturbance propagating linearly through the composite image implies that the disturbance, in addition to the fluid surrounding
the disturbance, are moving at a constant velocity and are not accelerating. It follows from observation (i) above that the fluid surrounding the Rayleigh disturbances experiences zero acceleration, that is, it can be assumed that net forces surrounding the Rayleigh disturbances are zero.

The lines in Fig. 3.5 begin in the lower right at the visible start of the Rayleigh disturbance\(^1\) and follow the disturbances as they progress to the upper left. A measurement to observation (ii) above estimates the first Rayleigh disturbance appearing at 2.5 mm from the nozzle exit. It is therefore reasonable to set a bound on distance from the nozzle, above which inertial forces surrounding a Rayleigh disturbance are dominant.

The fanning behavior observed when tracing the disturbances from right to left further demonstrates that the liquid filament is acting as a sequence of distinct fluid particles with each particle traveling on its own constant-velocity path. The speed and direction of the particle can only be constant once the net force acting on the particle is effectively zero.

The spacing between two adjacent liquid jets in Fig. 3.4 remains constant along the length of the jet and across all jets. This implies that the fluid particles are not accelerating in a direction normal to the filament and additionally the magnitude of the normal velocity is constant across all particles.

In the tangential direction of the liquid filament local acceleration of fluid particles can be observed. In particular where the Rayleigh disturbances grow and lead to detachment. At this point the surface tension forces dominate locally and cause the ends of the detached filament to pull together and form a droplet. However, based on observation (i), the local behavior is not significant enough to affect the arc-shape of the liquid jet as a whole.

From the three observations above we conclude that the Rayleigh disturbance lines trace the path of a fluid particle in the inertial frame of reference. Moreover, since the rotational speed and pixel size are known, it is possible to calculate the inertial velocity of a fluid particle along a disturbance line as discussed in the following subsection.

**Velocity components**

The image results in Fig. 3.4 can be used to validate the model described in Section 2 by comparing the liquid filament trajectory in this image with the trajectory predicted

\(^1\)The visible start of the Rayleigh disturbances were taken as viewed from the unscaled composite 512 pixel × 500 pixel image on the computer screen, which may not reflect what is visible in the displayed figure.
Table 3.2: Analysis results of high-speed video capture of a liquid filament exiting a rotary spray nozzle for near-nozzle (RA08) and remote-nozzle (RA20) measurements.

<table>
<thead>
<tr>
<th>Analysis results</th>
<th>RA08</th>
<th>RA20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nozzle exit speed, $w_0$ (m/s)</td>
<td>2.72</td>
<td>5.49</td>
</tr>
<tr>
<td>Rotor X-coordinate, $X_0$</td>
<td>1.04</td>
<td>0.27</td>
</tr>
<tr>
<td>Rotor Y-coordinate, $Y_0$</td>
<td>-0.94</td>
<td>-1.41</td>
</tr>
<tr>
<td>Initial phase angle, $\theta_0$ ($^\circ$)</td>
<td>102.8</td>
<td>78</td>
</tr>
<tr>
<td>Phase angle rate, $\Delta\theta$ ($^\circ$/fr)</td>
<td>1.23</td>
<td>1.03</td>
</tr>
<tr>
<td>Rossby number, $R_b$</td>
<td>0.74</td>
<td>1.49</td>
</tr>
<tr>
<td>Reynolds number, $Re$</td>
<td>7</td>
<td>13</td>
</tr>
<tr>
<td>Weber number, $We$</td>
<td>27</td>
<td>110</td>
</tr>
<tr>
<td>Froude number, $Fr$</td>
<td>22</td>
<td>90</td>
</tr>
</tbody>
</table>

by Eq. (3.3). To do so, a more accurate value of the nozzle exit radial speed $w_0$ is needed, since the estimated mean fluid speed $\bar{w}_0$ of 2.5 m/s is not sufficiently accurate.

It follows from the above results that the speed of a fluid particle in the inertial frame of reference, $w_I$, can be calculated from a disturbance line. Selecting the two points, highlighted with open circles in Fig. 3.5, the Rayleigh disturbance travels 538 pixels in 33 frames giving a value for $w_I$ of 4.6 m/s.

As a result of Eq. (3.7) and dimensional scaling, $w_I$ relates to nozzle exit speed, $w_0$, and the speed of the nozzle tip, $r_0\omega$, as follows:

$$w_I^2 = w_0^2 + r_0^2 \omega^2. \quad (3.11)$$

Applying $w_I$ and the nozzle tip speed of 3.68 m/s yields a better estimate for $w_0 = 2.72$ m/s. This result in turn yields a Rossby number, $R_b = 0.74$, which indicates that both the Coriolis force and inertial forces play a role in determining the filament arc-shape. This value of the Rossby number is in agreement with Partridge et al. (2005); Wong et al. (2004) as discussed in Section 3.1.

Using $w_0$ as the characteristic velocity and the nozzle radius, $a_0 = 0.15$ mm, as the characteristic length, the resulting Reynolds number, $Re = \rho w_0 a_0 / \eta$, and Weber number, $We = \rho w_0^2 a_0 / \gamma$ are 7 and 27, respectively. These values are summarized in Table 3.2 along with $R_b$ and $w_0$. 

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3 Filament arc-shape in rotary spraying

Center of rotation for near-nozzle analysis

Analysis of the filament trajectory requires that a coordinate system be assigned to the image capture window, where the center of rotation of the rotary sprayer is accurately placed at the origin. However, since the field of view of the high-speed camera is limited, the center of rotation is not visible in any image capture of the filament trajectory. A method is presented here, which utilizes the slope of the tangent line for each filament trajectory to produce an arc of constant radius. The center of rotation relative to the image capture window is then determined from the arc of constant radius.

A diagram representing the non-dimensional positioning of the image capture window relative to the center of rotation is shown in Fig. 3.6. In this diagram the center of rotation is given as \((X_0, Y_0)\) and the position of the nozzle exit is represented by the arc, which is scaled to have radius 1 for the non-dimensional problem. The liquid filaments are separated by a change in phase angle, \(\Delta \theta = \omega / \text{rate}\), which represents the change in rotor angular position from one image frame to the next. The tangential angle, \(\phi\), is defined as the arctangent of the slope of tangent line, where the slope of the tangent line is determined by the filament derivative.

If the filament trajectories in the image frames vary from one another only as simple rotation about the fixed point \((X_0, Y_0)\), then their rotation angle must be \(i \Delta \theta\), where \(i\) represents the number of image frames of separation between two filaments and thus represents the number of rotations applied to align two filaments. Furthermore, it follows that the location where \(\phi_i = \phi_0 + i \Delta \theta\) will be the same distance from \((X_0, Y_0)\), \(i.e.,\) a constant radius from \((X_0, Y_0)\). In order to have the tangential angle available for calculation, an interpolation or best-fit polynomial is necessary for each filament. Repeating calculations for each filament yield an arc of constant radius, from which the coordinates of the center of rotation can be calculated.

The process diagramed by Fig. 3.6 for calculating the origin using tangent angles is summarized as follows:

1. Beginning with the individual video frames, each containing only one liquid filament, scale to non-dimensional coordinates.
2. Calculate a best-fit quadratic polynomial for each liquid filament, enabling the tangent angle, \(\phi\), to be calculated at every point along each filament.
3. Select a point on a filament toward the center of the capture window and record its position as \((x_0, y_0)\) and its tangent angle as \(\phi_0\).
4. Determine for each filament in the capture window the location, \((x_i, y_i)\), such that \(\phi_i = \phi_0 + i \Delta \theta\).
5. Perform a least squares fit, optimized to \(X_0 - x_i = r \cos(i \Delta \theta)\) and \(Y_0 - y_i = r \sin(i \Delta \theta)\).
Figure 3.6: Conceptual diagram demonstrating the calculation of the origin by matching the slope of the tangent line. The open circles indicate the advancing tangent angle, $\phi_i$, which lie on a circular arc.
6. Shift the coordinate system of the image capture window by \((-X_0, -Y_0)\), thus forcing the center of rotation to be located at the origin, \((0, 0)\).

This method fails if the filaments in the capture window are no longer rotationally symmetric, more specifically, the method fails if the best-fit filament curves do not lead to an accurate calculation of the locations \((x_i, y_i)\).

This methodology has been applied to the RA08 experiment as shown in Fig. 3.7. The thinner black curves, running primarily vertically represent the best-fit quadratic curves for each filament. The open circles represent the calculated positions \((x_i, y_i)\) corresponding to the target value of each \(\phi_i\). The data points on the left-hand filaments and right-hand filaments have been excluded, since the assumption that they are rotationally symmetric does not hold in this region. The positional data result in the best fit circle with center \((X_0, Y_0) = (1.04, -0.94)\) and radius 1.37 as denoted by the heavy black line. The center of rotation is included in Table 3.2.

Following the positional calculation of the center of rotation, the image capture window was translated so that the new center of rotation is at \((0, 0)\). The initial phase angle, \(\theta_0\), was optimized for angular position of the nozzle of the first filament resulting in \(\theta_0 = 103^\circ\). The phase angle, \(\theta_i\), of any subsequent filament was calculated according to \(\theta_i = \theta_0 + (i - 1)\omega/f_{\text{rate}}\), where \(i\) is the frame number and \(f_{\text{rate}}\) is the frame rate of 5000 fr/s. Filament trajectories, which were generated using Eq. (3.3), were placed over the composite image for comparison as shown in Fig. 3.8. For clarity purposes, only seven trajectories were displayed, however the fitting characteristics of the omitted trajectories are in agreement with the represented trajectories.

Good alignment has been achieved though the middle of the image. This is expected, since the best-fit arc was optimized through the middle of the image. The model matches very closely on the right half of the image, where the nozzle is close. This serves a good validation of the model. The model deviates slightly from the filament in the bottom left region. However, the nozzle is already a large distance from the field of view as the filament enters the image. Farthest from the nozzle at the top of the image as magnified in Fig. 3.9, the trajectory alignment deviates by approximately 1 mm from the measured filament. The deviation of the trajectory from the measurement is primarily caused by two factors, the influence of non-inertial forces and measurement error, specifically sensitivity to measurement error.

Non-inertial forces, *e.g.* viscous forces, surface tension and wind resistance, are in reality nonzero. Therefore, using an inertial-only model to fit the data will lead to a non-perfect fit. The degree of influence viscous forces and surface tension have on the quality of fit depends on the material properties of the liquid. The influence wind resistance has on the overall fit depends on the inertial speed of the liquid in addition to material properties of both the liquid and surrounding air Kitamura and Takahashi (1976); Nonnenmacher and Piesche (2004).
Figure 3.7: A sequence of best-fit curves of the filament image data from experiment RA08. The open circles, whose positions are calculated from the best-fit curves, indicate where the tangent angle advances. A best-fit circular arc to these positions results in an arc of radius 1.37 and center \((X_0, Y_0) = (1.04, -0.94)\), yielding the center of rotation.
Figure 3.8: Near-nozzle composite image, where the orange curves are the computed trajectories.
Figure 3.9: The enlargement indicated by the square in the near-nozzle composite image. The axes have been scaled to milimeters to indicated absolute dimensions.
Measurement error and sensitivity to measurement error is likely to play a bigger role in the quality of fit. The position of a fluid particle at some distance after the nozzle exit is highly sensitive to the determined center of rotation and starting angle of the nozzle. The calculation of center of rotation and nozzle exit are, in turn, sensitive to accuracy of the image scale, the correctness of the Rossby number, etc., and still remains an approximation thereof.

Nevertheless, the quality of fit shows good overall agreement between the model and measurement data. It is therefore a useful means for calculating values of quantities not directly or accurately available from the measurement, e.g. Rayleigh breakup length and fluid velocities, both in an inertial frame and a rotating frame of reference.

3.4.2 Remote-nozzle analysis of the liquid filament

The remote-nozzle measurements, labeled RA20 in Table 3.1, resulted in an image composed of the superposition of 39 consecutive frames of the video capture of a liquid filament exiting a rotary sprayer as shown in Fig. 3.10. The image scaling remains the same, using a scale factor of $1.64 \times 10^{-3}$ px$^{-1}$ to produce a non-dimensional image.

In the composite image several Rayleigh disturbances have been traced and are highlighted by white lines shown in Fig. 3.11. The Rayleigh disturbance lines exhibit the same qualitative behavior as those in the near-nozzle composite image. Therefore, following the same reasoning, the inertial forces dominate and determine the arc-shape of the liquid filament.

The inertial speed is calculated for each of the Rayleigh disturbance lines shown in Fig. 3.11 and their average yields $w_I = 6.61$ m/s. Using Eq. (3.11) the resulting nozzle exit speed is $w_0 = 5.49$ m/s and Rossby number is $Rb = 1.49$. The resulting Reynolds number and Weber number are 13 and 110, respectively. These data are listed in Table 3.2.

Center of rotation for remote-nozzle analysis

The first method for locating the center of rotation of the rotary sprayer requires a rotational symmetry about the point $(X_0, Y_0)$, since the calculated location of each $\phi_i$ is sensitive to the curve fit to the liquid filament. Thus, if the liquid filaments in the field of view are no longer rotational transformations of one another, then the first method for finding the center of rotation will be inaccurate. To handle this situation a second, more robust albeit less accurate, method that locates the center
Remote-nozzle trajectories with non-dimensional scaling

Figure 3.10: Remote-nozzle image sequence displayed as a superposition of 39 video frames scaled to non-dimensional coordinates. The time sequence moves from right to left.
Figure 3.11: Remote-nozzle composite image, where the white lines in the image trace visible Rayleigh disturbances and the white circles indicate measured positions at the intersection between filament and disturbance line.
Consider the simplified diagram of a rotary sprayer as shown in Fig. 3.12, where the center of rotation is specified by \((X_0, Y_0)\) and the arc with radius 1 represents the nozzle exit in a non-dimensional coordinate system. The darkened rectangle represents the image capture window containing the composite image of superimposed liquid filaments represented by the dotted curves. The darkened lines represent the visible Rayleigh disturbances and the points, \(pt_1\) through \(pt_4\), represent known pixel coordinates, which lie on the Rayleigh disturbance lines.

Suppose the composite image of superimposed liquid filaments displays Rayleigh disturbances traveling in straight lines. Then, as already asserted, the disturbance lines represent motion of a fluid particle in the inertial frame of reference and inertial forces acting on the fluid particle dominate. If we assume that the inertial forces continue to dominate as the fluid particle is traced back to the nozzle, then the Rayleigh dis-
turbance lines can be extended to pass through the position of the nozzle exit as demonstrated by extending the line formed from $pt_1$ to $pt_2$ downward to the nozzle. Furthermore, the line formed from $pt'_1$ to $pt'_2$ will extend through $(X_0, Y_0)$, as will the line formed from $pt'_3$ to $pt'_4$. Therefore, the intersection of these two lines will locate the center of rotation. It remains to discuss how the shifted points, $pt'$, are calculated.

After nozzle exit a fluid particle has a known direction of travel given by the angle $\theta + \beta_0$ as discussed in Subsection 3.2.1. Therefore a rotation of the Rayleigh disturbance line by $-\beta_0$ and scaling it to a magnitude of 1 will define the shifting calculation. This results in a formula for the shifted positions, $pt'$, as follows:

$$pt'_i = pt_i + \left( \frac{pt_j - pt_i}{\|pt_j - pt_i\|} \right) \mathbf{rot}^\top (-\beta_0)$$

$$pt'_j = pt_j + \left( \frac{pt_j - pt_i}{\|pt_j - pt_i\|} \right) \mathbf{rot}^\top (-\beta_0),$$

where the $\|\cdot\|$ operator is the magnitude, $pt_i$ represents the point on the disturbance line farther from the nozzle exit and $pt_j$ represents the closer of the two.

Since $\sin \beta_0 = 1/\sqrt{1 + Rb^2}$ and $\cos \beta_0 = Rb / \sqrt{1 + Rb^2}$ the equation simplifies to:

$$pt'_i = pt_i + \frac{1}{\sqrt{1 + Rb^2}} \left( pt_j - pt_i \right) \begin{pmatrix} Rb & -1 \\ 1 & Rb \end{pmatrix},$$

(3.12)

where the same calculation applies to $pt_j$.

Using Eq. (3.12) the center of rotation can, therefore, be estimated by the intersection of two or more of the translated disturbance lines. This leads to a process for determining the center of rotation from the scaled non-dimensional image as follows:

1. Draw two Rayleigh disturbance lines on opposing sides of the image capture window.
2. Calculate a known start point and end point for each of the Rayleigh disturbance lines, where the end point lies closer to the center of rotation.
3. Translate each Rayleigh disturbance line using Eq. (3.12).
4. Calculate the intersection of the translated disturbance lines. This value represents $(X_0, Y_0)$, the center of rotation.
5. Translate the coordinate system of the image capture window by $(-X_0, -Y_0)$, thus forcing the center of rotation to be located at the origin, $(0, 0)$. 

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Figure 3.13: Overlay of the remote-nozzle model particle paths onto the composite image with image coordinates adjusted by $(-0.27, 1.41)$ so that the center of rotation lies at the origin.

This method has been applied to intersect all the disturbance lines displayed in Fig. 3.11. The mean average of all calculated center of rotations gave an initial estimate of $(0.22, -0.96)$. Particle paths based on center of rotation and Rossby number were plotted and superimposed over Fig. 3.10 to verify the calculation of $(X_0, Y_0)$. A manual adjustment of the center of rotation was required to improve the alignment of particle paths with the Rayleigh disturbance lines. The particle paths best aligned with the composite image are shown in Fig 3.13 and correspond to a center of rotation located at $(X_0, Y_0) = (0.27, -1.41)$.

A plot of filament trajectories is superimposed onto the translated composite image and shown in Fig. 3.14. In the figure the $\theta_0$ parameter was optimized, such that the model trajectory intersected with the liquid jet image at $(0, 1.4)$, resulting in a value of $\theta_0 = 78^\circ$, which is listed in Table 3.2 along with the center of rotation.

Figure 3.14 demonstrates a good qualitative agreement between remote-nozzle model fit and the composite image. The fit nearest the nozzle matches the image data most closely. This is in part because the value $\theta_0$ was optimized to result in a best fit nearest the nozzle. The model deviates more significantly with an increase in distance from the nozzle exit in comparison to the near-nozzle fit. This is to be expected, since we demonstrated in the near-nozzle fit that the quality of fit decreases with distance from...
Figure 3.14: Overlay of the remote-nozzle model trajectories onto the composite image, where the center of rotation lies at the origin. The orange curves are the computed trajectories.
the nozzle exit. One notable difference in the remote-nozzle fit is that the curvature of the model trajectories deviates more significantly from the image data. This is likely caused by the effects from wind resistance.

Overall, the model does a good job representing the image data, thereby making quantities available, which are not directly available from the initial measurements. The Rayleigh breakup length is of particular interest for the remote-nozzle measurements, since more droplets appear in this regime in comparison to near-nozzle measurements.

### 3.4.3 Horizontal rotational axis

In a more practical application of the rotational sprayer, the rotational axis would be vertical. However, in order to protect the high-speed camera in our study, a bench top design with a horizontal rotational axis was used as shown in Fig. 3.3. This arrangement eliminated the problem of fluid raining down on the camera and allowed for the mathematical model to be described in a 2-dimensional plane.

If gravity is included in the model and the tension term remains neglected, then Eq. (3.2) using a horizontal rotational axis becomes:

\[
\ddot{X}(T) = \frac{X(T)}{R_b^2} + \frac{2}{R_b} \dot{Y}(T)
\]

\[
\ddot{Y}(T) = \frac{Y(T)}{R_b^2} - \frac{2}{R_b} \dot{X}(T) - \frac{1}{Fr},
\]

(3.13)

where \(Fr = \frac{w_0^2}{rg}\) is the Froude number and \(g\) is the acceleration due to gravity. For the respective RA08 and RA20 measurements the resulting Froude number calculations were \(Fr = 22\) and \(Fr = 90\). In each case there was negligible difference between the results of Eq. (3.3) and the solution to Eq. (3.13) when superimposed over the images. The solutions were in agreement regardless of the nozzle angular position, \(\theta\), given as an input condition. Therefore, the Froude number was large enough to neglect and Eq. (3.3) can be used to model the filament arc-shape.

Further justification for using Eq. (3.3) comes from tracing the Rayleigh disturbances. If gravitational forces were significant, this would be visible in the composite image. In particular, the Rayleigh disturbances would not move at a constant velocity in the composite image. Either the spacing would change, or the path would no longer be a straight line, or both. Since the Rayleigh disturbances are moving at a constant velocity, Eq. (3.3) can be used to model the filament arc-shape.
3.5 Summary and outlook

Using a composite image created from high-speed video capture of a liquid filament jetting from a rotary sprayer under laminar conditions, we were able to demonstrate that Rayleigh disturbances can act as a tracer in determining fluid velocity within the filament. Since the disturbances were moving in straight lines across the image, we could conclude that inertia dominates the shape of the filament curve. Moreover, though important to Rayleigh breakup of a liquid filament, the viscosity, surface tension and wind resistance are significantly less important in determining the arc-shape of the liquid filament under these conditions.

A mathematical model was developed in a rotating frame of reference using the balance of Coriolis, centrifugal and tension forces. When viscosity, surface tension and wind resistance are neglected, the arc-shape of the liquid jet is based entirely on the Rossby characteristic number. Applying this model to a composite image of near-nozzle high-speed camera data showed a close match, which further supports that viscosity, surface tension and wind resistance can be neglected from the model defining arc-shape of the liquid filament under the conditions of this experiment.

In the general case, the tension term from Eq. (3.2) may not necessarily be insignificant. If this is the case, it would be visible in the composite image, since the zero net force assumption would not hold. That is, the Rayleigh disturbances would no longer travel in a straight line at a constant speed in the composite image. In such a case it would be necessary to include additional terms to the dimensionless equation, Eq. (3.2). That is, if surface tension were to play a role, there would be a term containing the Weber number, We, and if viscous forces were to play a role, there would be a term containing the Reynolds number, Re. In particular, the models of Gramlich Gramlich and Piesche (2012) and Părău Părău et al. (2007) could be readily adapted to Eq. (3.2), which demonstrates the flexibility of our modeling approach.

The model agreed well with a composite image of remote-nozzle high-speed camera data, thereby indirectly making data, such as fluid velocity and Rayleigh breakup length, available that are not directly available from the measurements. One can therefore eliminate the use of tracer particles to determine fluid velocity. Moreover, since the resolution high-speed cameras are presently a limiting factor, one can study high-speed video of the Rayleigh breakup regime without the center of rotation being included in the camera’s field of view.

The presented model greatly simplifies the equations defining arc-shape of the liquid filament jetting from a rotary sprayer. It applies only when viscous forces, surface tension and wind resistance can be neglected, as is the case in this study. It remains to be determined how far the model can be applied beyond the conditions considered here; in particular, if the model can be applied to the entire laminar rotary spraying
3 Filament arc-shape in rotary spraying

regime. A possible approach to this end could be a comparison with the models of Gramlich Gramlich and Piesche (2012) and Părău Părău et al. (2007).
4 Video analysis of liquid filament breakup from rotary spraying

4.1 Introduction

The Rayleigh breakup of laminar rotary jets is of interest, since experiments show that shear sensitive materials preserve structure under these gentle conditions (Dubey, 2013). It is known that a rotational device coupled with Rayleigh breakup offers the advantage of a narrow drop-size distribution and a reduced drop size as the result of filament stretching (Schröder and Walzel, 1998; Walzel, 2010).

The pressure driven RRBN was developed in order to capitalize on the above-mentioned structure preserving quality, while maintaining a narrow drop-size distribution and offering a smaller drop size through filament stretching compared to the Rayleigh breakup of an unstretched jet. The problem remains as to how to optimize the device in terms of rotational speed and flow rate for optimum drop size and drop size distribution. This requires a method for measuring the spray drop size in a rotational system.

The spray drop size distribution in a standard system can be analyzed using a spray particle size analyzer (PSA), such as the Malvern Spraytec. Such systems apply laser diffraction on a spray plume to analyze the particle sizes. In a standard setup the PSA is positioned such that the spray plume is centered at the cross section of the applied laser beam, which optimizes the amount of drops entering the measurement field of the PSA. This method works well for a motionless spray device, such as a standard gas-assisted atomizer.

In our experiment an attempt was made to measure the drop size distribution using the Malvern Spraytec. Since the spray nozzles are rotating in the RRBN, there was no possibility of centering a PSA onto a spray plume. The number of drops crossing the measurement field was limited to at most only a few drops per nozzle per revolution. In general, there were not enough drops crossing the measurement field to register a measurement.

We therefore used high-speed videography as a method for determination of spray drop sizes at different operating conditions when using the RRBN. This chapter discusses the image processing techniques to detect and identify spray drops. The
results of these drop size data are then compared to operating conditions of the RRBN to gain insight into the spray breakup behavior of a rotary liquid jet under Rayleigh breakup conditions.

### 4.2 Mathematical model

According to Rayleigh breakup theory of a liquid filament, perturbations or disturbances on the surface of the liquid filament tend to grow or shrink based on the wavelength, $\lambda$, of the disturbance (Rayleigh, 1878). Rayleigh determined that the wavelength of the fastest growing disturbance, $\lambda_{\text{opt}}$, ultimately determines the size of the resulting drops. Furthermore, he calculated the wavelength of the fastest growing disturbance for a cylindrical inviscid liquid filament with no body forces present as follows:

$$\lambda_{\text{opt}} = d_f \pi \sqrt{2},$$

where $d_f$ is the filament diameter.

Later Weber, 1931, and Chandrasekhar, 1961, extended the calculation of $\lambda_{\text{opt}}$ to a viscous liquid filament, see (Ashgriz and Yarin, 2011). This resulted in a value for $\lambda_{\text{opt}}$ as follows:

$$\lambda_{\text{opt}} = d_f \pi \sqrt{2}(1 + 3 \text{ Oh})$$  \hspace{1cm} (4.1)

$$\text{Oh} = \frac{\eta}{\sqrt{d_f \rho \gamma}},$$  \hspace{1cm} (4.2)

where Oh is the Ohnesorge number, $\eta$ is the viscosity, $\gamma$ is the surface tension and $\rho$ is the density of the liquid.

Since the liquid jet is cylindrical, the volume of the resulting drop must be $V_{\text{drop}} = \lambda_{\text{opt}} d_f^2 \pi / 4$. The diameter of the resulting drop is calculated from the volume, which yields:

$$d_{\text{drop}}^3 = 1.5\pi \sqrt{2} d_f^3(1 + 3 \text{ Oh}).$$

Assuming that the liquid filament has the same diameter as the nozzle, that is $d_f = d_{\text{nozzle}}$, then the dimensionless drop diameter can be written as follows:

$$D_{\text{We}}^3 = 1.5\pi \sqrt{2}(1 + 3 \text{ Oh}),$$  \hspace{1cm} (4.3)

where $D_{\text{We}} = d_{\text{drop}}/d_{\text{nozzle}}$ is the dimensionless drop diameter that results from the breakup of an unstretched viscous filament according to Weber theory.
4.3 Materials and methods

The measurements discussed in this chapter are a continuation of the experiment discussed in the Chapter 3. The dimensions of the RRBN and the fluid properties remain the same as described in Section 3.3 and are listed in Table 4.1.

Table 4.1: Table of experiment conditions for measuring liquid filament breakup in a rotary system. The experiment conditions include dimensions and settings of the test apparatus, material properties of the liquid being sprayed and experimental control variables.

<table>
<thead>
<tr>
<th>Experiment conditions</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of nozzles installed on RRBN</td>
<td>2</td>
</tr>
<tr>
<td>Rotor radius to nozzle exit, ( r_0 ) (mm)</td>
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</tr>
<tr>
<td>Nozzle orifice diameter, ( a_0 ) (mm)</td>
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</tr>
<tr>
<td>Nozzle orifice area, ( \text{mm}^2 )</td>
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</tr>
<tr>
<td>Zero-shear-rate viscosity, ( \eta_0 ) (Pa s)</td>
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</tr>
<tr>
<td>Surface tension, ( \gamma ) (N/m)</td>
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</tr>
<tr>
<td>Liquid density, ( \rho ) (kg/m(^3))</td>
<td>980</td>
</tr>
<tr>
<td>Ohnesorge number, ( \text{Oh} )</td>
<td>0.55</td>
</tr>
<tr>
<td>Dimensionless drop diameter (Weber), ( D_{\text{We}} )</td>
<td>2.6</td>
</tr>
<tr>
<td>High-speed camera capture rate, (fr/s)</td>
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</tr>
<tr>
<td>Pixel size (( \mu \text{m/px} ))</td>
<td>76.5</td>
</tr>
<tr>
<td>Equivalent speed of 1 px/fr, (m/s)</td>
<td>0.765</td>
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</table>

Control variables

<table>
<thead>
<tr>
<th>Control variables</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid feed rate, (mL/min)</td>
<td>12–38</td>
</tr>
<tr>
<td>Rotational speed, (rpm)</td>
<td>500–4000</td>
</tr>
</tbody>
</table>

The Ohnesorge number, \( \text{Oh} = 0.55 \), was calculated using Eq. 4.2 in which the viscosity \( \eta \) was taken to be the zero-shear-rate viscosity. The resulting dimensionless drop diameter of an unstretched filament is then \( D_{\text{We}} = 2.6 \) based on Eq. (4.3).

The high-speed camera has been positioned downstream from the liquid filament breakup, so that drops resulting from breakup are visible in the camera’s field of view (FOV). The capture rate of the high-speed camera was set to a frame rate of 10000 fr/s, yielding a working image FOV of 512 pixels wide \( \times \) 216 pixels high once header and footer information were cropped from the video.

At the start of measurements a length scale was placed in the FOV for dimensional reference in subsequent measurements. It was determined that 15 mm spanned 196 pixels, yielding a pixel size of 76.5 \( \mu \text{m} \). The equivalent dimensionized speed of 1 px/fr
corresponded to 0.765 m/s, which was obtained by applying the pixel size and the frame rate of 10000 fr/s (see Table 4.1). The dimensionalized FOV was determined to be $39 \text{ mm} \times 16.5 \text{ mm}$.

In these measurements, the rotational speed of the rotor was adjusted to 500, 1000, 2000, 3000 and 4000 rpm. The volumetric feed rate was adjusted to 12, 21, 29 and 38 mL/min, which corresponds to an inlet pressure of 1, 2, 3 and 4 bar, respectively. The feed rate and rotational speed are listed in Table 4.1 as control variables.

A test matrix was constructed accordingly to handle all possible combinations of rotational speed and volumetric flow rate. For bookkeeping purposes the prefix $\text{RAXX}$ was assigned to each test case, where $XX$ is a numeric placeholder, which is set according to the test conditions as shown in Table 4.2. The test cases $\text{RA06}$, $\text{RA12}$, $\text{RA18}$ and $\text{RA24}$ are not listed, since measurements at 5000 rpm were not taken.

Table 4.2: Test matrix and corresponding experiment list for measuring liquid filament breakup using a high-speed camera. There were two control variables used in the experiments: rotational speed of the Rotary Rayleigh Breakup Nozzle and liquid feed rate into the device.

<table>
<thead>
<tr>
<th>Feed rate $\text{mL/min}$</th>
<th>Rotational speed [rpm]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>500</td>
</tr>
<tr>
<td>12</td>
<td>RA01</td>
</tr>
<tr>
<td>21</td>
<td>RA07</td>
</tr>
<tr>
<td>29</td>
<td>RA13</td>
</tr>
<tr>
<td>38</td>
<td>RA19</td>
</tr>
</tbody>
</table>

Using the high-speed video camera, several rotations of the RRBN were recorded for each test case within the test matrix. The resulting videos were analyzed to determine particle size behavior as a function of the two control variables: nozzle velocity and rotational speed, where nozzle velocity is directly proportional to and determined by the volumetric feed rate setting.

The resulting nozzle velocities are 1.4, 2.5, 3.4 and 4.5 m/s for the feed rate of 12, 21, 29 and 38 mL/min, respectively. Details are given in Table 4.3 in Section 4.4.2.
4.4 Results and discussion

4.4.1 Qualitative results from high-speed videography

For each test case in Table 4.2 high-speed video captured several rotations of the RRBN using a frame rate of 10000 fr/s. In particular, the high-speed camera was positioned so that the FOV was downstream from where the liquid filament breaks up into drops. The resulting high-speed videos display a fixed FOV with drops moving through the FOV as the image frames progress. An example of this progression is illustrated in Fig. 4.1.

Figure 4.1: A composite image from the high-speed video of drops after liquid filament breakup recorded at 10000 frames per second. The entire image represents the camera field of view of one data collection, whereas the dashed lines represent a transition to a new video frame. The drops are located at their actual position in the field of view at the given frame (fr) number.

Figure 4.1 is a composite image created from 9 frames of high-speed video capture during the RA07 test case. The image represents a superposition of the drops captured in each video frame, so that all drops visible in the 9 frames are composed into one image. Since the drops are moving throughout the video capture, it was possible to divide the composite image into regions of interest based on drop location in a particular video frame. This is indicated by dashed lines, which separate the regions of interest based on frame number. In other words, the dashed lines represent a temporal separation. Furthermore, since the frame number increments by 10 across each dashed line, the time increments by 1 ms across each dashed line.

To clarify, two drops enter the FOV in the lower-right corner of Fig. 4.1. After 1 ms the drops have moved vertically in the FOV to the region separated between dashed
lines, which is designated as frame 11. The two drops are beginning to coalesce and three additional drops have entered the FOV.

The composite image illustrates several characteristics of the high-speed video capture. First, the regions of interest are progressing from right to left as a result of the RRBN rotating in a counterclockwise direction relative to the camera FOV. Second, the drops move more-or-less at a constant velocity, that is they are moving in a constant direction at a constant speed. Finally, the tangential direction of the (no longer existing) filament can be visualized from the drops in an individual frame, that is, the dashed lines run approximately parallel to the filament direction. Furthermore, there is both a tangential and normal component to the velocity of a drop with respect to the filament direction.

This superpositioning method was applied to the same video sequence over 87 frames, which resulted in the image shown in Fig. 4.2. The image has been scaled to millimeters as illustrated by the axes.

![Superposition of all video frames following filament breakup](image)

**Figure 4.2:** A composite image of drops following liquid filament breakup is displayed as a superposition of 87 video frames recorded at 10000 frames per second. The image represents the field of view of the high-speed camera scaled to millimeters.

Since there are two nozzles on the RRBN, the composite image was produced from all drops produced in a half revolution of the RRBN. The white space visible in the upper-left corner illustrate that the video sequence was truncated to 87 frames, however there would be drops visible several frames that follow.
Figure 4.2 better illustrates the constant velocity behavior of the drops after breakup. In particular, the straight path lines are visible, which demonstrate a constant direction for most drops with the exception of the coalescing drops on the right side of the image. These drops do not hold a constant direction, since cohesive forces are causing a change in momentum. Moreover, the banding pattern along each path line represents the spacing of the same drop at two consecutive image frames. Since the frame rate remains constant and the banding pattern appears constant, the drop speed is approximately constant over the image sequence.

4.4.2 Processing results from high-speed videography

Using the constant velocity behavior of the drops recorded in video, we developed a method for detecting and analyzing the drops from the high-speed videography. The method can be broken into two parts: drop detection from video and identifying individual drop trajectories from the list of detected drops.

The built-in functions in Mathematica were used to detect drops on a frame-by-frame basis from the high-speed video. In particular, the process for detecting drops was as follows:

1. Each video frame was processed individually as an image. Contrary to Fig. 4.1, the background was dark and the drops were light.
2. A binary image was created from each image using the MorphologicalBinarize function with a threshold value of 0.4. This value was tuned based on a sample set of the images.
3. Drops were detected in the binary image using the function SelectComponents based on two criteria: 2 < pixel area < 500 and elongation < 0.2. The pixel area requirement removed small and large image artifacts from the list of drops including the background. Elongation is defined as $1 - \frac{\text{width}}{\text{height}}$ as determined by principal axes of the best fitting ellipse (Wolfram Research, 2015). The elongation requirement was used to remove components, such as filament strands and coalescing drops, from the list of detected drops.
4. Drops that lie on or are touching the image border were removed using the function DeleteBorderComponents, since the drop area is not represented in its entirety.
5. The equivalent circle of each drop, that is the pixel coordinates of the center of the circle and the pixel radius of the best-fit circle were calculated using the function ComponentMeasurements.
6. The resulting data were tabulated and exported as image frame number, pixel coordinates $(x, y)$ and pixel radius.
The results of the drop detection method are shown in Fig. 4.3. Drop position and pixel radius have been scaled to millimeters. Demonstrated in this figure is the removal of border components, that is no circles lie on the edge of the image. Also demonstrated by the coalescing drops on the right side of the image is that the two drops are ignored until they coalesce, since their elongation is out of range. The figure illustrates that hundreds of drops have been detected across the entire video sequence, however, visually one can see that there are 16 unique detected drops. Therefore, further processing is required to isolate individual drops in order to draw meaningful conclusions regarding drop sizes.

![Overlay of detected drops onto composite image](image)

Figure 4.3: The results of drop detection are overlayed onto a composite image of drops after liquid breakup. The size and position of detected drops are indicated accordingly by the circles. The circles are colored based only on frame number to indicated that individual drops have not been identified.

The second part of the method concerns isolating and identifying individual drops based on trajectory. More specifically, each drop is identified by a frame in which it first appears, a coordinate position within that frame, and a speed and direction in which it moves. One difficulty in particular, is that two drops could potentially occupy the same space and travel at the same speed and direction, but at different times. In this situation, they two must be identified as different drops.

The method for tracking the drops based on trajectory is as follows:

1. Assign all detected drops a unique identifier.
2. Starting with the first frame number calculate a line from the pixel coordinates of each drop in the first frame extended to the center of each drop in the second frame. This represents all possible drop trajectories of drops originating in the first frame. Thus, if there are \( m \) drops in the first frame and \( n \) drops in the second frame, then there will be \( m \times n \) potential trajectories between the two frames.

3. Extend each trajectory forward through all the frames until it exits the FOV. List drops by its identifier which intersect each trajectory. Intersection is based on the Euclidean distance between trajectory position at a given frame number and the drop center at the same frame number. If the Euclidean distance is less than some threshold, then the two intersect. In these calculations a threshold of 5 pixels was used.

4. Repeat steps 2 and 3 incrementing the frame number until all frames, other than the last two, serve as the starting frame.

5. Start with the trajectory achieving the highest number of intersections from step 3. All intersections to this trajectory, including the two originating drops, are grouped together as one drop and identified accordingly. These drops are removed from the list of potential intersections. Furthermore, the list from step 3 must also be adjusted since drops may have been removed from this list.

6. Repeat step 5 using the next highest number of intersections from the list from step 3. Continue down the list repeating step 5 until only trajectories remaining containing two or less intersections, including the two originating drops.

This method assigns the highest weight to trajectories having the most intersections. Furthermore, since drops are removed from the intersection list once they are uniquely identified, it reduces the risk that the drops will falsely be assigned to the wrong trajectory. Results of the trajectory tracking algorithm were visually verified and corrected manually across all video sequences.

The results of the trajectory tracking algorithm are displayed in Fig. 4.4. The colors are now assigned to individual trajectory groups, thus demonstrating a successful grouping based on trajectory.

Once the resulting drop groups have been uniquely identified, mean position and drop size are calculated as well as mean velocity. These results are shown in Fig. 4.5. The circles indicate the mean position and mean drop size calculated for each group. The arrows represent the velocity vectors in m/s. The velocity vectors show that the mean speed, displayed as the length of an arrow, is approximately constant for all drops. Both Figs. 4.4 and 4.5 show good agreement in size and position of the resulting drops compared to the images.

Multiple revolutions of the RRBN were included in high-speed video for each of the test cases from Table 4.2. The high-speed videos were truncated to limit each
video sequence to one half revolution and to include only frames in which drops appeared. Thus, multiple half revolution videos were analyzed using the method described above. The resulting number of drops determined for each test case are summarized in the third column of Table 4.3.

The rotational speed measurement of the RRBN was known to be inaccurate in the experiments. Since the high-speed videos contained multiple revolutions for each test case, a more accurate rotational speed could be determined based on the duration of a revolution. Using the lower left corner of the FOV as a reference point the total number of frames were determined from the crossing of the reference point in the first revolution to the crossing of the reference point in the last revolution. From the total number of revolutions, the duration of one revolution could be determined. These results are summarized in Table 4.3.

Figure 4.4: Particle tracking results overlayed onto a composite image of drops after liquid breakup. The size and position of drops were tracked over 87 video frames. Individual drops were identified based on trajectory across the video frames and are distinguished in the plot based on color.
Figure 4.5: The summarized results after particle tracking was used to determine mean drop position, drop radius and velocity of individual drops. Each individual drop’s position, size and velocity were averaged across all frames, in which the drop was detected. The mean position and size are displayed as circles and the mean velocity is shown as a vector.
Table 4.3: Results from analysis of video and calculations. Rotational speed of the RRBN was measured from high-speed video. Nozzle velocity was calculated from the feed rate based on two 0.3 mm nozzles. The number of drops detected in high-speed video used for drop size analysis is recorded under sample size.

<table>
<thead>
<tr>
<th>Test case</th>
<th>Meas’d rot. rpm</th>
<th>Feed rate mL/min</th>
<th>Nozzle vel. m/s</th>
<th>Sample size</th>
</tr>
</thead>
<tbody>
<tr>
<td>RA01</td>
<td>514</td>
<td>12</td>
<td>1.4</td>
<td>153</td>
</tr>
<tr>
<td>RA02</td>
<td>1023</td>
<td>12</td>
<td>1.4</td>
<td>51</td>
</tr>
<tr>
<td>RA03</td>
<td>2028</td>
<td>12</td>
<td>1.4</td>
<td>140</td>
</tr>
<tr>
<td>RA04</td>
<td>3030</td>
<td>12</td>
<td>1.4</td>
<td>79</td>
</tr>
<tr>
<td>RA05</td>
<td>3982</td>
<td>12</td>
<td>1.4</td>
<td>46</td>
</tr>
<tr>
<td>RA07</td>
<td>515</td>
<td>21</td>
<td>2.5</td>
<td>137</td>
</tr>
<tr>
<td>RA08</td>
<td>1020</td>
<td>21</td>
<td>2.5</td>
<td>90</td>
</tr>
<tr>
<td>RA09</td>
<td>2017</td>
<td>21</td>
<td>2.5</td>
<td>99</td>
</tr>
<tr>
<td>RA10</td>
<td>3072</td>
<td>21</td>
<td>2.5</td>
<td>55</td>
</tr>
<tr>
<td>RA11</td>
<td>4067</td>
<td>21</td>
<td>2.5</td>
<td>251</td>
</tr>
<tr>
<td>RA13</td>
<td>514</td>
<td>29</td>
<td>3.4</td>
<td>315</td>
</tr>
<tr>
<td>RA14</td>
<td>1007</td>
<td>29</td>
<td>3.4</td>
<td>141</td>
</tr>
<tr>
<td>RA15</td>
<td>2024</td>
<td>29</td>
<td>3.4</td>
<td>164</td>
</tr>
<tr>
<td>RA16</td>
<td>3016</td>
<td>29</td>
<td>3.4</td>
<td>173</td>
</tr>
<tr>
<td>RA17</td>
<td>4043</td>
<td>29</td>
<td>3.4</td>
<td>81</td>
</tr>
<tr>
<td>RA19</td>
<td>518</td>
<td>38</td>
<td>4.5</td>
<td>172</td>
</tr>
<tr>
<td>RA20</td>
<td>1006</td>
<td>38</td>
<td>4.5</td>
<td>67</td>
</tr>
<tr>
<td>RA21</td>
<td>2024</td>
<td>38</td>
<td>4.5</td>
<td>31</td>
</tr>
<tr>
<td>RA22</td>
<td>3023</td>
<td>38</td>
<td>4.5</td>
<td>58</td>
</tr>
<tr>
<td>RA23</td>
<td>4036</td>
<td>38</td>
<td>4.5</td>
<td>7</td>
</tr>
</tbody>
</table>
4.4.3 Resulting drop size distributions

The RA13 test case was selected for illustrational purposes, since the sample size of 315 was comparatively large. The drop sizes determined from video analysis were nondimensionalized by dividing the drop diameter by the nozzle diameter, or \( D = \frac{d_{\text{drop}}}{d_{\text{nozzle}}} \). It is important to clarify that the nondimensional scaling used here differs from that in Chapter 3, where the scaling was based on the rotor diameter.

The resulting dimensionless drop sizes from the RA13 results were binned using a bin width of 0.05 and plotted in the histogram in Fig. 4.6. The dimensionless bins are located on the x-axis and their corresponding bin counts are on the primary y-axis.

![Histogram and smoothed PDF results of test case](image)

Figure 4.6: Resulting dimensionless drop diameter of 315 detected drops detected from high-speed video capture of the RA13 experiment. The histogram (primary axis) displays actual tabulated results of dimensionless drop diameter. The probability density function (PDF) (secondary axis) is the result of applying a smoothing kernel with a bandwidth of 0.05 to the histogram and scaled so that it integrates to have a probability of one.

Using the built in functions in Mathematica a Gaussian smoothing kernel with a bandwidth 0.05 was applied to the dimensionless drop size results from RA13. A probability density function (PDF) was generated from the resulting smoothed data. This resulting PDF is plotted over the histogram in Fig. 4.6 using the secondary y-axis. The secondary y-axis has been scaled by the bin width and total count so that the amplitudes of the two plots are the same.

A comparison of the histogram and PDF in Fig. 4.6, demonstrate that PDF well represents the resulting drop size histogram. The PDF has the advantage that it
compares directly with PDFs from other test cases. Whereas in the case of the histogram, both scaling and aesthetics make direct comparisons between two histograms already difficult, with difficulty compounding as the number of histograms increase.

A cumulative histogram was constructed from the histogram in Fig. 4.6 and plotted in Fig. 4.7. The primary y-axis represents the total counts of dimensionless drops having the given diameter or below. The cumulative distribution function (CDF), calculated as the integral of the PDF, was plotted on the secondary y-axis in Fig. 4.7. The secondary axis was scaled so that an amplitude of 1 on the secondary corresponds to an amplitude of 315, the sample size.

Cumulative histogram and CDF results of test case

Figure 4.7: Resulting dimensionless drop diameter of 315 detected drops detected from high-speed video capture of the RA13 experiment. The cumulative histogram (primary axis) displays actual accumulated results of dimensionless drop diameter. The cumulative distribution function (CDF) (secondary axis) is the integral of the probability density function curve.

A comparison between the cumulative histogram and the CDF demonstrate good qualitative agreement. The CDF offers the same comparative advantages over the cumulative histogram as the PDF does over the histogram. Moreover, the probability that a drop diameter falling within a particular range can be calculated directly from the CDF. Therefore, the CDF in place of the cumulative histogram will be primary means of comparison of drop size data among the different cases. Likewise, the PDF will be used in place of the histogram.

The weighting scheme plays a role in comparing drop size distributions as illustrated in Figs. 4.8 and 4.9. Three weighting schemes are considered here: number-weighted...
or unweighted, volume-weighted or mass-weighted and diameter-weighted. The unweighted scheme, already used in Figs. 4.6 and 4.7, represents the frequency of occurrence of a drop. The unweighted scheme tends to amplify the contribution of small drops, since the scheme assigns equal weighting to a small drop as to a large drop.

**Volume-, diameter- and number-weighted PDFs**

![Volume-weighted PDFs](image)

Figure 4.8: Comparison of the volume-weighted, diameter-weighted and number-weighted PDF curves using the 315 detected drops from high-speed video capture of the RA13 experiment. The dimensionless diameter, $D = d_{\text{drop}}/d_{\text{nozzle}}$ is used for the weighting schemes. Volume-weighting uses a weighting scheme depending on $D^3$, diameter-weighting requires $D^1$ and the number-weighted PDF represents the unweighted frequency of occurrence.

The volume-weighted scheme assigns a weighting based on $D^3$, where $D$ is the dimensionless drop size. That is, the PDF and CDF are adjusted so that probabilities are based on volume. Given an arbitrary drop with diameter $D_0$ the CDF represents the proportion of volume of drops having a diameter less than $D_0$. The volume-weighted scheme tends to amplify the contribution of large drops, since large portions of the total mass are contained in individual large drops.

The diameter-weighted scheme assigns a weighting based on $D^1$. This weighting scheme reduces the contribution of small drops in comparison to an unweighted scheme. Furthermore, it reduces the contribution of large drops in comparison to a volume-weighted scheme. Despite this balancing, the volume-weighted CDF and PDF were chosen to serve as the primary weighting scheme for subsequent analysis. Volume-weighting was chosen primarily because the properties of resulting spray-processed powders are often measurement using a volume-weighting scheme.
4 Video analysis of liquid filament breakup from rotary spraying

Vol. weighted
Diam. weighted
No. weighted

Figure 4.9: Comparison of the volume-weighted, diameter-weighted and number-weighted CDF curves using the 315 detected drops from high-speed video capture of the RA13 experiment. The volume-weighted, diameter-weighted and number-weighted CDFs are the integrals of their corresponding PDFs from Fig. 4.8.

4.4.4 Drop diameter versus rotational speed

In analyzing the effect of rotational speed on drop diameter, the test cases were considered in which the rotational speed was varied from 500 rpm through 4000 rpm while the nozzle velocity was held constant at 1.4 m/s. The resulting volume-weighted drop size CDFs are compared in Fig. 4.10.

The drop diameter, at which the volume-weighted cumulative distribution curve intersects the 0.9 value dashed line is denoted by $\bar{D}_{90,3}$ as highlighted on the 500 rpm curve. Ninety percent of the total volume (or mass) is contained in drops having a diameter $\bar{D}_{90,3}$ or smaller. Similarly, $\bar{D}_{50,3}$ and $\bar{D}_{10,3}$ curve indicate the diameter at which the curve intersects the 0.5 dashed line and 0.1 dashed line, respectively. Thus, $\bar{D}_{50,3}$ represents the volume-weighted mean diameter and is denoted by a symbol on each distribution curve.

Except for the transition from 3000 rpm to 4000 rpm, the plot shows that the mean drop diameter decreases as rotational speed of the RRBN increases. The increased rotational speed causes an increase in the stretching of the liquid filament in its tangential direction, causing a narrowing of the filament. The narrower filament breaks up into drops, which are smaller in diameter. Likewise, except for the transition
Figure 4.10: Volume-weighted cumulative distributions of the dimensionless drop diameter, \( D = \frac{d_{\text{drop}}}{d_{\text{nozzle}}} \), from experimental results using a nozzle exit velocity of 1.4 m/s and rotational speed as the control variable. The 10% value \( \bar{D}_{10,3} \), mean value \( \bar{D}_{50,3} \), and 90% value \( \bar{D}_{90,3} \) are highlighted on the 500 rpm curve.

from 3000 rpm to 4000 rpm, there is a reduction in drop diameter across the entire distribution as rotational speed increases.

The mean drop diameter remains the same from 3000 rpm to 4000 rpm, which indicates that the added filament stretching provided by the increased rotational speed provides no additional reduction in drop size. This is discussed in more detail in Chapter 5.

The volume-weighted median drop-size diameter, \( D_{50,3} \), in addition to the 90th percentile diameter, \( D_{90,3} \), and 10th percentile diameter, \( D_{10,3} \), were plotted against rotational speed as shown in Fig. 4.11. Note that the \( D_{(\cdot),3} \) values are calculated based on the sampled data, whereas the \( \bar{D}_{(\cdot),3} \) are calculated based on the smoothed probability distribution.

Figure 4.11 reasserts the observations above, however the overall trend is more visible. In particular, the \( D_{50,3} \), \( D_{90,3} \) and \( D_{10,3} \) curves all show a reduction in drop diameter as rotational speed increases from 500 rpm to 2000 rpm, followed by a diminished reduction when rotational speed is increased to 3000 rpm. There is no size reduction when rotational speed is increased from 3000 rpm to 4000 rpm. The \( D_{90,3} \) value increases from 3000 rpm to 4000 rpm, which indicates an increase in the production of large drops at the higher rotational speed.
Figure 4.11: A summary of experimental results showing the volume-weighted dimensionless drop diameter versus rotational speed using a nozzle exit velocity of 1.4 m/s. Three metrics were used to calculate drop diameter: The median drop diameter (closed circle), the \( D_{90,3} \) diameter (closed square) and the \( D_{10,3} \) diameter (closed diamond) are plotted versus rotational speed. The span, indicated by the bargraph, is plotted on the secondary axis.
The span, \( \text{span} = (D_{90,3} - D_{10,3})/D_{50,3} \), indicates how narrow the drop size distribution is. It shows a narrowing of the distribution as rotational speed increases from 500 rpm to 1000 rpm. This is followed by a constant span from 1000 rpm through 3000 rpm. From 3000 rpm to 4000 rpm the span increases again.

Based on Figs. 4.10 and 4.11 the optimum rotational speed for reduced drop size and a narrow drop size distribution occurs near the 3000 rpm operating condition. However, operating at 2000 rpm also produces good results and may be worth the tradeoff of operating at a lower rotational speed.

The results of drop size versus rotational speed for the remaining three test cases is summarized in Fig. 4.12. In addition, the median drop diameter versus rotational speed for all four test cases is shown in Fig. 4.13.

The behavior of the remaining test cases is similar in comparison to the 1.4 m/s nozzle velocity test case. However, there is a notable improvement in drop diameter at 500 rpm for the 3.4 m/s and 4.5 m/s test cases. Furthermore, the drop size behavior at 4000 rpm showed better results for nozzle velocities of 2.5 m/s and 3.4 m/s. There were only 7 drops detected in the 4.5 m/s - 4000 rpm test case, which explains the change in behavior under these conditions. Generally, the optimum rotational speed in terms of span and drop diameter was 2000 rpm to 3000 rpm.

The dimensionless drop diameter for an unstretched liquid filament was calculated to be \( D_{\text{We}} = 2.6 \) using the zero-shear-rate viscosity as the viscosity of the liquid jet. The largest median drop diameters came from the 500 rpm test cases with nozzle velocities of 1.4 m/s and 2.5 m/s. From these two test cases, the median dimensionless drop diameter was approximately 2.5. Since the filament stretching due to the lower rotational speed, these results agree well with the calculation for \( D_{\text{We}} \). This confirms the methodology developed herein to calculate drop diameters from high-speed videography.

The lower limit of the dimensionless median drop diameters achieved here was approximately 1.9. This is a drop diameter reduction of approximately 25%, which corresponds to a drop volume reduction of approximately 60%.
Summary of drop diameters versus rotational speed

(a) Drop size CDF for $u_{\text{nozzle}} = 2.5$ m/s

(b) Diameter vs. rpm for $u_{\text{nozzle}} = 2.5$ m/s

(c) Drop size CDF for $u_{\text{nozzle}} = 3.4$ m/s

(d) Diameter vs. rpm for $u_{\text{nozzle}} = 3.4$ m/s

(e) Drop size CDF for $u_{\text{nozzle}} = 4.5$ m/s

(f) Diameter vs. rpm for $u_{\text{nozzle}} = 4.5$ m/s

Figure 4.12: Experimental results for dimensionless drop diameter versus rotational speed of the RRBN. The cumulative drop-size distributions in (a), (c) and (e) are for nozzle exit velocities of 2.5 m/s, 3.4 m/s and 4.5 m/s, respectively. Corresponding dimensionless drop diameters versus rotational speed are shown in (b), (d) and (f), respectively.
4 Video analysis of liquid filament breakup from rotary spraying

Figure 4.13: A summary of results from experiment of the dimensionless median drop diameter versus rotational speed of the RRBN. The results are summarized for nozzle exit velocities of 1.4 m/s (closed circle), 2.5 m/s (closed square), 3.4 m/s (closed diamond) and 4.5 m/s (closed triangle).

4.4.5 Drop diameter versus nozzle exit velocity

Using the CDF we make a examine the drop diameter versus nozzle exit velocity when the RRBN is operating at 2000 rpm as shown in Fig. 4.14. In addition, the resulting $D_{10.3}$, $D_{50.3}$, $D_{90.3}$ values were plotted for the 2000 rpm test cases as shown in Fig. 4.15.

Both figures illustrate that there is no significant change in drop diameter when varying the nozzle exit velocity and holding the rotational speed constant. This result is reasonable for two reasons. First, filament stretching is primarily driven by rotational forces and not by nozzle velocity. Thus changing the velocity should not affect stretch-driven drop diameter reduction. Second, according to Eq (4.3), the drop diameter is independent of the nozzle velocity.
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Figure 4.14: Volume-weighted cumulative distributions of the dimensionless drop diameter, \( D = \frac{d_{\text{drop}}}{d_{\text{nozzle}}} \), from experimental results using a rotational speed of 2000 rpm and nozzle exit velocity as the control variable.

Figure 4.15: A summary of experimental results showing the volume-weighted dimensionless drop diameter versus nozzle exit velocity using a rotational speed of 2000 rpm. Three metrics were used to calculate drop diameter: The median drop diameter (closed circle), the \( D_{90,3} \) diameter (closed square) and the \( D_{10,3} \) diameter (closed diamond) are plotted versus rotational speed. The span, indicated by the bargraph, is plotted on the secondary axis.
4.5 Summary

Image processing was used in conjunction with high-speed videography to calculate drop sizes resulting from liquid filament breakup in a Rayleigh breakup regime under rotating conditions. Analysis of videography was necessary, since rotary spraying limited the sampling capabilities of a spray PSA.

This chapter discussed the methodology developed to effectively utilize high-speed videography to determine drop diameters. Furthermore, the methods developed led to calculated drop sizes that were in agreement with Rayleigh and Weber theory regarding the breakup of viscous liquid jets.

Analysis showed that the pressure driven RRBN generated smaller spray drops than occur in irrotational liquid filament breakup. Furthermore, we were able to show additional drop size reduction with increased rotational speeds.

Based on the resulting drop size measurements, we were able to recommend 2000 rpm to 3000 rpm as an optimum rotational speed in order to produce dimensionless drop diameters of approximately 2.0 with a narrow drop-size distribution.

Further analysis showed that the drop diameters were not significantly affected by nozzle exit velocity. Therefore, the RRBN can be tuned for optimum drop size using rotational speed of the device, whereas throughput can be tuned separately using the feed pressure. However, care must be taken to spray at sub critical Weber numbers in order to maintain the integrity of the shear sensitive materials being sprayed.
5 Simulation of Rayleigh breakup

5.1 Introduction

Complex fluid structures such as emulsions and multiple emulsions experience structure loss as a result of high shear stresses during spray processing. Previous experiments show that allowing the liquid filament to breakup in a Rayleigh breakup regime significantly reduces the structure loss in emulsions. Moreover, applying rotational forces to a liquid jet undergoing Rayleigh breakup reduces spray drop-size and narrows the drop-size distribution while only slightly affecting structure.

We simulate the Rayleigh breakup of a liquid filament under the stretching conditions existing in a pure centrifugal field. Filament breakup length, drop size and drop size distribution are determined from the simulation results for varying rotational speeds and flow rates. These results are compared with measurements taken from a rotary sprayer under similar operating conditions.

The simulations show good qualitative agreement with measurement results when considering Rayleigh breakup length and resulting spray drop size distribution versus rotational speed. However, a direct quantitative comparison between measurement and simulation data was not possible, since the simulation model does not include the degradation of the centrifugal field induced by filament bending as a result of Coriolis force, which is present and is not negligible in the physical rotary sprayer.

5.2 Computational methods

5.2.1 Simulation

Simulations were performed using the OpenFOAM-2.1.x finite volume platform (Jasak, 1996; OpenFOAM Foundation; Weller et al., 1998). The volume of fluid (VoF) solver, interFoamWithSources (Gschaidner and ICEStrömungsforschung GmbH) was used for simulating the two-phase problem with the capability of including an additional momentum source term supplied at run-time.
5 Simulation of Rayleigh breakup

Simulation domain

Simulations of the liquid filament breakup were performed on an axisymmetric simulation domain divided radially into two regions as shown in Fig. 5.1. The domain is a wedge with axial length of 25 mm in the x-direction, radius of 0.5 mm extending in the y-direction, and a wedge half-angle of 2.5° symmetric with the xy-plane. The lower region from \( y = 0 \) mm to \( y = 0.15 \) mm represents the liquid filament with an inlet patch at \( x = 0 \) mm and an outlet patch at \( x = 25 \) mm. The upper region represents the atmospheric air with an air inlet patch at \( x = 0 \) mm, an outlet patch at \( x = 25 \) mm and an atmospheric patch at \( y = 0.5 \) mm.

![Axisymmetric Simulation Domain](image)

Figure 5.1: Description of the axisymmetric simulation domain used for simulating liquid filament breakup under Rayleigh breakup conditions

The simulation domain was divided into mesh cells. Under the standard configuration, or base configuration, the domain was divided into 3000 equally sized cells in the axial direction. The radial direction was composed of two regions: a filament region and an atmosphere region. The filament region was divided radially into 48 equally sized cells. The atmosphere region was divided into 60 cells using a nonuniform grading, where the cells touching the filament region were 1/2 the size of the outer cells. This resulted in a base mesh of 324000 mesh cells. A mesh independence analysis was performed and is discussed in detail in Sec. 5.3.3.

The patches were initialized to boundary conditions for velocity (U), modified pressure (\( p_{\text{rgh}} = p - \rho gh \)), and the phase fraction (\( \alpha_1 \)) as shown in Table 5.1. The Neumann boundary condition is assigned the value zeroGradient to corresponding patches. Likewise, the Dirichlet boundary condition is assigned a fixed value scalar to corresponding patches for \( \alpha_1 \) and \( p_{\text{rgh}} \) and a fixed value vector to corresponding patches for velocity. The internal fields for velocity, \( p_{\text{rgh}} \) and \( \alpha_1 \) are initialized to fixed values according to the table. In particular, the internal field for \( \alpha_1 \) is initialized with a value of 1 for liquid filament according to Fig. 5.1 and a value of 0 elsewhere.
Derived boundary conditions are also described in Table 5.1. The inletOutlet boundary condition describes the boundary condition, which acts as a fixed value if the flux is directed inward and zeroGradient if the flux is directed outward. The pressureInletOutletVelocity boundary condition on the velocity similarly assigns a fixed value to the velocity if the flux is directed inward, otherwise the velocity is calculated from the pressure. For more details see (OpenFOAM Foundation, 2011a)

Table 5.1: Table of boundary conditions used as initial conditions to the OpenFOAM two-phase VoF solver.

<table>
<thead>
<tr>
<th>Patch</th>
<th>( \mathbf{u} \ (\text{m/s}) )</th>
<th>( p_{\text{rgh}} )</th>
<th>alpha1</th>
</tr>
</thead>
<tbody>
<tr>
<td>inlet</td>
<td>(1,0,0)</td>
<td>zeroGradient</td>
<td>I/O 1^a</td>
</tr>
<tr>
<td>aInlet</td>
<td>(1,0,0)</td>
<td>zeroGradient</td>
<td>I/O 0</td>
</tr>
<tr>
<td>atmos</td>
<td>p I/O (0,0,0)</td>
<td>0</td>
<td>I/O 0</td>
</tr>
<tr>
<td>outlet</td>
<td>p I/O (1,0,0)</td>
<td>zeroGradient</td>
<td>I/O 0</td>
</tr>
<tr>
<td>internal</td>
<td>(0,0,0)</td>
<td>0</td>
<td>^c</td>
</tr>
</tbody>
</table>

^a InletOutlet boundary condition (I/O)

^b PressureInletOutlet boundary condition (p I/O)

^c Filament is assigned \( \alpha_1 = 1 \), \( \alpha_1 = 0 \) elsewhere

**Momentum source terms**

The additional momentum source term was the momentum supplied due to centrifugal acceleration. The centrifugal acceleration source term was an input calculated based on a center of rotation located at \( x = -31.5 \) mm and the rotational speed of the rotor. The rotational speed of the rotor was a control variable and was varied from 1000 rpm to 4000 rpm in increments of 500 rpm. The centrifugal acceleration is multiplied by the density, \( \rho \), to yield the resulting momentum source term, \( r \omega^2 \rho \ \text{kg/(m}^2 \text{s}^2) \). The momentum source term is calculated at run-time using the dictionary file momentumSourceDict. The momentumSourceDict for the 1000 rpm simulation is in included in Appendix B for additional information.

Since the simulations are axisymmetric, the gravity contribution to the momentum source term is set to zero in the non-axial y-direction and z-direction. A simulation at 1000 rpm was performed with and without gravity in the axial direction (x-direction) showed that gravity did not influence the results. Analysis of the Froude number, defined by \( Fr = \omega\sqrt{r/g} \), where \( g \) is the gravity in the axial direction shows that \( Fr = 18.8 \) at 1000 rpm and thus \( Fr \gg 1 \) for all simulations. This calculation further verified that gravity in the axial direction does not play a significant role for these simulations.
5.2.2 Simulation conditions

The conditions for the simulation of liquid filament breakup in a gaseous medium is summarized in Table 5.2. The simulations were performed using the model fluids water and air, where a water liquid filament having a diameter of 0.3 mm undergoes Rayleigh breakup in a continuous gas phase composed of air. The diameter of the rotor, i.e., the position of the nozzle exit relative to the center of rotation was at 31.5 mm for all simulations. The material properties of water, air and the surface tension between water and air are recorded in the table.

The primary control variable for the simulations was the rotational speed, which was set in the momentum source term. A secondary control variable was mesh size, which was used to verify mesh independence. The post-processing parameter, phase fraction threshold $\alpha_{th}$ was also varied to verify independence of the threshold value.

Table 5.2: Summary of simulation conditions and material properties used for liquid filament breakup simulations

<table>
<thead>
<tr>
<th>Simulation parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filament diameter, (mm)</td>
<td>0.3</td>
</tr>
<tr>
<td>Radial-position nozzle at tip, (mm)</td>
<td>31.5</td>
</tr>
<tr>
<td>Fluid velocity, (m/s)</td>
<td>1.0</td>
</tr>
<tr>
<td>Kinematic viscosity water, (cSt)</td>
<td>1.000</td>
</tr>
<tr>
<td>Kinematic viscosity air, (cSt)</td>
<td>1.526</td>
</tr>
<tr>
<td>Fluid density water, (kg/m$^3$)</td>
<td>1000</td>
</tr>
<tr>
<td>Fluid density air, (kg/m$^3$)</td>
<td>1.204</td>
</tr>
<tr>
<td>Surface tension, (mN/m)</td>
<td>72.9</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Control variables</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh size</td>
<td>coarse, base, fine</td>
</tr>
<tr>
<td>Phase fraction threshold</td>
<td>0.1, 0.5</td>
</tr>
<tr>
<td>Rotational speed, (rpm)</td>
<td>1000 – 4000</td>
</tr>
</tbody>
</table>

Numerical schemes

A second-order one-point Gauss quadrature scheme was used to approximate the integrals in the FV formulation of the problem. Gradients, such as $\nabla \cdot (\nu \text{grad } \mathbf{u})$, and Laplacians, such as $\nabla \cdot (\mathbf{u})$, were discretized using a second-order linear interpolation, or central differencing scheme. Surface gradients were discretized using an explicit non-orthogonal correction. Different methods were used for the various divergence terms. For example, convection terms $\text{div}(\rho \mathbf{u} \mathbf{u})$ were discretized using a second order linear
interpolation with a limiting velocity. The volume fraction equation was discretized using a total variation diminishing (TVD) second order discretization with a vanLeer limiter, which limits the volume fraction value between 0 and 1. Interface compression was used for contribution of the interface to the volume fraction equation. A first-order implicit Euler method was used for temporal discretization. For general face to point interpolations a central differencing second order linear discretization was used.

Table 5.3 summarizes the numerical schemes used in these simulations. The \textit{fvSchemes} file is included in Appendix B for a detailed listing of the numerical schemes used in these simulations. See (Deshpande et al., 2012; Jasak, 1996; OpenFOAM Foundation, 2011a) for additional details on these methods.

Table 5.3: Description of the numerical schemes used for simulations

<table>
<thead>
<tr>
<th>Numerical scheme</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>gradSchemes</td>
<td>Gauss linear</td>
</tr>
<tr>
<td>laplacian</td>
<td>Gauss linear corrected</td>
</tr>
<tr>
<td>snGradSchemes</td>
<td>corrected</td>
</tr>
<tr>
<td>\text{div}(\rho\phi,U)</td>
<td>Gauss limitedLinearV 1</td>
</tr>
<tr>
<td>\text{div}(\phi,\alpha)</td>
<td>Gauss vanLeer</td>
</tr>
<tr>
<td>\text{div}(\phi_r,\alpha)</td>
<td>Gauss interfaceCompression</td>
</tr>
<tr>
<td>ddtSchemes</td>
<td>Euler</td>
</tr>
<tr>
<td>interpolationSchemes</td>
<td>linear</td>
</tr>
</tbody>
</table>

**Execution**

The two-phase FV-VoF solver, \texttt{interFoamWithSources} was used to solve the filament breakup problem. A write time of 0.10 ms simulation time was used, outputting $U$, $p_{\text{rgh}}$ and $\alpha_1$ at each write. The simulations for the base mesh were completed at 30 ms of simulation time.

Adjustable time stepping using a maximum Courant number of 0.7 and alpha-Courant number of 0.5 were used for all simulations. This resulted in a typical time steps settling down to the order of $1.0e-6$ to $1.0e-7$. Time steps smaller than $1.0e-7$ typically indicated unusually high velocities in the continuous phase, see Sec. 2.2.4. Execution times for the base mesh simulations are displayed in Table 5.4. For a more detailed list of the solver settings for these simulations see the \texttt{fvSolution} file included in Appendix B.
Table 5.4: Resulting simulation execution times for liquid filament breakup simulations using the base mesh and varying the rotational speed. The maximum Courant number, on which the time-step is based, was held constant at 0.7.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Cores</th>
<th>Dur.</th>
<th>Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000 RPM</td>
<td>4 x 2.3\textsuperscript{a}</td>
<td>30 hr</td>
<td>0.64 µs</td>
</tr>
<tr>
<td>1500 RPM</td>
<td>4 x 2.3\textsuperscript{a}</td>
<td>42 hr</td>
<td>0.46 µs</td>
</tr>
<tr>
<td>2000 RPM</td>
<td>8 x 2.3\textsuperscript{b}</td>
<td>39 hr</td>
<td>0.37 µs</td>
</tr>
<tr>
<td>2500 RPM</td>
<td>8 x 2.3\textsuperscript{b}</td>
<td>42 hr</td>
<td>0.30 µs</td>
</tr>
<tr>
<td>3000 RPM</td>
<td>8 x 2.3\textsuperscript{b}</td>
<td>56 hr</td>
<td>0.25 µs</td>
</tr>
<tr>
<td>3500 RPM</td>
<td>8 x 2.3\textsuperscript{b}</td>
<td>63 hr</td>
<td>0.21 µs</td>
</tr>
<tr>
<td>4000 RPM</td>
<td>16 x 2.3\textsuperscript{b}</td>
<td>44 hr</td>
<td>0.18 µs</td>
</tr>
</tbody>
</table>

\textsuperscript{a} i7-3615QM CPU @ 2.30GHz

\textsuperscript{b} i7-3615QM CPU @ 2.30GHz

5.2.3 Post-processing

The resulting simulation time files are post-processed using dropSizeCalc (Case \textit{et al.}, 2012), an in-house tool built in the OpenFOAM-2.1.x platform, which partitions the mesh based on the \texttt{alpha1} file and the input parameter $\alpha_{th}$. The mesh undergoes a segregation process, which isolates individual simulation drops. Once drops are isolated, the post-processing tool calculates for each drop the centroid to be used as location, drop volume, and diameter of a sphere of equivalent volume. This calculation is performed on all simulation time directories.

Following the drop isolation step, additional criteria are applied to ensure the resulting isolated drops are the result of Rayleigh breakup. In particular, the criteria used to exclude undesired drops are:

- Time directories occurring before a stabilized Rayleigh breakup
- Drops too small to be well resolved by the mesh
- Liquid filament, which are identified by a volume or radius larger than some threshold
- Drops, which are upstream from a segment of liquid filament, since these signify an incomplete Rayleigh breakup.

Drops remaining after post-processing were tabulated using Wolfram Mathematica version 10.1 to evaluate drop-size statistics, such as drop-size distribution and span.
5.3 Results and discussion

Simulations resulted in a series of time steps with the pressure, velocity and \( \alpha_1 \) fields recorded as individual files stored at each time step. Visualizations of the liquid phase and gas phase were obtained from the \( \alpha_1 \) field, where the interface separating the liquid and gas phases was determined by a constant phase fraction contour.

5.3.1 Rayleigh breakup

The simulations resulted in the Rayleigh breakup of the liquid jet into droplets as demonstrated in Fig. 5.2. Rayleigh disturbances propagate from the nozzle exit on the left-hand side (not shown) and increase in amplitude over time. The net effect is that the disturbances grow in amplitude as the distance increases from the nozzle. In this example, the surface tension forces begin to dominate near 15 mm and the filament pinches off to form drops. The drops continue moving axially to the right until leaving the simulation domain.

Figure 5.2 was generated from simulations of liquid filament breakup with a rotational speed of 3500 rpm supplying the centrifugal acceleration and the interface was defined using \( \alpha_{th} = 0.1 \). The destabilization of the liquid filament is highlighted in (a), where Rayleigh-Plateau disturbances are growing from the left-hand side of the figure and begin to dominate approximately 15 mm from the nozzle exit. The disturbances continue to grow in amplitude, which is demonstrated well in (d). Further increase in disturbance amplitude leads pinch-off, which is well illustrated in (f), the moment before pinch-off occurs, and (g), the moment after pinch-off occurs.

Figure 5.2 (b) shows the progression of breakup of a liquid segment into droplets even though the segment is detached from the primary liquid filament. Since the amplitude of disturbances is large enough, pinch-off occurs more rapidly than formation of a single large drop. The high velocity of the liquid phase is also visible in (b). In particular, one can observe that (b) moves from 17.2 mm to 18.6 mm from time \( t = 17.0 \) ms to \( t = 17.1 \) ms, resulting in a mean velocity of 14 m/s. The high velocity is a consequence of the high accelerations imposed by the centrifugal-only accelerational field and the high rotational speed. The formation of a satellite droplet is also highlighted in (b).

Although the simulation model does not include a physical model for coalescence, it is observed in (c). In the simulation recoalescence occurs when interfaces of two drops overlap in the same mesh cell while the drops are closing in on each other. Whereas in the physical model, other factors, such as elastic collisions, must also be considered.
Well highlighted in (e) is the reshaping of drops as the result of a force balance between wind resistance, surface tension and viscosity. The modified Taylor analogy breakup (mTAB) model, see (Liang et al., 2016), describes this deformation in more detail. In particular, surface tension tends to cause the drops to form spheres in order to minimize surface energy. Whereas, wind drag tends to cause a deformation of the spheres. This deformation process is dynamic and tends to oscillate between over deformed and under deformed as is observed in (d). At time step $t = 17.2 \text{ ms}$ the two drops are stretched axially, which over relaxes after breakup –as visible by the elongation in the radial direction at time $t = 17.3 \text{ ms}$. At time $t = 17.4 \text{ ms}$ the left-hand drop is again elongated axially. As further evidence, the left-hand drop has a gas Weber number of $\text{We}_{\text{gas}} = 2.4$, and the right-hand drop has a gas Weber number of $\text{We}_{\text{gas}} = 3.7$. Thus, one would expect a greater level of deformation at time $t = 17.3$, however, since the drop deformation is oscillating, the contrary is true.

The disappearance of small droplets is observed in (e). This disappearance is often a consequence of the VoF method, since the droplet is diffused across several mesh cells. Further diffusion of the droplet causes the phase fraction of the mesh cells to drop below $\alpha_{th}$ making it no longer traceable. However, in other cases, the small droplets being in close proximity to larger drops may recoalesce, or figuratively speaking, be consumed by the larger drops.

Slipstreaming is illustrated in (g), that is, the upstream drop is traveling in the wake of a nearby downstream drop. Since both drops are moving faster than the surrounding air, the downstream drop experiences a higher wind drag than the upstream drop causing a relative decrease in position between the two drops. If traced beyond the domain boundary, these two drops would likely coalesce.

Drops resulting from the Rayleigh breakup simulations were post-processed using dropSizeCalc to calculate spheres of equivalent volume including position and radius of the spheres. Figure 5.2 illustrates the post-processing of Rayleigh breakup simulations (top) into drops (middle). The superposition of the equivalent spheres over the simulation results at the bottom of Fig. 5.2 demonstrates qualitatively that volume is conserved on a per droplet basis. Furthermore, the total drop volume after post-processing was 3.173e-3 mm$^3$ and the total liquid volume across the entire mesh was 3.173e-12 m$^3$, which verifies quantitatively that volume is conserved during using dropSizeCalc.
Simulation of Rayleigh breakup

Rayleigh breakup simulation results

Figure 5.2: Time evolution results from simulation of Rayleigh-Plateau breakup of a liquid filament using a rotational speed of 3500 rpm. The interface is calculated using the threshold value $\alpha_{th} = 0.1$. The simulation captures many aspects of liquid filament breakup, including: (a) the destabilization of a liquid filament, (b) the breakup of a segment into droplets, (c) the recoalescence of two drops, (d) complete destabilization of the liquid jet and formation of droplets, (e) reshaping of droplets, (f) moment before pinch-off, (g) slipstreaming and (h) moment following pinch-off.
Rayleigh breakup simulation with drop calculations

Figure 5.3: Results from simulation. Simulation results of liquid filament breakup under Rayleigh conditions (top). Results after isolating drops and calculating equivalent drop diameters (middle). Superposition of the two for comparison (bottom).

5.3.2 Phase fraction independence

The phase fraction, $\alpha_1$, of a mesh cell determines phase properties of that cell. In these simulations a mesh cell is in the liquid phase if it has an $\alpha_1 = 1$. Likewise, a mesh cell is in the gaseous phase if it has an $\alpha_1 = 0$. Therefore, $\alpha_1$ can also be considered as the liquid volume fraction of a mesh cell in this context.

Mesh cells, particularly those at or near the interface, will often have a liquid volume fraction that is greater than 0 but less than 1. It is therefore necessary to determine which mesh cells are treated as liquid cells in order to segregate drops and calculate the volume of each drop. This is done by using a threshold value for $\alpha_1$ denoted as $\alpha_{th}$. Mesh cells having an $\alpha_1$ value at or exceeding $\alpha_{th}$ are considered liquid. Otherwise, they are considered gaseous. Exclusion or inclusion of a mesh cell as part of a drop, therefore, often depends on the value of $\alpha_{th}$. It follows that the calculated size of each spray droplet is directly dependent on $\alpha_{th}$.

The locations of the contours in Fig. 5.4 demonstrate the dependence of included cells based on the phase transition threshold value. In particular, as $\alpha_{th}$ increases, the liquid area contained within a closed contour region decreases. Thus, increasing $\alpha_{th}$ will reduce the overall drop sizes. In some cases, as can be seen in Fig. 5.4, small droplets may sometimes be completely excluded from calculations. However, due to their small size, many of these droplets would be automatically excluded from the drop-size distribution based on the criteria discussed in Sec. 5.2.3.

Rather than calculating the drop size volume based on the total volume of mesh cells exceeding $\alpha_{th}$, a weighted average is used to calculate the total liquid volume...
Figure 5.4: An illustration of drop size dependence based on three values of $\alpha_{th}$. The comparison is done using the fine mesh for more intricate detail.
5 Simulation of Rayleigh breakup

exceeding $\alpha_{th}$ for each mesh cell, according to the formula:

$$V_{drop} = \sum_{\alpha_i \geq \alpha_{th}} \alpha_i V_i,$$  \hspace{1cm} (5.1)

where $\alpha_i$ is the volume fraction of liquid in a mesh cell and $V_i$ is the cell volume.

The resulting liquid volume of each droplet is then tabulated from this weighted volume, resulting in a reduced drop size volume dependence on $\alpha_{th}$. This can be seen in Fig. 5.5, where the drop-size PDF and drop-size CDF are compared using $\alpha_{th}$ values of 0.1 and 0.5. The comparison clearly demonstrates volume fraction independence when Eq. (5.1) is applied.

**Drop size dependency on $\alpha_{th}$**

![Figure 5.5: Volume-weighted drop-size distributions used to demonstrate drop-size independence compared to critical threshold value, $\alpha_{th}$](image)

5.3.3 Mesh independence analysis

Mesh independence of liquid filament breakup in the classical sense – where further refinement of the mesh does not change the velocity, pressure, and phase fraction fields – is at least difficult and, more probably, impossible to achieve. There are several factors why this is the case. These include the physical process of liquid filament breakup through propagation of Rayleigh-Plateau instabilities, handling of small droplets and numerical diffusion.

According to Rayleigh breakup theory of a liquid filament (Rayleigh, 1878), perturbations in the liquid jet will tend to grow or shrink based on their wavelength and
contribution to a force balance satisfying the Young-Laplace equation. In a physical system perturbations are caused by fluctuations in the liquid jet, such as variations in pressure or viscosity. In numerical simulations numerical error, such as round-off error or truncation error, is one means of inducing perturbations. Refinement of the mesh will inherently cause differences in numerical error among different mesh refinements. As a consequence, this leads to different perturbations, which results in different filament breakup behavior.

Subsequent smaller refinement of the mesh allows for formation of ever-smaller satellite droplets and improves the traceability of small droplets that are composed of only a few liquid mesh cells. Thus, true mesh independence cannot be achieved unless droplets of all sizes can be properly resolved. A similar argument is made by (Li and Soteriou, 2013), in which the authors determine mesh resolution based on the smallest liquid structures of interest.

Numerical diffusion also plays a role, since it contributes to numerical error, which heavily affects the development and propagation of Rayleigh-Plateau disturbances as previously described. Furthermore, if the mesh is too finely refined, numerical diffusion becomes dominant and can lead to the degradation quality of the simulation.

Therefore, rather than showing mesh independence of the liquid filament breakup simulations, we focus on a less restrictive requirement for mesh independence by considering mesh independence of the drop-size distribution of simulation results.

Evaluation of mesh independence

To evaluate mesh independence simulations were performed on three different mesh sizes labeled coarse, base and fine. The corresponding cell count in the axial direction (x-direction), and radial direction (y-direction) for both filament and atmosphere cells, and total cell count for each label are detailed in Table 5.5. Relative to the coarse mesh, the cell count is adjusted for the base mesh and fine mesh by the respective amounts of +20% and +40% in each the x and y dimensions. The simulations were run using the 3000 rpm simulation conditions. These conditions were chosen, since the stretching force was high causing smaller drops and simulations could be run to completion for all three mesh sizes.

In order to accurately capture the liquid filament breakup, the mesh cells must be sufficiently small, so that smaller drops will each occupy multiple mesh cells. However, sufficiently small is a relative term. The guideline adopted in these simulations is to have a cell size smaller than $d_{\text{nozzle}}/20$, that is, a normalized cell size smaller than 1/20. It can be seen from the normalized cell lengths in Table 5.5 that this guideline has been achieved for all three mesh refinements.
Table 5.5: Summary of cell counts and cell lengths in the axial and radial directions for the coarse, base and fine meshes.

<table>
<thead>
<tr>
<th></th>
<th>Coarse</th>
<th>Base</th>
<th>Fine</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. axial cells</td>
<td>2500</td>
<td>3000</td>
<td>3500</td>
</tr>
<tr>
<td>No. radial cells (filament)</td>
<td>40</td>
<td>48</td>
<td>56</td>
</tr>
<tr>
<td>No. radial cells (atmosphere)</td>
<td>50</td>
<td>60</td>
<td>70</td>
</tr>
<tr>
<td>Cell count</td>
<td>225000</td>
<td>324000</td>
<td>441000</td>
</tr>
<tr>
<td>Axial cell length(^a)</td>
<td>1/30</td>
<td>1/36</td>
<td>1/42</td>
</tr>
<tr>
<td>Filament radial cell length(^a)</td>
<td>1/80</td>
<td>1/96</td>
<td>1/112</td>
</tr>
<tr>
<td>Atmosphere mean radial length(^a)</td>
<td>1/43</td>
<td>1/51</td>
<td>1/60</td>
</tr>
</tbody>
</table>

\(^a\) Cell lengths are normalized using: cell length / nozzle diameter

The resulting diameter-weighted and volume-weighted drop-size distributions for the mesh study analysis are shown in Fig. 5.6. From the diameter-weighted drop-size distribution in Fig. 5.14a, we see that the coarse mesh has not yet converged with regards to production of small drops. Furthermore, the volume-weighted drop-size distribution in Fig. 5.14b shows that the large drops also have not converged for the coarse mesh.

The results of both drop-size distributions show that the base mesh and the fine meshes are in agreement concerning their distributions. Therefore, we conclude that mesh independence has been sufficiently achieved using the base mesh. Moreover, simulations results from this point forward result from simulations using the base mesh.
Mesh indepedence study using drop size distribution

![Mesh-size comparison on drop-size distribution](image1)

(a) Diameter-weighted drop size distribution

![Mesh-size comparison on drop-size distribution](image2)

(b) Volume-weighted drop size distribution

Figure 5.6: Evaluation of mesh independence using the drop size distribution as a benchmark for determining convergence. The diameter-weighted drop size distribution (a) highlights discrepancies in small drops, whereas the volume-weighted drop size distribution (b) highlights discrepancies in larger drops.

### 5.3.4 Velocity at detachment

The velocity fields of their corresponding Rayleigh breakup simulations are available as part of the simulation results. From this the dimensionless mean velocity, $W^*$, of the first detached drop is calculated by averaging the velocity field over the entirety of that particular drop followed by dividing by the nozzle exit velocity $w_0$. Mathematically this takes the following form:

$$W^* = \frac{1}{V_{\text{drop}}} \sum_{i \in \text{drop}} \frac{u_i}{w_0} \alpha_i V_i,$$

where $V_{\text{drop}}$ is defined by Eq. (5.1) and $u_i$ is the axial component of the velocity in mesh cell $i$. The results from Eq. (5.2) are shown in Fig. 5.7 (closed-circles).

Moreover, by applying the assumption that the viscous forces, surface tension and wind resistance are small relative to the centrifugal forces, an underlying assumption concluded in Chapter 3, the drop velocity at detachment can be calculated using the centrifugal accelerational field. Setting up a differential equation describing motion in a centrifugal accelerational field, $a_c = \omega^2 x$, yields:

$$\omega^2 x = \frac{du}{dt} = \frac{dv}{dx},$$

where $V_{\text{drop}}$ is defined by Eq. (5.1) and $u_i$ is the axial component of the velocity in mesh cell $i$. The results from Eq. (5.2) are shown in Fig. 5.7 (closed-circles).
where $\omega$ is the rotational speed, $x$ is the axial position relative to the rotor origin, and $u$ is the axial component of the velocity. After scaling, the non-dimensional equation becomes:

$$X = Rb^2 W \frac{dW}{dX},$$

where $X$ and $W$ are dimensionless position and velocity as described in Chapter 3. The velocity, $W$, at position $X$ can be solved from the initial conditions $X_0 = 1$ and $W_0 = 1$ as follows:

$$W^2 - 1 = \frac{1}{Rb^2} (X^2 - 1), \quad (5.3)$$

which is identical to Eq. (3.9).

Since the position of the first detached droplet, $X^*$, can be determined (as later discussed in Fig. 5.12), the velocity of the detached drop, $W^*$, can be calculated from Eq. (5.3). The results are displayed in Fig. 5.7 (closed-squares).

**Mean simulation drop velocity at breakup**

![Mean simulation drop velocity at breakup](image)

Figure 5.7: Results from simulation showing the dimensionless mean velocity, $W^*$, of the first detached drop versus the simulation control variable, rotational speed. The velocity curve depicted by closed-circles represents the mean fluid velocity of the drop. The velocity curve depicted by close-squares represents the fluid velocity calculated based on drop position accelerating in a centrifugal-only field without regard to surface tension, wind resistance or viscosity.

The close similarity between the two curves illustrated in Fig. 5.7 confirm the earlier assumption leading to Eq. (5.3) that under the given simulation conditions, the
viscous forces, surface tension and wind resistance are insignificant relative to the centrifugal force field.

Per simulation conditions, the filament diameter and fluid velocity at the nozzle exit are known to be \( d_{\text{nozzle}} = 0.3 \) mm and \( w_0 = 1 \) m/s, respectively. According to conservation of mass, \( \frac{\pi}{4} d_f^2 w = \text{const} \), where \( d_f \) is the filament diameter and \( w \) is fluid velocity at the location. In scaled terms the conservation of mass is written as follows:

\[
D_f^2 W = 1,
\]

where \( D_f = d_f / d_{\text{nozzle}} \) represents the non-dimensional filament diameter and \( W \) is the dimensionless fluid velocity.

Although Eq. (5.4) applies strictly to the liquid filament before Rayleigh-Plateau disturbances affect the cross-sectional area, we apply this assumption to estimate what the filament diameter would be at the position of the detached drop. In particular, since the velocity of the detached drop is known to be \( W^* \), the dimensionless filament diameter \( D_f^* \) is estimated from Eq. (5.4). This equation is applied in later analysis.

### 5.3.5 Drop size dependency on rotational speed

Simulations were performed, during which the rotational speed was varied from 1000 rpm to 4000 rpm in increments of 500 rpm. The volume-weighted drop-size CDF was calculated for each simulation and combined in Fig. 5.8. The \( \bar{D} \) diameter, mean diameter \( \bar{D}_{90,3} \) and \( \bar{D}_{10,3} \) diameter a highlighted on the 1000 rpm distribution (see 4.4.4 for their definitions). As rotational speed increases, there is a reduction in overall drop-size. This is visible by a left-hand shift in the drop-size distribution with an increase in rotational speed. In particular, the mean drop-size decreases as rotational speed increases.

The volume-weighted median drop-size diameter, \( D_{50,3} \), in addition to the 90th percentile diameter, \( D_{90,3} \), and 10th percentile diameter, \( D_{10,3} \) were plotted against rotational speed as shown in Fig. 5.9. As rotational speed increases, there is a reduction in drop-size. However, we can see from all three curves that the drop-size reduction decreases with diminishing returns, that is, there is significant reduction in mean drop-size when there is an increase from 1000 rpm to 1500 rpm, however, there no significant reduction in drop-size as rotational speed increases from 3500 rpm to 4000 rpm. In fact, \( D_{90,3} \) curve shows an increase in drop-size from 3500 rpm to 4000 rpm. This is also visible in Fig. 5.8.

The span = \( (D_{90,3} - D_{10,3}) / D_{50,3} \) was calculated at each rotational speed and is shown Fig. 5.9 on the secondary axis. The span tends to increase with rotational speed, that
Figure 5.8: Volume-weighted cumulative distributions of the dimensionless drop-size diameter from simulation results with rotational speed as the control variable. A left-hand shift in the curve corresponds to a reduced drop diameter, $D = d_{\text{drop}}/d_{\text{nozzle}}$. The $D_{10.3}$ value, mean value ($D_{50.3}$) and $D_{90.3}$ are highlighted on the 500 rpm distribution. Distributions were generated using smoothing kernel with a bandwidth of 0.05 and a sample size of 201 drops.
Simulation of Rayleigh breakup

Simulation drop diameter vs. rotational speed

Figure 5.9: Results from simulation showing the volume-weighted dimensionless drop diameter versus rotational speed. Three metrics were used to calculate drop diameter: The median drop diameter (solid-circle), the $D_{90,3}$ diameter (closed-square) and the $D_{10,3}$ diameter (closed-diamond) are plotted versus rotational speed. The span, indicated by the bargraph, is plotted on the secondary axis.
is, the drop-size distribution widens as rotational speed increases. The increase in span is caused, in part, by the reduction in drop-size. However, the absolute span, \textit{i.e.}, the distance between the $D_{90}$ curve and $D_{10}$ curve also increases, which points to a widening of the drop-size distribution. The improvement in span from 1000 rpm to 1500 rpm perhaps indicates that the drop production process may not have fully stabilized at 1000 rpm.

The resulting volume-weighted dimensionless drop diameters versus rotational speed are summarized in Table 5.6. Included in the table is the span.

Table 5.6: Summary of volume-weighted drop-size statistics versus rotational speed.

<table>
<thead>
<tr>
<th>rpm</th>
<th>Median</th>
<th>$D_{90,3}$</th>
<th>$D_{10,3}$</th>
<th>Span</th>
<th>Mean</th>
<th>$D_{90,3}$</th>
<th>$D_{10,3}$</th>
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<tr>
<td>1000</td>
<td>1.30</td>
<td>1.23</td>
<td>1.44</td>
<td>0.16</td>
<td>1.30</td>
<td>1.43</td>
<td>1.17</td>
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<tr>
<td>1500</td>
<td>1.04</td>
<td>0.98</td>
<td>1.09</td>
<td>0.10</td>
<td>1.04</td>
<td>1.12</td>
<td>0.96</td>
</tr>
<tr>
<td>2000</td>
<td>0.98</td>
<td>0.90</td>
<td>1.08</td>
<td>0.18</td>
<td>0.98</td>
<td>1.11</td>
<td>0.87</td>
</tr>
<tr>
<td>2500</td>
<td>0.85</td>
<td>0.71</td>
<td>0.98</td>
<td>0.32</td>
<td>0.85</td>
<td>0.99</td>
<td>0.70</td>
</tr>
<tr>
<td>3000</td>
<td>0.79</td>
<td>0.65</td>
<td>0.90</td>
<td>0.33</td>
<td>0.79</td>
<td>0.94</td>
<td>0.63</td>
</tr>
<tr>
<td>3500</td>
<td>0.70</td>
<td>0.57</td>
<td>0.85</td>
<td>0.41</td>
<td>0.70</td>
<td>0.87</td>
<td>0.55</td>
</tr>
<tr>
<td>4000</td>
<td>0.70</td>
<td>0.55</td>
<td>0.91</td>
<td>0.52</td>
<td>0.70</td>
<td>0.91</td>
<td>0.54</td>
</tr>
</tbody>
</table>

The advantage of the RRBN is that the rotational speed, and therefore, centrifugal force is controllable. Centrifugal force causes axial velocity of the jetted liquid to increase with distance from the nozzle. Due to conservation of mass, the filament diameter must then decreases with respect to distance from the nozzle. The net result produces a stretching effect. This stretching process continues until Rayleigh disturbances coupled with surface tension dominate and cause pinch-off and droplet formation.

The dimensionless filament diameter $D_f$ is estimated from Eq. (5.4) and compared to the mean drop diameter in Fig. 5.10. As the rotational speed increases, centrifugal force increases and the diameter near drop break off decreases. Therefore, with increasing rotational speed, drop diameter decreases. However, since the rate of decrease in filament diameter is reduced at higher rotational speeds, it follows that the rate of decrease in drop diameter is also reduced at higher rotational speeds, \textit{i.e.}, diminishing returns on drop-size at higher rotational speeds. This phenomenon is discussed more in detail below in the context of Fig. 5.13.
5 Simulation of Rayleigh breakup

Filament diameter compared to drop diameter

Figure 5.10: Results from simulation showing the volume-weighted dimensionless mean drop diameter, $D_{50.3}$ (left axis) and dimensionless diameter of the filament at breakup, $D_\ast_f$ (right axis). Both the drop diameter and filament diameter at breakup were scaled by nozzle diameter for dimensionless values.

5.3.6 Rayleigh breakup length

The filament breakup length, $l_{\text{breakup}}$, from the simulation results is estimated using the position of the first drop after filament breakup relative to the nozzle exit. The non-dimensional breakup length, $L$, is the scaling of the breakup length by the nozzle diameter, $L = l_{\text{breakup}} / d_{\text{nozzle}}$. The dimensionless breakup length over simulation time is shown in Fig. 5.11. The plot captures the breakup length at each write time from the simulation. For clarity the plot was broken into a lower half and an upper half using 2500 rpm as a reference between the two halves. The lower half of the plot displays the breakup length for rotational speeds 1000 rpm through 2500 rpm. The upper half of the plot displays the breakup length for rotational speeds 2500 rpm through 4000 rpm. All measurements before 10 ms were disregarded, to allow for fully developed drop production.

The upper half of Fig. 5.11 shows that for high rotational speeds, the breakup length has converged to $L \approx 60$. The lower half indicates the breakup length increases with increasing rotational speed. Furthermore, the breakup length results for the 1000 rpm simulation indicate that drop production is not fully developed until 15 ms of simulation time.

The breakup length results for the 1500 rpm simulation show an oscillation in the
Figure 5.11: Scatter plot of dimensionless filament breakup length, $L^*$, from simulation results with rotational speed as the control variable. The lower part (left axis) illustrates simulation results for rotational speeds 1000 rpm through 2500 rpm, where breakup length is progressively increasing with rotational speed. The upper part (right axis) shows that breakup length is stabilized for rotational speeds from 2500 rpm through 4000 rpm. The results from the 2500 rpm simulation is displayed twice for reference.
breakup length with respect to time. The oscillation indicates a resonating effect on the filament caused by drop detachment. A possible explanation is that drop detachment induces a wave, e.g. pressure wave, in the filament, which in turn induces a Rayleigh-Plateau disturbance of a particular wavelength. The disturbance leads to eventual breakup after some time delay, which depends on how quickly the disturbance grows. Since the growth rate of the disturbance depends on its wavelength and the wavelength depends on the detachment position, thus leading to resonant behavior.

The mean breakup length, $L^*$, was calculated for each rotational speed and displayed in Fig. 5.12. Corresponding to the breakup length is the mean breakup position, $X^*$ labeled on the secondary axis. The mean breakup position is the position of detachment relative to the rotor position and scaled by the rotor radius, that is, $X^* = x_{\text{breakup}} / r_{\text{rotor}}$. When calculating filament breakup, $L^*$ is useful, where $X^*$ is useful in calculating rotational forces.

**Simulation breakup length vs. rotational speed**

![Simulation breakup length vs. rotational speed](image)

Figure 5.12: Results from simulation displaying the mean dimensionless breakup length, $L^*$, based on the centroid position of the first detached drop as a function of rotational speed. The primary- or left-axis displays breakup length relative to the nozzle exit and is scaled by nozzle diameter. The secondary- or right-axis displays breakup position relative to the rotor origin and is scaled by the rotor radius.

The breakup length increases with rotational speed, however the increase in breakup length is more pronounced at lower rotational speeds. The cause of this is better illustrated in Fig. 5.13, which compares $L^*$ with the dimensionless filament diameter at breakup, $D_f^*$. As rotational speed increases the higher centrifugal forces cause
filament stretching resulting in a narrowing of the liquid filament near breakup. This decrease in filament diameter causes the onset of Rayleigh breakup to happen over a shorter distance. That is, because of the smaller filament diameter, Rayleigh disturbances need not grow as much in amplitude before they lead to drop formation. This in turn leads to diminishing returns in terms of both Rayleigh breakup length and filament diameter reduction. Furthermore, it explains the limitation on drop size reduction with increasing rotational speeds.

**Comparison of breakup length and filament diameter**

![Graph](image)

Figure 5.13: Results from simulation displaying the mean dimensionless breakup length, $L^*$, on the primary axis and the dimensionless filament diameter at breakup, $D_f^*$, on the secondary axis.

### 5.3.7 Rayleigh breakup simulations compared to measurements

The resulting plots of drop diameter versus rotational speed from simulation and from measurement are compared side by side in Fig. 5.14. For comparison, the primary axis of the measurement plot is scaled to double that of the simulation plot, whereas the scaling of the secondary axis is the same in both plots.

The material properties of the liquid in simulation and the liquid in experiment vary significantly. The viscosity of the liquid used in simulation was $\eta = 1.0 \text{ mPa.s}$, whereas in the experiment the zero-shear-rate viscosity was $\eta_0 = 60 \text{ mPa.s}$. Thus the theoretical drop diameter resulting from the Rayleigh breakup of an unstretched filament also differed between the two. Applying Eq. (4.3) resulted in drop diameters of 1.9 and 2.6 for simulation and experiment, respectively. Therefore, a better comparison
Comparison of drop diameter from simulation and measurements

![Comparison of drop diameter from simulation and measurements](image)

Figure 5.14: Side by side comparison between drop size results from simulation and drop size results from measurement. The volume-weighted dimensionless drop diameters and span versus rotational speed from (a) simulation with a nozzle velocity of 1.0 m/s and (b) measurements with a nozzle velocity of 1.4 m/s. The primary axis scale in (b) is doubled, however the secondary axis is the same for both plots.

results by normalizing the drop diameter curves by their respective theoretical drop diameters as illustrated in Fig. 5.15.

Figure 5.15 compares the results of drop diameter versus rotational speed from simulation to the experimental results. The simulations were based on a centrifugal only field, whereas Coriolis forces in measurements lead to filament bending, thus greatly reducing the net forces acting in the axial direction of the liquid filament. As a consequence, the filament stretching and therefore, filament diameter reduction, is more significant in the simulations. This accounts for the discrepancy in drop diameters between the two curves. The nozzle exit velocity in simulations was set to 1.0 m/s, whereas the nozzle exit velocity from the experiment was 1.4 m/s. However, as discussed in Section 4.4.5, the nozzle exit velocity does not significantly affect the resulting drop diameter.

Despite the centrifugal-field-only simulation model overestimating the filament stretching in comparison to the experimental results, the results behave qualitatively quit similarly. In particular, drop diameter in both cases reduces with respect to an increase in rotational speed, however at a decreasing rate. The resulting spans agree closely in magnitude, although measurements show no widening in the drop-size distribution as rotational speed increases.
5 Simulation of Rayleigh breakup

5.4 Summary and outlook

In chapter 5 we simulate liquid filament breakup under low Weber numbers in a centrifugal accelerational field. The simulations demonstrate that Rayleigh-Plateau instabilities form numerically without being induced, presumably by numerical error such as round-off error and truncation error. Furthermore, the instabilities grow in amplitude and lead to filament breakup.

We developed a post-processing tool, which isolates individual drops from the $\text{alpha1}$ field. Once isolated, the tool calculates particle size, position and velocity of each drop. Using these results, we were able to focus on the drop-size distribution of drops produced from Rayleigh breakup simulations. The drop-size distribution was used as a metric to verify independence of the choice of $\alpha_{th}$ and establish a mesh independence criteria based on drop-size distribution, which when applied, determines the necessary simulation mesh size.

The resulting drop-size tabulations were used to establish a relationship between drop-size and the centrifugal accelerational field determined by rotational speed. In particular, as rotational speed increase, particle size decreases. However, improvement in drop-size reduction is most significant at low rotational speeds.
Mean fluid velocity at detachment and filament breakup length were also available from simulations. The fluid velocity at breakup was used to confirm that viscous forces, surface tension and wind resistance were insignificant in comparison to centrifugal force under the simulation conditions.

Fluid velocity was useful to determine the ideal limiting behavior of the filament diameter at pinch-off. The limiting behavior gave insight as to why breakup length increases, but at a decreasing rate with respect to rotational speed. Furthermore, resulting drop-size showed a strong correlation to the limiting behavior of the filament diameter at pinch-off.

The simulation drop-size results were compared to measurement results. There was good qualitative agreement between the two results. In measurements filament bending led to a decrease in filament stretching in the axial direction, which was not included in the centrifugal-only simulations. This led to a discrepancy in quantitative behavior, when considering drop-size reduction as a function of rotational speed.

A logical step in future analysis is to include a more physical accelerational field in the axisymmetric simulations for liquid filament breakup. Instead of the centrifugal-only field acting in the axial direction, the accelerational field should be adjusted, since bending reduces the amount of stretching in the axial direction.
6 Conclusions

The work in this thesis is centered around the analysis and modeling of the Rayleigh breakup of liquid filaments, which jets from a rotating nozzle under laminar conditions. The objective of this study was to characterize the liquid filament as it exits the pressure driven Rotary Rayleigh Breakup Nozzle (RRBN), determine the spray drop size distribution as a function of the RRBN’s operating conditions, and develop a Computational Fluid Dynamics (CFD) model that accurately predicts the spray drop size distribution from the given operating conditions.

A method for analyzing high-speed videography of the RRBN was developed within this work, which was based on the superposition of the high-speed video frames. The method was applied to both the analysis of the liquid filament and the drop formation, which occurs downstream from the filament breakup.

The analysis of high-speed video showed that inertia dominated the arc shape of the filament under the operating conditions of the RRBN and for the given material properties of the fluid. This led to a means of accurately calculating the nozzle exit velocity without the need for tracer particles. It also led to a model based only on the Rossby characteristic number, which could be applied to a filament image to determine nozzle position, fluid velocity and acceleration in a rotating frame of reference and in an inertial frame of reference.

High-speed videography was also used to analyze the drop breakup behavior resulting from jet disintegration in a rotary system, in which a particle size analyzer (PSA) could not be used. The results showed agreement in drop size with Rayleigh breakup theory. Furthermore, results demonstrated a drop size dependence on rotational speed, but no dependence on nozzle exit velocity. Finally, based on the drop size distribution and median drop size, an optimum rotational speed of 2000 rpm to 3000 rpm was recommended.

An axisymmetric two-phase CFD model was developed to determine the drop size distribution for a given rotational speed and nozzle velocity. Although the simulations excluded the Coriolis force, the drop size results were in good agreement with experimental results. Moreover, the simulations provided additional value, since the velocity field and breakup length are available from the simulation results.
6 Conclusions

6.1 Outlook

The CFD model described in this work shows good results in comparison to the experimental data. However, further improvements are suggested below, which could lead to a CFD model that is in better quantitative agreement with experimental data. Moreover, additional work can be done to explore the response of the dispersed phase to the operating conditions of the spray nozzle.

The model for filament arc shape described in this work provides a method for calculating the acceleration acting in the direction of the filament using only the Rossby number. Therefore, the tangential acceleration, or stretching field, can be calculated as a function of arc length. This calculation can be applied to the axisymmetric CFD model, whereby the accelerational field no longer increases linearly with the distance from the center of rotation. A more accurate accelerational field would resolve two shortcomings with the present model. First, the velocity field is artificially high in the present model, since the acceleration does not reduce. Second, filament stretching is also exaggerated. As a consequence, the present model results in spray drops that are too small in diameter. Both issues would be improved by a better representation of the rotary spray nozzle. Furthermore, the improved model for the accelerational field would maintain the advantage of reduced computational costs in comparison to a 3-dimensional simulation model.

Due to high viscosity ratios between the liquid phase and the gas phase, high velocities in the gas phase are induced. The high velocities cause the local Courant number to increase, which leads to a time step reduction in an adaptive time-stepping simulation as described in 2.2.4. If the velocities are high enough it leads to unreasonably long simulation times. Resolution of this issue would lead to simulations in which the material properties of the fluid used in simulation matches those from experiments.

Simulations of emulsions, which show the response of the dispersed droplets in the continuous phase inside a spray nozzle have been detailed in the work of (Baniabdulrahman, 2015). This same approach can be applied simulating the dispersed phase within the liquid filament during Rayleigh-Plateau breakup. This would tie together the work presented here with the experimental work of (Dubey, 2013).
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Appendix
A DropSizeCalc Algorithm

Two-phase CFD simulations, in which drop breakup behavior is studied, require a method to identify and separate mesh cells according to which drop they belong. Once mesh cells have been assigned to their respective drops, all the data describing the state of a mesh cell becomes available to its respective drop. This document describes the post-processing tool, dropSizeCalc, which was written using the OpenFOAM C++ platform in order to perform these prescribed calculations.

OpenFOAM simulations using a two-phase solver, such as interFoam, generate the alpha1 at each write time along with other files that describe simulation domain, mesh cell attributes such as position, dimensions and state variables of the simulation. The OpenFOAM platform provides classes and routines, which readily give access to this information.

The dropSizeCalc tool uses the alpha1 file along with mesh information to identify mesh cells based on phase fraction and to assign the mesh cells to their corresponding drops. Following this, the tool utilizes mesh information and state variables describing each mesh cell to determine the characteristics of its respective drop, such as drop volume, mean velocity and drop centroid.

A.1 Partitioning of alpha1 file

For each time directory, the alpha1 file contains the phase fraction information of the two-phase problem. A simple thresholding is applied to the alpha1 file, where the threshold value \( \alpha_{th} \) determines the cut-off value for each mesh cell. Mesh cells having a phase fraction at or above \( \alpha_{th} \) are considered in the disperse phase and mesh cells having a phase fraction below \( \alpha_{th} \) are considered in the continuous phase.

Since only the disperse phase is considered for drop formation, a list is generated containing all mesh cells in the disperse phase and their adjacent neighbors, particularly only those neighbors who are in the disperse phase. The list is structured such that the mesh cell and its adjacent neighbors are grouped together as an ordered set and the list itself is also ordered. For example consider the sample mesh in Table A.1. The highlighted regions represent mesh cells that exceed the cut-off threshold. This will generate a list of droplets. The list of droplets is conclusive but redundant. In
order to determine drop size and centroid, the list must be fully reduced, so that each
droplet is contained entirely in one set and each set contains no element more than
once.

Each set is ordered numerically in ascending order and the list itself is also ordered
numerically in ascending order. Structuring the list of droplets in this manner allows
for the reduction algorithms to take advantage of structure in order to speed up
reduction time. Since sorting is relatively computationally inexpensive, the advantage
in reduction time outweighs the added time to sort.

Table A.1: Mesh cells exceeding threshold converted to a list

<table>
<thead>
<tr>
<th>List</th>
<th>Sorted</th>
</tr>
</thead>
<tbody>
<tr>
<td>{0,1,5}</td>
<td>{0,1,5}</td>
</tr>
<tr>
<td>{1,0}</td>
<td>{0,1}</td>
</tr>
<tr>
<td>{5,0,10}</td>
<td>{0,5,10}</td>
</tr>
<tr>
<td>{10,5,11}</td>
<td>{5,10,11}</td>
</tr>
<tr>
<td>{11,10}</td>
<td>{10,11}</td>
</tr>
<tr>
<td>{13,18}</td>
<td>{13,18}</td>
</tr>
<tr>
<td>{17,18}</td>
<td>{17,18}</td>
</tr>
<tr>
<td>{18,13,17,19,23}</td>
<td>{13,17,18,19,23}</td>
</tr>
<tr>
<td>{19,18}</td>
<td>{18,19}</td>
</tr>
<tr>
<td>{23,18}</td>
<td>{18,23}</td>
</tr>
</tbody>
</table>

A.1.1 Backward Simplify \textit{bwdSimplify} Algorithm

The backward simplify algorithm, \textit{bwdSimplify}, reduces the sorted list of droplets
quickly, but incompletely. The algorithm loops once through the list of droplets
assigning a set as the active set. Likewise, the algorithm selects a set for comparison
from the remaining sets that have not yet been activated. There is one argument
used by \textit{bwdSimplify}, which is used to determine the basis for set comparison. The
last element of the active set is compared to the \( p \)th element of the comparison set,
where \( p \) is the input argument. If the two elements are not equal the comparison
set is advanced until all comparisons are made. At which time the active set will
be advanced and the process repeated. However, if the two elements are equal the
sets are merged and stored at the location of the comparison set. The active set is
advanced and the comparison process continues. The algorithm is demonstrated in
Algorithm 1 and Table A.2.
A DropSizeCalc Algorithm

Algorithm 1 bwdSimplify(p)

Require: \( A = \{a_0, a_1, \cdots, a_{n-1}\}^T \) is a collection of sets, \( a_i = \{\gamma_{i,0}, \gamma_{i,1}, \cdots, \gamma_{i,m_i}\} \).

Require: The collection \( A \) and the sets \( a_i \) are sorted in numerical order.

\[
\text{for } i = 0 \text{ to } n-2 \text{ do}
\]
\[
j \leftarrow i + 1
\]
\[
\text{while } j < n \text{ and } a_i \neq \emptyset \text{ do}
\]
\[
\text{if } \gamma_{j,p} = \gamma_{i,m_i} \text{ then}
\]
\[
a_j \leftarrow a_j \cup a_i
\]
\[
a_i \leftarrow \emptyset
\]
\[
\text{end if}
\]
\[
j \leftarrow j + 1
\]
\[
\text{end while}
\]
\[
\text{end for}
\]

return \( A \)

Table A.2: Demonstration of bwdSimplify algorithm

<table>
<thead>
<tr>
<th>Start</th>
<th>bwdSimplify(1)</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>{0,1,5}</td>
<td>{0,1,5}</td>
<td>{}</td>
</tr>
<tr>
<td>{0,1}</td>
<td>{0,1}</td>
<td>{0,1}</td>
</tr>
<tr>
<td>{0,5,10}</td>
<td>{0,5,10} \rightarrow {0,1,5,10}</td>
<td>{}</td>
</tr>
<tr>
<td>{5,10,11}</td>
<td>{5,10,11} \rightarrow {0,1,5,10,11}</td>
<td>{}</td>
</tr>
<tr>
<td>{10,11}</td>
<td>{10,11}</td>
<td>{0,1,5,10,11}</td>
</tr>
<tr>
<td>{13,18}</td>
<td>{13,18}</td>
<td>{13,18}</td>
</tr>
<tr>
<td>{17,18}</td>
<td>{17,18}</td>
<td>{17,18}</td>
</tr>
<tr>
<td>{13,17,18,19,23}</td>
<td>{13,17,18,19,23}</td>
<td>{}</td>
</tr>
<tr>
<td>{18,19}</td>
<td>{18,19}</td>
<td>{18,19}</td>
</tr>
<tr>
<td>{18,23}</td>
<td>{18,23}</td>
<td>{13,17,18,19,23}</td>
</tr>
</tbody>
</table>

A.1.2 Forward Simplify fwdSimplify Algorithm

The forward simplify algorithm, fwdSimplify, is similar in operation to the bwdSimplify algorithm. However, it reduces the sorted list of droplets by comparing the first element of the active set to the \( p^{th} \) element of the comparison set. Since the list of droplets is sorted the active set is selected last to first in order to take advantage of structure. The fwdSimplify algorithm is demonstrated in Algorithm 1 and Table A.2.
**Algorithm 2** fwdSimplify(p)

**Require:** $A = \{a_0, a_1, \ldots, a_{n-1}\}$ is a collection of sets, $a_i$, where $a_i = \{\gamma_{i,0}, \gamma_{i,1}, \ldots, \gamma_{i,m_i}\}$.

**Require:** The collection $A$ and the sets $a_i$ are sorted in numerical order.

for $i = n - 1$ to 1 step -1 do
  $j \leftarrow i - 1$
  while $j \geq 0$ and $a_i \neq \emptyset$ do
    if $\gamma_{j,p} = \gamma_{i,0}$ then
      $a_j \leftarrow a_j \cup a_i$
      $a_i \leftarrow \emptyset$
    end if
    $j \leftarrow j + 1$
  end while
end for

return $A$

---

Table A.3: Demonstration of fwdSimplify algorithm (last row first)

<table>
<thead>
<tr>
<th>Start</th>
<th>fwdSimplify(0)</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>{0,1,5}</td>
<td>{0,1,5}</td>
<td>{0,1,5,10}</td>
</tr>
<tr>
<td>{0,1}</td>
<td>{0,1}→{0,1,5,10}</td>
<td>{}</td>
</tr>
<tr>
<td>{0,5,10}</td>
<td>{0,5,10}</td>
<td>{}</td>
</tr>
<tr>
<td>{5,10,11}</td>
<td>{5,10,11}</td>
<td>{5,10,11}</td>
</tr>
<tr>
<td>{10,11}</td>
<td>{10,11}</td>
<td>{10,11}</td>
</tr>
<tr>
<td>{13,18}</td>
<td>{13,18}</td>
<td>{13,17,18,19,23}</td>
</tr>
<tr>
<td>{17,18}</td>
<td>{17,18}</td>
<td>{17,18}</td>
</tr>
<tr>
<td>{13,17,18,19,23}</td>
<td>{13,17,18,19,23}</td>
<td>{}</td>
</tr>
<tr>
<td>{18,19}</td>
<td>{18,19}</td>
<td>{18,19,23}</td>
</tr>
<tr>
<td>{18,23}</td>
<td>{18,23}</td>
<td>{}</td>
</tr>
</tbody>
</table>

---

**A.1.3 Full Simplify fullSimplify Algorithm**

The fullSimplify algorithm operates in a similar manner to the other two simplification methods, however instead of comparing a single element from the active set to a single element in the comparison set, it compares all elements of each set. Thus the method is complete, but slow. In practice the other two simplification methods are employed with different inputs in order to significantly reduce the size of the droplet list. Following this speedy but incomplete reduction, the fullSimplify algorithm is employed to reduce the list completely. The algorithm is demonstrated in Algorithm 3 and Table A.4.
A.2 Calculation of drop characteristics

Once isolating the individual drops in terms of their mesh cells is complete, the calculation of volume and centroid as well as other quantities is somewhat straightforward. The OpenFOAM platform provides access to quantities such as volume, phase fraction and the centroid for each mesh cell denoted as $V_i$, $\alpha_i$ and $(x_i, y_i, z_i)$, respectively. The volume and centroid can be calculated without considering the phase fraction in the calculation or the by weighting with phase fraction values. The resulting unweighted and weighted formulas for volume of an individual drop are as
A DropSizeCalc Algorithm

follows:

\[
V_{\text{noweight}} = \sum V_i \\
V_{\text{weight}} = \sum V_i \alpha_i, \tag{A.1}
\]

where the summation is performed over all mesh cells defining the isolated drop. Likewise, the weighted and unweighted centroid of an individual drop are calculated using:

\[
(x, y, z)_{\text{noweight}} = \frac{\sum (x_i, y_i, z_i) V_i}{V_{\text{noweight}}} \\
(x, y, z)_{\text{weight}} = \frac{\sum (x_i, y_i, z_i) V_i \alpha_i}{V_{\text{weight}}}. \tag{A.2}
\]

A.2.1 Adjusting the Centroid for Axisymmetric Case

The centroid lies along the axis of symmetry in the axisymmetric case, however the resulting centroid calculated above is the centroid of the wedge. Thus the corrected centroid results from projecting the wedge centroid onto the axis of symmetry, yielding:

\[
(x, y, z) = [(x, y, z)_{\text{wedge}} \cdot e_{\text{axial}}] e_{\text{axial}}, \tag{A.3}
\]

where \( e_{\text{axial}} \) is the unit vector pointing in the axial direction, that is in the direction of the axis of symmetry.

A.2.2 Radius Calculation for 2D, 3D and Axisymmetric Cases

In order to calculate the radius of a drop, the assumption is made that the drop has a circular cross section with a volume as calculated in Eq. (A.1). The radius of each droplet can then be calculated from the drop volume and the dimension of the domain, i.e., 2-dimensional, 3-dimensional or axisymmetric. In the 2D case the drop volume is treated as a cylinder with a small thickness determined by the thickness of the simulation domain. In the 3D case the drop volume is treated as a sphere. In the axisymmetric case to drop volume is treated as a spherical wedge with the wedge angle determined by the simulation geometry.
Radius calculation for the 2D domain

The drop volume calculated in Eq. (A.1) is assumed to be contained in a cylinder, thus for a thickness $\Delta s$ the radius is calculated as follows:

$$V_{cyl} = \pi r^2 \Delta s$$

$$r = \sqrt{\frac{1}{\pi} \Delta s V_{cyl}}$$

$$r = \sqrt{k_{2D} V_{cyl}}$$

$$(A.4)$$

$$k_{2D} = \frac{1}{\pi \Delta s},$$

where $k_{2D}$ represents an intermediate simplification.

Radius calculation for the 3D domain

In the 3D calculation the droplet is assumed to be spherical, so that the radius can be calculated using

$$V_{sphere} = \frac{4}{3} \pi r^3$$

$$r = \sqrt[3]{\frac{0.75}{\pi} V_{sphere}}$$

$$r = \sqrt[3]{k_{3D} V_{sphere}}$$

$$k_{3D} = \frac{3}{4\pi}.$$  

(A.5)

Radius calculation for the axisymmetric domain

The volume calculated in Eq. (A.1) for the axisymmetric case is that of a circular wedge, where the circular wedge represents a fraction of a rotation of a semicircle determined by the wedge angle, $\theta$ in radians. Thus, the radius can be calculated using

$$V_{wedge} = \frac{\theta}{2\pi} V_{sphere} = \frac{2\theta}{3} r^3$$

$$r = \sqrt[3]{1.5 \frac{\theta}{\theta} V_{wedge}}$$

$$r = \sqrt[3]{k_{axi} V_{wedge}}$$

$$(A.6)$$

$$k_{axi} = \frac{3}{2\theta}.$$
Combined radius calculation

When combining the three cases, it results in the a radius calculation as follows

\[
    r = \begin{cases} 
        \sqrt{k_{2D}V_{cyl}}, & k_{2D} = \frac{1}{\pi \Delta s} \\
        \sqrt[3]{k_{3D}V_{sphere}}, & k_{3D} = \frac{3}{4\pi} \\
        \sqrt[3]{k_{axi}V_{wedge}}, & k_{axi} = \frac{3}{2\theta} 
    \end{cases}
\]  

(A.7)

This format allows for a cleaner approach, providing easy separation between the class function that determines the dimension of the simulation domain and the class function that calculates the radius from a known volume.
B OpenFOAM Files

MomentumSourceDict

---
FoamFile
{
    version 2.0;
    format ascii;
    class dictionary;
    location "constant";
    object momentumSourceDict;
}

UEqn
{
    variables
    {
        "rpm=1000;"
        "center=vector(-0.0315, 0, 0);" // [m] Center of rotation
        "twoPi=2*atan1*4;" // [-] 2*Pi = 6.28...
        "omega=twoPi*rpm/60;" // [rad/s] Rotational velocity
        "r=vector(pos().x, 0, 0) - center;" // [m] Calculate radius as a vector
        "accel=r^omega^omega;" // [m/s/s] Calculate centripetal accel.
    };
    expression "accel*rho";
    dimensions [1 -2 -2 0 0 0 0];
}

// ************************************************************************* //
fvSchemes

FoamFile
{
    version 2.0;
    format ascii;
    class dictionary;
    location "system";
    object fvSchemes;
}

// ************************************************************************* //

ddtSchemes
{
    default Euler;
}

gradSchemes
{
    default Gauss linear;
}

divSchemes
{
    div(rho*phi,U) Gauss limitedLinearV1;
    div(phi,alpha) Gauss vanLeer;
    div(phib,alpha) Gauss interfaceCompression;
}

laplacianSchemes
{
    default Gauss linear corrected;
}

interpolationSchemes
{
    default linear;
}

snGradSchemes
{
    default corrected;
}

fluxRequired
{
    default no;
    p_rgh;
    pcorr;
    alpha1;
}

// ************************************************************************* //
fvSolution

FoamFile
{
    version 2.0;
    format ascii;
    class dictionary;
    location "system";
    object fvSolution;
}

solvers
{
    pcorr
    {
        solver PCG;
        preconditioner DIC;
        tolerance 1e-10;
        relTol 0;
    }
    p_rgh
    {
        solver PCG;
        preconditioner DIC;
        tolerance 1e-07;
        relTol 0.05;
    }
    p_rghFinal
    {
        $p_rgh;
        tolerance 1e-07;
        relTol 0;
    }
    U
    {
        solver PBiCG;
        preconditioner DILU;
        tolerance 1e-06;
        relTol 0;
    }
}

PIMPLE
{
    momentumPredictor no;
    nCorrectors 5;
    nNonOrthogonalCorrectors 0;
    nAlphaCorr 1;
    nAlphaSubCycles 2;
    cAlpha 1;
}

// ************************************************************************* //