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A physical insight into electrospray process in cone-jet mode: Role of operating parameters

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ABSTRACT

This article investigates the formation of cone-jet structure in an electrospray process based on a two-phase numerical simulation. The numerical approach takes account of the coupled governing equations of fluid flow and electrostatics in conjunction with the charge conservation equation and a VOF interface tracking method on the basis of a CSF model. The temporal and spatial evolutions of the cone-jet mode are examined in connection with the operating parameters, i.e. liquid flow rate and electric potential. Under the influence of these parameters, this study elucidates the physical aspects of the geometrical growth and extension along with the electric charge dispersion within the cone-jet structure. Furthermore, the flow patterns developed in the two-phase flow are studied revealing how orderly the operating parameters can alter the flow configuration. The results are compared with experimental data indicating good agreements, which, in turn, confirm the effectiveness of the simulation methodology concerning the electrospray phenomenon.

1. Introduction

Electrohydrodynamics (EHD) would be deemed as a branch of fluid mechanics that deals with the effects of electrical forces on liquids (Castellanos, 1998). In this context, electrospray can be regarded as that part of the EHD, which is especially involved with the electrical charging of liquids for the generation of liquid droplets. A typical electrospray arrangement consists of two major elements, i.e. emitter and electrode, held at different electric potentials. The main aspect of the electrospray concerns the liquid flow deformation at the emitter exit acquiring a conical structure referred to as a Taylor cone (Taylor, 1964). When the apex of the Taylor cone emits a jet of liquid leading to the breakup and generation of droplets, this is termed a cone-jet mode of the electrospray operation.

The electrospray process is used in a variety of applications, a few of which include mass spectrometry as an ionization technique (Fenn et al., 1989; Chetwani et al., 2010; Banerjee and Mazumdar, 2012), electrospinning for nanofiber production (Yu et al., 2008; Agarwal et al., 2013; Ghelich et al., 2016), surface coating based on accurate deposition (Salata, 2005; Jaworek and Sobczyk, 2008; Yoon et al., 2011; Sweet et al., 2014) and electrohydrodynamic printing (Park et al., 2007). The functioning of an electrospray process is dependent on various factors. These factors would be divided into four groups comprising operating parameters, physical properties, geometrical features and surrounding conditions. Depending on the factors, especially the operating parameters inherent in the liquid flow rate and electric potential, the electrospray process would take different modes. The diversity of the modes may encompass the states of dripping, micro dripping, spindle, multiple spindle, oscillating-jet, precession, cone-jet and multi-jet (Jaworek and Krupa, 1999a, b; Cloupeau and Prunet-Foch, 1990).

Among the electrospray modes, the cone-jet is the most important and widely used mode since it is approved as a very useful technique to generate the monodisperse sprays with droplet diameters in the range of tens of nanometers to hundreds of microns depending on the liquids used (Cloupeau and Prunet-Foch, 1989; Chen et al., 1995; Gamero-Castano, 2008). However, the formation of the cone-jet mode requires minimum magnitudes of the electric potential and the liquid flow rate. The minimum electric potential, namely the onset voltage, can be estimated as given by (Morris et al., 2013),

$$\Phi_{on} = \sqrt{\frac{\gamma d_e}{2\varepsilon_0}}\, ln\left(\frac{4L}{d_e}\right) \tag{1}$$

where d_e and L, respectively represent the emitter diameter and the emitter to ground electrode distance, γ is the surface tension coefficient and ε_0 denotes vacuum permittivity equal to $8.854 \times 10^{-12}\,CV^{-1}m^{-1}$.

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Nomenclature

C	Volume fraction;
Ca	Capillary number;
D_{32}	Sauter mean diameter (m);
d_{disk}	Disk diameter (m);
$d_{i,\ e}$	Emitter inner diameter (m);
$d_{i,\ o}$	Emitter outer diameter (m);
$\overrightarrow{E}$	Electric field vector (Vm^{-1});
$\overrightarrow{F_{ES}}$	Electric force vector (Nm^{-3});
$\overrightarrow{F_{ST}}$	Surface tension force vector (Nm^{-3});
$\overrightarrow{g}$	Gravity acceleration (ms^{-2});
$\overrightarrow{J}$	Electric charge flux (Cm^{-2}s^{-1});
K	Electrical conductivity (Sm^{-1});
l	Characteristic length (m);
L_{c-j}	Cone jet length (m);
$\overrightarrow{n}$	Normal vector;
$\hat{n}$	Unit normal vector;
P	Pressure (Pa);
Q	Flow rate (m^{3}s^{-1});
r	Radial coordinate (m);
Re	Reynolds number;
t_e	Electric relaxation time (s);
t_m	Magnetic characteristic time (s);
$\overrightarrow{u}$	Velocity vector (ms^{-1});
We	Weber number;
z	Axial coordinate (m).

Greek symbols

γ	Surface tension coefficient (Nm^{-1});
ε_0	Vacuum permittivity (CV^{-1}m^{-1});
ε_r	Relative permitivity;
κ	Curvature of interface (m);
μ	Viscosity (Pa s);
μ_m	Magnetic permeability (Hm^{-1});
ρ	Density (kgm^{-3});
ρ_e	Volume electric charge density (Cm^{-3});
ρ_S	Surface electric charge density (Cm^{-2});
Φ	Electric potential (V);
χ	Taylor number.

Subscripts

$c-j$	Cone-jet surface;
g	Gas;
j	Jet;
l	Liquid;
on	Onset;
VC	Vortex center.

In addition, the minimum liquid flow rate would be estimated using the following relation (Rosell-Llompart and De La Mora, 1994);

$$Q_{min} = \frac{\gamma\varepsilon_r\varepsilon_0}{\rho K} \quad (2)$$

where ρ, ε_r and K are the density, relative permittivity and electrical conductivity of liquid, respectively.

The research work on electrospray can be divided into experimental and theoretical studies. The experimental work of Zeleny (1914, 1917) would be acknowledged as the first systematic study on the electrospray whereon the following research studies to-date are based and evolved (Taylor, 1969; De La Mora and Loscertales, 1994; Gañán-Calvo et al., 1997; López-Herrera et al., 2004; Yu et al., 2016). In contrast, the theoretical study of Taylor (1964) can be distinguished as a leading methodical attempt that founded a robust basis for the subsequent analytical and numerical investigations until present.

Although the succeeding theoretical efforts in the electrospray initially focused on analytical methods, particularly oriented towards the instability of liquid jets (Chaudhary and Redekopp, 1980; Setiawan and Heister, 1997; Cherney, 1999; Hartman et al., 2000), this was the numerical simulation which has drawn the attention of research studies during the recent decades mainly owing to the tremendous advancements achieved in computing facilities. Nevertheless, it seems that the first numerical simulations on electrically charged liquids can be tracked back to three decades ago with a main focus on the formation of a stable liquid meniscus from which no jet was emerged. In fact, this viewpoint would be thought as a zero flow rate limit for the cone-jet mode that does not encounter the singularity at the cone apex due to the liquid jet emanation. In this connection, Joffre et al. (1982) initiated an axisymmetric equilibrium approach based on a balance among the forces arising from the surface tension, hydrostatic pressure and electric field, which could determine the liquid shape profile. They further extended the model to include the corona discharge from the meniscus surface inserting the space charge effects in the meniscus formation process (Joffre and Cloupeau, 1986). Following on from these works, Pantano et al. (1994) employed the same electrohydrostatic equilibrium strategy by taking account of a small perturbation analysis to overcome the mathematical singularity in the liquid meniscus profile with a pointed apex. This also led to a profounder study on the electrospray physics by Gañán-Calvo (1997) who described the transition between Taylor cone and jet regions proposing asymptotic universal scaling laws for both the jet size and the issued electric currents.

The first simulations of electrically charged jets were inspired by numerical models on uncharged liquid jets (Jeong and Moffatt, 1992; Eggers and Dupont, 1994; Brenner et al., 1997). Hartman et al. (1999b) developed a physical model to simulate the electrospray cone-jet mode based on a steady state one-dimensional axial momentum equation. This equation was established over a balance among the hydrodynamic potential and kinetic sources of energy, tangential electric stress and the dissipation viscous stress, which could ultimately determine the cone-jet shape. Although they also proposed another model using a Lagrangian approach to predict drop dynamics (Hartman et al., 1999a), the model was not an extension of their cone-jet model and solely relied on the experimental data as the input information.

Yan et al. (2003) simulated the formation of a liquid meniscus and the arising liquid jet due to an electric field in the cone-jet mode. This model would be considered as an extension of the work of Hartman et al. (1999b) to an axisymmetric two-dimensional model based on employing the Navier–Stokes equations and the Gauss law (except for the liquid-gas interface). The interface was dealt with by a current balance to accommodate the jump in the normal electric field.

Lastow and Balachandran (2006) employed the commercial code CFX to numerically model the cone-jet mode using the Navier–Stokes equations in conjunction with the Laplace equation. The simulation did not include the parts of current and conductivity in the governing equations implying the insert of a dielectric body in an electric field with no charge flow.

The aforementioned models did not comprise the liquid jet breakup into drops and, thus, appeared to require subsequent extensions with a particular focus on intricacies of the liquid free surface. These goals were pursued by taking account of various numerical schemes developed for the multiphase flows to scrutinize the moving interfaces between the different fluid phases (Puckett et al., 1997; Tryggvason et al., 2001). In this respect, Lim et al. (2011) simulated the cone-jet mode involved with the jet breakup and drop formation based on a two