Abstract

Liu, Xiao, Ph.D., Purdue University, May, 2023. Filament generated droplets during drop breakup, sheet rupture, and drop impact. Major Professor: Osman A. Basaran.

Free surface flows, characterized by a deformable interface between two immiscible fluids or between a liquid and a gas, play a pivotal role in numerous natural phenomena and industrial processes. The fluid-fluid interface dynamics, governed by the complex interplay of forces such as inertia, capillary force, viscous force, and possibly elastic force, significantly influence the behavior of the fluids involved. Examples of free surface flows can be observed in everyday situations, such as droplet formation from a faucet, propagation and breaking of ocean waves, and tear films that coat the eye. An in-depth understanding of free surface flows and fluid-fluid interface dynamics has extensive implications for optimizing applications like inkjet printing, coating, spraying, and droplet formation while providing insights into the intricate behavior of natural fluid systems. Most of these applications, except for coating, involve abrupt and catastrophic topological changes of interfaces present in processes such as drop breakup, sheet rupture, and drop impact, where small droplets form from liquid sheets or filaments.

This thesis examines the dynamics of contracting liquid filaments through computational means. Previous computational simulations have assumed that initially the fluid within the filament is quiescent which, however, may not typically be the case in practical applications. Here, the effect of a realistic, non-zero initial velocity profile is considered with the hypothesis that the fact that the fluid is already in motion when it starts to contract may result in significant alterations in the filament's final fate vis-à-vis whether it breaks up into multiple small droplets or contracts into a sphere as its ends retract toward each other. The transient system of governing equations, the three-dimensional but axisymmetric (3DA) Navier-Stokes and continuity equations subjected to interfacial boundary conditions, are solved using rigorous and robust numerical algorithms in both fully 3DA and one-dimensional (1D) settings using the Galerkin finite element (GFEM) method. The simulation results are then used to construct comprehensive phase diagrams to delineate regions where filaments break up into smaller droplets from those where filaments contract to spheres without breakup.

Polymer additives are often present in practical applications involving filament contraction and breakup. The presence of polymer molecules in an otherwise Newtonian solvent gives rise to non-Newtonian rheology. In this thesis, the dynamics of filaments containing polymer

additives are analyzed using a 1D algorithm that is developed specifically for simulating viscoelastic free surface flows where the fluid's rheology is described by the oft-used Oldroyd-B model. In real-world applications, filaments produced from nozzles are expected to be prestressed at the instant when they are created and begin to contract. It is demonstrated that the retraction velocity of tips of highly viscous, prestressed filaments is significantly increased compared to filaments in which the polymer molecules are initially relaxed and Newtonian filaments. This enhancement is explained by examining the value of $\boldsymbol{\sigma} : \mathbf{D}$ ($\boldsymbol{\sigma}$: Elastic stress; $\mathbf{D}$: Rate-of-strain tensor), which can be positive or negative. This quantity is positive when the flow does work on the polymer molecules but negative when the molecules do work on the flow, i.e., when elastic recoiling or unloading takes place. In prestressed filaments, elastic unloading takes place because $\boldsymbol{\sigma} : \mathbf{D} < 0$. The elastic stresses work by pulling the fluid in axially and pushing it out radially, thereby drastically increasing the tip velocity. However, this enhancement in contraction velocity is not observed in low to intermediate viscosity prestressed filaments and whose Newtonian counterparts typically experience end-pinching. It has been established by others that end-pinching can be precluded in either filaments of intermediate viscosity or surfactant-laden filaments of low viscosity through a process known as escape from end-pinching. In this study, we demonstrate that a similar escape can also occur in prestressed viscoelastic filaments of low-to-intermediate viscosity, as revealed by one-dimensional numerical simulations and rationalized by examining when and where the elastic recoil takes place.

Beyond cylindrical filaments, thin liquid films or planar liquid sheets are also prevalent in atomization, curtain coating, and other processes where liquid sheet stability has been a subject of extensive research. Numerous authors have examined wave formation and growth leading to sheet breakup. Free liquid films or sheets without edges or caps at their two ends, which typically have two free surfaces and are surrounded by air or sometimes another liquid, can destabilize and rupture due to intermolecular van der Waals attractive forces, despite the stabilizing influence of surface tension. In this thesis, the dynamics of contracting free films or sheets with caps—two-dimensional (2D) drops—of Newtonian fluids is examined without considering van der Waals forces to confirm or refute the hypothesis that such systems can rupture due to finite-amplitude perturbations even in the absence of intermolecular forces. In particular, both two-dimensional and one-dimensional high-accuracy simulations are employed to demonstrate that unlike inviscid 2D drops that can rupture in the absence of van der Waals forces, 2D drops or sheets can escape from pinch-off due to the action of viscous forces which are present in real systems no matter how small their viscosity. The reopening of the interface and escape from pinch-off in 2D drops and sheets are explained by demonstrating the key role played by vorticity. New power-law relations or scaling laws are obtained as a function of Ohnesorge number (ratio of viscous to the square root of the product of inertial and capillary forces) for the value of the minimum film thickness for which 2D drops or sheets stop thinning and after which the interface begins to reopen. Simple yet powerful arguments are presented rationalizing these scaling laws. It is expected that these power-law relations should be of great interest to experimentalists who study such phenomena by high-speed visualization experiments.

Some of the motivation for this thesis research comes from crop spraying applications in which achieving zero or negligible drift is highly desirable. To further the understanding of fluid mechanics underpinning current and future drift reduction technologies, a simplified experimental setup is adopted to generate liquid sheets and analyze their disintegration into droplets. This new setup is both simpler and more universal than commonly utilized experimental systems that use single or multiple nozzles to generate liquid sheets and spray droplets from the disintegration of free liquid films. In the current experiments, droplets of test fluids are made to collide with or impact the top planar surface of a solid cylinder or rod. A series of MATLAB codes are developed and employed to extract droplet size distributions from images that are obtained from high-speed visualization experiments. The experimental setup and the means of data analysis are then used to probe the effect of fluid properties on the dynamics of sheet disintegration and droplet size distributions. It is hoped that future researchers will be able to combine what has been done in this thesis by simulations and in this chapter via experimental observations to develop an improved mechanistic understanding of spray formation.