Experimental and Numerical Studies of Droplet and Particle Formation in Electrohydrodynamic Atomization

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ABSTRACT

Electrohydrodynamic Atomization (EHDA) is an effective method to produce micro-droplets/particles in a controllable manner. In this paper, both experimental and numerical approaches are adopted to investigate the mechanism of various EHDA spray modes under different operating conditions. Especially, Computational Fluid Dynamics based numerical simulation is applied to investigate the Taylor cone-jet formation process. The numerical simulations solve the full Navier-Stokes equations for both liquid and gas phases, tracking the liquid / gas interface using a front tracking method, and taking into account the effects of electric stress on the interface. The operating parameters, e.g. the ring electric potential and surface charging density, are varied to study their effects on the Taylor Cone jet formation and the droplet size. The results show that the size of droplets / particles fabricated by the EHDA method can be controlled by adjusting the operating parameters.

Keywords: Electrohydrodynamic Atomization (EHDA), Computational Fluid Dynamics (CFD), two-phase flow, micro-fluidics, droplet and particle.

1 INTRODUCTION

Electrohydrodynamic atomization (EHDA) has been observed and documented for over a century [1] and recently there is a renewed interested in harnessing its ability to produce monodispersed liquid droplets for the fabrication of the monodispersed polymeric particle [2]. An electrohydrodynamic atomization system consists of a nozzle, a high voltage DC power supply attached to the nozzle to raise its electric potential to kilovolt range, and an earthed ground plate placed directly beneath the nozzle to act as the counter electrode in the system. When a liquid solution is pumped through the nozzle and the solution emerges the from the nozzle, electrical stresses on the surface of the solution accelerates the liquid, and a cone like structure, termed the Taylor Cone, is formed at the tip of the nozzle. A fine liquid jet then emerges from the tip of the Taylor Cone at high speed [3]. The jet may further break into micro-droplet due to the stability.

For the fabrication of polymeric particles, a solution containing organic solvent and polymeric solute is sprayed using the electrohydrodynamic spraying system. As the jet travels away from the nozzle, the volatile solvent will evaporates from the solution surface. Depending on the stability of the jet in the electrical field surrounding the nozzle, particles will be formed if the jet breaks into droplets before the solvent has fully evaporated.

In order to control the electrohydrodynamic spraying process properly to obtain the desired droplet and particle, it is essential to understand the interaction mechanism between electrical field and liquid flow, which may result in various patterns in the Taylor Cone formation and liquid jetting. The liquid jet stability in electrical field has been previously studied theoretically [4,5] and experimentally [2,3]. Recently, work has been done to investigate the formation of the Taylor Cone and jet through Computational Fluid Dynamics Simulation [6]. The recent development of Front Tacking / Finite Volume method [7] for multiphase flow provides a robust method for such simulations and analysis.

In this paper, both experimental and numerical approaches are adopted to investigate the formation of various EHDA spray modes under different operating conditions. First, we investigated the different spray modes in the EHDA process under various operating conditions. The spray modes observed in experiments is qualitatively revealed by the numerical simulations. Then, the numerical simulation is applied to investigate the formation process of Taylor cone and jet as well as the droplet size under the same operating conditions. The simulation results indicate that the numerical method proposed here can make reasonable prediction on the electrohydrodynamic spraying process, as well as the jet diameter and droplet size.

2 EXPERIMENTAL METHOD

The present experimental system is shown in Figure 1. A 29-gauge spinal tap needle from Becton Dickinson was flatted at the tip, and connected to the liquid pump to disperse liquid. It also serves as an electrode and is connected to a Glassman high voltage DC power supply (V_n). The needle nozzle has an outer diameter of 340 micron and an inner diameter of 220 micron. The second electrode was in the form of a ring. It was made from copper tube with outside diameter of 2 mm and formed into a ring with a diameter of 40 mm. The center of the ring electrode was placed 10 mm above the tip of the nozzle. The ring electrode was connected to a separated Glassman high voltage DC power supply (V_r). This arrangement enabled the nozzle electric potential and the ring electric potential to be varied independently. An additional 29 gauge spinal tap needle was located 100 mm below the tip of the nozzle. It was connected to ground and used as the counter electrode to the nozzle and the ring electrode. Thus, the electric potential settings to the nozzle electrode and the ring electrode could be adjusted independently to fine tune the electric field in the vicinity of the nozzle tip, which may contribute to the proper control of EHDA process.

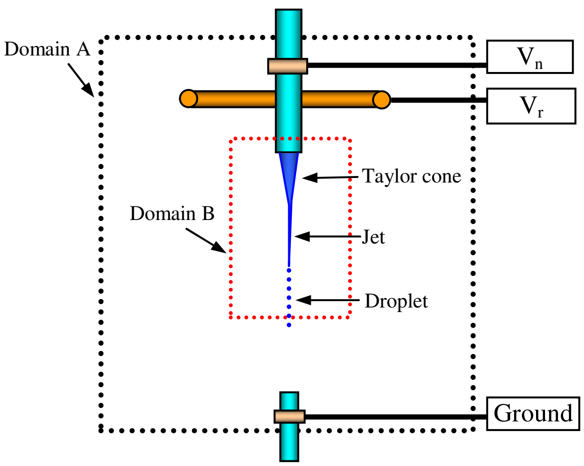

Figure 1: Schematics showing the experimental setup.

Ijsebaert [8] has previously made use of the ring electrode in his study of the production of aerosols, but the ring electric potential was set to a constant and was thought only to have the effect of focusing the spray. Here the ring acted as the means to control the electrical field strength nearby the tip of the nozzle where the Taylor Cone and jet will be formed.

3 NUMERICAL SIMULATION METHOD

3.1 Front Tracking Method

For the EHDA system, the system consist of two phase, a liquid phase which includes the Taylor Cone, jet and droplets, and a gas phase which is the ambient air. The novelty of the Front Tracking Method [7] is that the liquid-gas interface is considered to have a finite thickness of the order of the mesh size, instead of having zero thickness. In this transition zone, the physical properties of fluids change smoothly from the value on one side of the front to the value on the other side. Hence, there is no need to treat the two phases in different solution domains. There exists only one simulation domain, and a "one-fluid" formulation is adopted to describe the two-phase flow problem. The singular discontinuities on the interface such as interface tension and surface charge are distribute to the nearby control volume cell using Peskin interpolation for the solution of the governing equations.

Assuming the both liquid and gas phases to be incompressible, the conservation of mass equation can be simply written as

$$\nabla \cdot \vec{u} = 0, \tag{1}$$

where $\vec{u}$ is the velocity field.

The Navier-Stokes equation would need to be modified to take into account the additional stresses on the interface so that it and can be written as

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot \rho \vec{u}\vec{u} = -\nabla p + \nabla\left[\mu\left(\nabla \vec{u} + \nabla \vec{u}^T\right)\right] + \sigma^F \kappa \vec{n}\,\delta\left(\vec{x} - \vec{x}_f\right) + \rho \vec{g} + \vec{\sigma}^E, \tag{2}$$

where, ρ, p, μ, g and t are density, pressure, viscosity and gravitational acceleration and time, respectively. σ^F, κ and $\vec{n}$ denotes the interfacial tension coefficient, curvature and unit outward normal, respectively. $\delta(\vec{x} - \vec{x}_f)$ is the delta function where the value is one on the grid point where the interface lies and zero everywhere else. σ^E stands for the electric stress. Detail description of the numerical methods for solving the above governing equations will not be presented here, but can be found elsewhere [9].

3.2 Calculation of the electric field

The distribution of electric potential (ϕ) within the solution domain can be solved using the following equation as well as the electric field,

$$\nabla \cdot \varepsilon^* \nabla \phi = \rho^c \quad \text{and} \quad \vec{E} = -\nabla \phi. \tag{3}$$

where ε the fluid electric permittivity and ρ^c is the space change density. ρ^c is non zero due to the distribution of electrical charge on the interface (q), and ε is non constant since it will change as it crosses the moving interface from the liquid phase to gas phase.

The electrical volume stress [10] in equation (2) can be calculated as,

$$\vec{\sigma}^E = -\frac{1}{2} \vec{E} \cdot \vec{E} \nabla \varepsilon + \rho^c \vec{E} \cdot \tag{4}$$

3.3 Simulation strategy and boundary conditions

Accurate calculation of the electrical field strength near the tip of the nozzle is important to the success in modeling the EHDA process. Ideally, the calculation of the electrical field should be conducted in a large solution domain including the nozzle, ring electrode and the ground needle. However, it is not effective to calculate all governing equations for fluid flow and electric field in a domain big enough to encompass all these entities (domain A as shown in Figure 1). This is due to the fact that the electric field in the far field away from the nozzle will not be affected significantly by the presence of liquid jet and the detail flow field in the far field is not important to the EDHA process. Hence, we propose another modeling strategy. We first calculate the electric potential field only in large domain A. The nozzle electric potential and the ring electric potential are both taken into account, and the simulation geometry matches the actual production facilities. Once the electric potential field is calculated, the electric potential value on the boundary of the CFD simulation domain (Domain B as shown in Figure 1) is extracted from the calculated results, and applied to the CFD simulation as the boundary conditions for electric field calculation. The numerical tests have shown that if the electrical charge density on the Taylor Cone and jet in the CFD simulation is kept within a reasonable range, this method has negligible errors.

Figure 2 shows the small domain of an axis-symmetric cylindrical coordinate system for the detail CFD simulation of EHDA process. The length scale is normalized using the nozzle inner diameter. The bottom wall is the symmetry axis. The electric potential boundary conditions on the top, left and right wall are derived from the electric field calculation in the large domain A. The interfacial charge density is assumed to be constant for the model input, and is distributed to the control volume where the liquid gas boundary lies. Since there is no pre-simulation knowledge of the charge density on the liquid-gas interface, the charge density is estimated by trial and error and the comparison of the profiles of the Taylor Cone and jet obtained from the CFD simulations with those observed in the experiments.

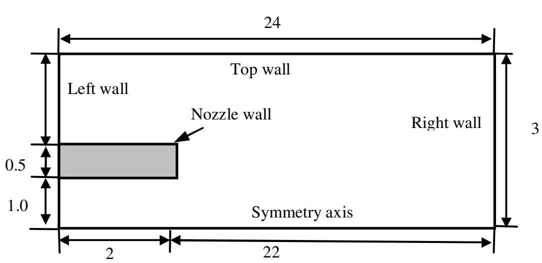

Figure 2: CFD simulation domain.

4 RESULTS AND DISCUSSION

4.1 Experimental observation and simulation on typical EDHA process

A typical case of Electrohydrodynamic Atomization of pure Dichloromethane is chose for this study. The electric potentials on the nozzle and ring electrodes are set to be 8.0 kV and 8.9 kV, respectively. The liquid flow rate is 6 ml/h. The interfacial charge density is determined to be 2.05×10^{-5} C/m^2 by fitting the simulated Taylor Cone and Jet profile to the experimental data. A Single Taylor Cone Single Jet mode was obtained from experiment and simulation result is also shown in Figure 3. The numerical simulation was able to replicate the major qualitative feature of the Taylor Cone and Jet reasonably well. The Taylor Cone is first formed near the tip of the nozzle. From the tip of the Taylor Cone, a jet is formed that has a diameter of around one order of magnitude smaller than the diameter of the nozzle. As the jet travels downward, surface instability sets in and droplets are then formed.

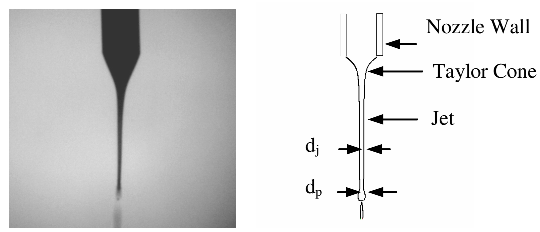

Figure 3: EHDA Taylor Cone and Jet observed in experiment (left) and predicted by simulation (right).

At the end of the jet where droplets are formed, CFD simulation has shown the formation of the unstable wave like structure before the breakup of the jet (Figure 4). This is similar to the formation of droplets in surface tension driven Rayleigh disintegration. Hohman [11] has reported the experimental observation of similar structure on the jet in EHDA. As the neck diameter decreases due to surface tension, the jet will break into droplets of similar size.

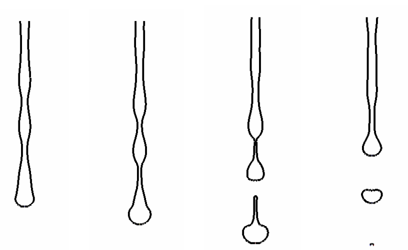

Figure 4: The evolution of unstable wave-like structure at the end of the liquid jet before pinch-off to form droplets. The interval between each frame is about 24 microseconds.

4.2 Effect of the ring electric potential on the Taylor Cone, jet and droplet formation

One of the most interesting observations made in the course of the study for droplet formation is the effect of the electric potential applied to the ring electrode on the EHDA process. In experiments, it was observed that in the Single Taylor Cone Single Jet mode, the cone angle decreases accordingly as the ring electric potential is increased.

Attempts have also been made to replicate such observation using CFD simulation. From the CFD simulation results, it is interesting to note that a constant charge density on the liquid-gas interface would not be able to give reasonable prediction on the changes of the Taylor cone angle. The simulation results would fit the experimental results best only when the interface charge density is reduced as the ring electric potential is reduced. This suggests that the ring electrode, although having no direct contact with the sprayed solution, have an effect on the liquid charging process.

As the ring electric potential changes, a change in the diameter of the jet is also observed in the CFD simulation results. As the ring electric potential is increased, there is an increase in the jet diameter as shown in Figure 5. The droplets size increases when the ring electric potential is increased.

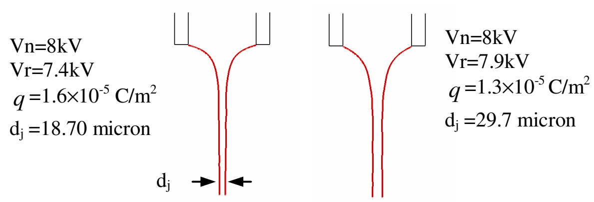

Figure 5: Changes in the jet diameter as the ring electric potential is increased. The liquid used is Dichloromethane and has a flow rate of 6ml/h. d_j represents the diameter of the jet.

5 CONCLUSION

The Electrohydrodynamic Atomization process has been studied through experiments and simulations. The ring electrode, acting as an additional electric potential field source, is found to be effective in controlling both the spray mode, and the droplet size. The Front Tracking has been shown to be a suitable approach for the simulation of the Electrohydrodynamic Atomization process, including Taylor Cone formation, jet formation and the droplet formation. Both the changes in the spray mode and the changes in droplet size can be reasonably predicted.

The simulation results also indicate that the interface charge density plays an important role in the EHDA process. It affects simulation accuracy on predicting the formation of Taylor Cone, jet and droplet. Hence, development of a first principle model to simulate the charging process on interface is highly essential in the future work.

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