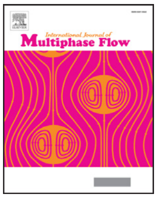
International Journal of Multiphase Flow 90 (2017) 46–56

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

journal homepage: www.elsevier.com/locate/ijmulflow



A multiphysics model for charged liquid droplet breakup in electric fields

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ARTICLE INFO

Article history:
Received 1 February 2016
Revised 8 November 2016
Accepted 22 November 2016
Available online 1 December 2016

Keywords:
Droplet breakup
Atomization
Electrohydrodynamics
Multiphysics
Two phase flow
Charge transport

ABSTRACT

A computational multiphysics model for simulating the formation and breakup of droplets from axisymmetric charged liquid jets in electric fields is developed. A fully-coupled approach is used to combine two-phase flow, electrostatics, and transport of charged species via diffusion, convection, and migration. A conservative level-set method is shown to be robust and efficient for interface tracking. Parametric simulations are performed across a range of fluid properties corresponding to commonly used liquids in inkjet printing and spray applications to examine their role in jet evolution and droplet formation. Specifically, the effects of electric potential drop, surface tension, viscosity, and mobility are investigated. Droplet velocity and size distributions are calculated, and the corresponding mean values are found to increase and decrease respectively with increasing electric field strength. The variations in droplet velocity and size are quantified, and droplet size and charge levels agree well with experimental values. Increasing mobility of charged species is found to enhance jet velocity and accelerate droplet formation by shifting charge from the liquid interior to the interface.

1. Introduction

The ability to predict and control the breakup and atomization of droplets from a liquid jet has critical implications in a wide variety of applications such as paint sprays, inkjet printing, and fuel injection (Okuda and Kelly, 1996). It is known that liquid droplets subjected to an electric field acquire a net electric charge, and that the magnitude of this charge depends on the conductivity of the liquid and the size of the droplet (Bailey, 1988; Kelly, 1978; Kelly, 1990). When the direction of the electric field is aligned with that of the liquid nozzle, the charged liquid experiences electrical forces that accelerate and deform the droplets. With sufficient electric field strength, the forces can be strong enough to significantly change the velocity of the droplets, as well as alter their size and shape owing to the distribution of forces between electrostatics, pressure, and surface tension. It is therefore theoretically possible to control the behavior of droplets by manipulating the electric field around it, and this is a key problem in the field of electrohydrodynamics (EHD). However, despite progress in understanding the underlying physical phenomena governing charged liquid droplet behavior, there is still far too much uncertainty to apply these concepts to real-world applications. This is due to the vast difference in length scales between the fundamental droplet breakup processes such as instability and polarization, and systems in which their effects are experienced. Individual droplets are typically a few tens of microns in diameter (Ganan-Calvo et al., 1997), whereas the dimensions of nozzles in electrospinning or electrospray applications may contain many individual jets spaced millimeters (Park et al., 2011) or centimeters apart (Theron et al., 2005). There are also a large number of important parameters related to operating conditions and material properties that may vary significantly depending on the application. These considerations highlight the difficulty of comprehensively modeling even a moderately complex liquid jet system.

Consequently, prior work in this area has tended to rely on experimental observation or simplified models. For example, approximate formulas for droplet properties such as size and charge have been obtained from electrostatic atomization experiments (Ganan-Calvo et al., 1997; Hines, 1966) and analytical solutions to simplified problems such as ligament-droplet systems (Toljic et al., 2010; Lefebvre, 1989). Nonetheless, the widespread applicability of liquid jets has motivated a broad body of research spanning a diverse range of disciplines. A recent review of the literature on physics of liquid jets has revealed research on phenomena such as instability, breakup, spraying, and non-Newtonian fluid behavior (Eggers and Villermaux, 2008). This research has included a significant amount of numerical modeling developments. One example is a model developed to analyze the electrohydrodynamic instability of a charged liquid jet by calculating induced forces from

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http://dx.doi.org/10.1016/j.ijmultiphaseflow.2016.11.009
0301-9322/

a magnetic field (Ruo et al., 2010). A subsequent model extended the analysis to non-Newtonian jets (Ruo et al., 2012). However, these models do not solve for the velocity or electric fields, and are thus unable to capture the evolution of the jet or formation of droplets. Similarly, a particle method has been developed to analyze breakup of suspended droplets, but and does not model how the droplets are initially formed (Nomura et al., 2001). Other prior literature on numerical modeling includes a model for two-phase charged droplets using volume-of-fluid (VOF) (Tomar et al., 2007) and level-set methods (Bjorklund, 2009). Although good agreement with theory was obtained in the validation simulations, the results are limited to cases in which steady-state forces are calculated only at the interface. Other models have been developed using a variety of methods such as a charge-conservative method (Lopez-Herrera et al., 2011), immersed interface method (Hu et al., 2015), and ghost fluid method (Paknemat et al., 2012), but simulations are limited to cases involving a single immersed droplet, and do not directly simulate the process of multiple droplet formation from a bulk liquid such as a stable jet.

A more general model has been formulated using a 3-D ghost fluid method that can calculate the electric field inside droplets (Van et al., 2010). Although a sample time-dependent simulation results of a single jet breakup is shown, no results for the charge distribution and droplet size or velocity range are provided, and the temporal evolution of droplet formation and atomization are not shown. Another numerical model has been developed to perform high-fidelity simulations of the evolution and breakup of uncharged liquid jets without electrostatic forces using a VOF method (Delteil et al., 2011). Various other interface tracking methods have been developed for multiphase flows such as the marker cell method (Sim and Shyy, 2012), but have yet to be demonstrated in coupled multiphysics contexts. To complement numerical modeling, researchers have also used experimental work to provide benchmark results for computational models. As an example, high speed photographs taken at various points in time have been used to understand the physics of liquid jets and droplets in inkjet applications, including charging, and droplet–surface interactions (Martin et al., 2008). The characteristic shape of droplets seen in these photographs are compared to simulation results in this present work.

Despite the numerous research efforts in the areas of charged liquids and multiphase flows, there remains a large gap between the current state of modeling and understanding, and what is needed to overcome the previously mentioned challenges and ultimately drive technology development in real world applications. This gap is exacerbated by the narrow range of operating conditions and fluid properties considered in much of the prior literature relative to the large differences between different studies. Although EHD problems are rich in scaling laws based on dimensional analysis (Saville, 1997; Schnitzer et al., 2013), robust models generalized for a wide range of scenarios are still needed. This article documents the development of a novel multiphysics model for a single charged liquid jet that accomplishes several objectives in resolving these limitations. First, multiphysics coupling is applied to directly model the transport of electrical charge from first principles, bypassing ad-hoc assumptions about the relationship between the charge and fluid fields. This approach allows the model to be scalable to larger systems of multiple jets. Second, the model is sufficiently flexible to allow a large number of parameters to be varied to systematically examine the effects of important fluid properties such as surface tension and viscosity, as well as the effect of varying the electric field strength. This makes the model suitable for simulating a wide range of scenarios corresponding to different applications. The model can also be used as a tool for tailoring fluids to achieve the desired droplet behavior for its application. Third, the simulation results give information about both the macroscopic behavior of droplets (size and velocity distribution), but also within the interior of the liquid to provide insight into how electric charges accelerate instability and necking in the jet that ultimately leads to droplet formation. Due to problem complexity, previous studies have been limited to examining individual aspects of charged liquid jet and droplet systems. In comparison, this model makes it feasible to perform high fidelity simulations of an entire charged jet, from initiation to instability, droplet formation, acceleration, and deposition.

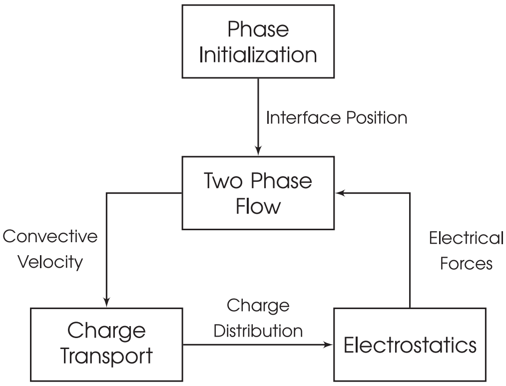

Fig. 1. Multiphysics coupling of individual physics models.

Next, the governing equations for the model are presented, including a discussion of important aspects of the numerical implementation and simulation platform. This is followed by presenting a set of representative results and a summary of the main findings. The paper concludes with a discussion of the major accomplishments and directions for future research.

2. Methodology

The multiphysics model consists of three coupled individual physics models, illustrated in Fig. 1. A two-phase flow model is used to compute the movement of the liquid jet and droplets in the presence of a gas phase by tracking the evolution of the interface between the phases. A charge transport model uses the velocity field produced by the two-phase flow model to calculate the distribution of electric charges, which convect with the liquid. This charge distribution is used to calculate the electric potential field using an electrostatics model. Finally, the potential field is used to calculate a field of electrical forces acting on the fluids in the two-phase flow model. Note that although the individual physics models are shown separately in Fig. 1 to illustrate the coupling relationships between them, the multiphysics model is treated as a fully-coupled system by the numerical solver. This means that a single system matrix is generated to solve the entire multiphysics system of equations simultaneously. This section presents the governing equations for each portion of the multiphysics model, including the choice of boundary and initial conditions. Important details of the numerical implementation are also discussed.

The governing equations for both phases of the two-phase flow model are the incompressible Navier–Stokes equations:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{F}. \tag{2}$$

The flow regime being modeled is of a laminar jet of conducting liquid surrounded by a stationary gas phase. Due to the small characteristic length scale of the problem, the flow in both phases can safely be assumed to be laminar and a turbulence model is