Computational Eletrohydrodynamics

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1 Conducting drop in electric field

Figure 1 shows the configuration for an axisymmetric conductive drop attached to a conductive surface and subject to a uniform background electric field. The problem is motivated by the phenomena characteristic of electrospinning of nanofibers and other topics. The interplay between viscous, capillary, and electric forces create various evolutions of the drop, such as steady shape, jetting, and dripping off, dependent on initial contact angle α and other parameters. The flow inside the drop is governed by Navier-Stokes equations while the outside space is governed by Laplace equation for the electric potential. The dynamic boundary condition on the free surface reads

$$T_\tau = 0,$$
$$T_n = \kappa + \frac{B_{0E}}{8\pi}(\frac{\partial \phi}{\partial n})^2,$$

where T_τ and T_n stand for tangent and normal traction, κ denotes curvature, and B_{0E} is the electric Bond number, defined as

$$B_{0E} = \frac{a_0 E_\infty^2}{\gamma},$$

where γ represents the surface tension coefficient and a_0 is the radius of an equivalent sphere which has the same volume as the drop. Tentatively, it is assumed the contact angle α remains constant.

A developed finite element method will be used to solve the flow inside the drop and the electric field is to be solved by a boundary element method. The free surface is tracked through the kinematic boundary condition by a Direct Boundary Tracking method.

2 Micro Encapsulation

2.1 Introduction

Production of nano and micro size drops or particles encapsulated by a different material has been of great interest due to its many industrial applications such as food additives, targeted drug delivery, special material processing to isolate an unstable component from an aggressive environment, to avoid decomposition of a labile compound under certain atmosphere, to deliver a given substance to a particular receptor, etc. In some treatments of lung diseases medicines are better to be directly inhaled into lung tissues, and only those in nano and micro sizes can well

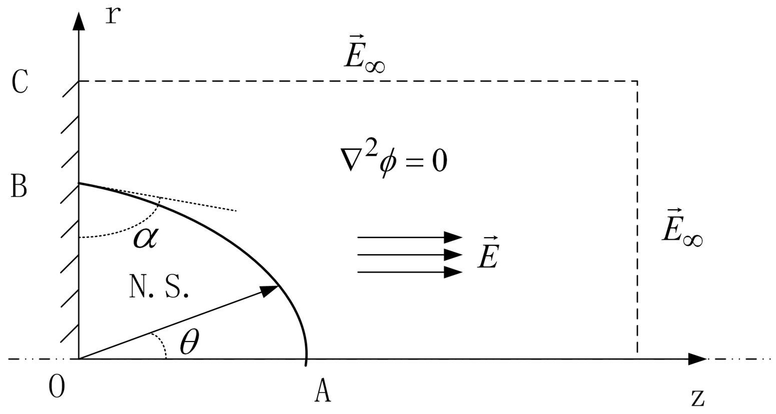

Figure 1: Conducting drop in electric field

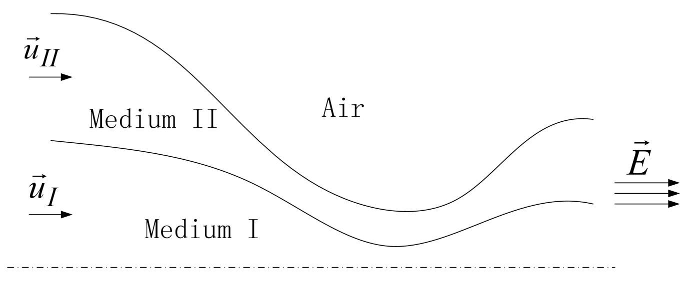

Figure 2: Configuration for Micro Encapsulation

attach to or penetrate into tissues to fulfil the task. A variety of techniques of producing micro size encapsulated drops and particles are available, such as a technique described in [8] where a liquid jet is placed underneath the surface of another liquid. Although each of these methods is able to produce encapsulated particles with well-defined size range, good control over thickness of coating, or a specific size of coated particles, they are unable to accomplish all three of the desired parameters. Moreover, droplets of nano size are difficult to be achieved employing these techniques and dispersion of size in this case is quite large. In this project, a technique to achieve micro/nano encapsulation via coaxial electrified liquid jets is investigated numerically. In brief, we will use electro-hydrodynamic forces to generate coaxial jets of immiscible liquids with diameters in the nanometer range. It is experimentally observed that an applied electric field is credited for generating much smaller droplets by several orders. The spray generated from the varicose breakup of the jets consists of mono disperse compound droplets, which can reach sizes well below the micrometer range. The experimental aspect of this method appeared first in Loscertales *et al.* [10] where good improvement compared with previous methods was demonstrated. However, the method still suffers from stability control over electrified compound jets, a judicious way of choosing appropriate liquid flow rate and applied voltage is still absent, the complex electro-fluid-mechanical scenario is merely poorly understood, and size dispersion of droplets of about 100 nm in diameter is still beyond tolerance.[10] The proposed study will lead to better fundamental understanding and practical improvement of the process.

The behavior of electrified fluid drops/jets has attracted the attention of scientists for generations. In a theoretical analysis, Rayleigh [17] calculated the characteristic frequencies for small-amplitude oscillations of a charged conducting drop in an insulating medium and established the amount of charge necessary to induce disruption of the drop surface. Without an externally applied electric field, the experimentally observable steady equilibrium shape of charged drop is always spherical. Steady shape deformations of a fluid drop can usually be observed in an external electric field, where the electric stress at the fluid interface tends to elongate the drop in the direction of the electric field, as described in the well established electrohydrostatics (see for example, Miksis [14]). Most of the electrostatic studies adopted either insulating dielectric model with no free charges present at the fluid interface or perfectly conducting model for liquid inside while the surrounding fluid is insulating. For a drop with zero net electric charge, the electrohydrostatics predicts that the drop surface is always deformed into a prolate spheroid in a uniform external electric field.

To explain the experimentally observed oblate spheroid, Taylor [19] proposed the theory of electrohydrodynamics (EHD) based on the leaky dielectric model, along with a linear asymptotic analysis. In a review by Melcher and Taylor [12] the Taylor-Melcher leaky dielectric model finally settled. The leaky dielectric model yielded results in qualitative agreement with experimental data but serious quantitative discrepancies were noticed.[20]. Higher-order correction was introduced later and an electrokinetic model (for very low scale) was used to replace leaky dielectric model, but neither could resolve discrepancies. Vizika and Saville [21] carried out a further experimental investigation and their results appeared to agree better with the model. The original Taylor-Melcher leaky dielectric model involves approximation at several levels but still finds support in most of experimental studies to date.

In order to take into account the nonlinearities arising from significant deformation of drop interface, Feng and Scott [6] performed an extensive computational analysis with Galerkin finite element method. The computed relation between the drop deformation parameter and the square of the dimensionless electric field strength was found to be typically nonlinear, whereas linearized theory merely provides an approximation for drops with vanishingly small asphericity at relatively low field strength. Notz and Basaran [15] also used Galerkin finite element method and carried out an investigation on pendant drops in an electric field based on an inviscid and perfectly conducting liquid model. The results confirmed that as the strength of the applied field increases, the mode of drop formation changes from simple dripping to jetting, to so-called microdripping, which were observed experimentally. Feng [3] included flow-induced charge convection effects on the electrohydrodynamic behavior of electrified drops and concluded that charge effect reduces the intensity of eletcrohydrodynamic flow and as a consequence enhances prolate drop deformation, which is in an agreement with experimental observations.

Extensive studies have also been conducted on the formation of Taylor cone which was first analyzed by Taylor [19]. Taylor showed that as the strength of the external electric potential is increased above a critical value, jetting initiates from the tip of a conducting drop. At the critical potential, the drop assumes a cone shape with a semi-angle of 49.3^o. Further studies on Taylor cone can be found in literature, for example [9].

Although the first research on electrified drops/jets appeared more than one century ago, relatively intensified research merely started from 1960s after Taylor-Melcher leaky dielectric model was introduced. Due to the interdisciplinary nature of electrohydrodynamics, the literature on this subject is yet very limited. Castellanos' four chapters [1] on electrohydrodynamics is thus far one of the best available introductory material directly on the subject. Several other helpful books [13, 16, 11] are also available. Feng published a sequence of papers [6, 7, 3, 4, 5, 2] on the subject of electrified drops and jets. The review papers by Melcher and Taylor [12] and Saville [18] are among the most relevant to the subject.

The main goal of this work is to improve the recently devised encapsulation process[10] by providing a fundamental understanding of various phenomena involved and to explore the application of the process to a problem of great interest, namely drug encapsulation. This goal could be accomplished by conducting well-coordinated concurrent experimental and computational studies. More specifically, the computational work will shed light on the mechanisms of Taylor cone formation and the breakup of the ensuing liquid jet. The role played by electric forces on the great reduction of sizes of drops will be investigated quantitatively. The computational modelling must overcome several challenges for accurate description of the two-fluid, compound flow under the influence of an external electric field and to capture the evolution of the liquid free surface. A main difficulty in the modelling is the large variation in length scales, from the needle assembly to the liquid jet, by orders of magnitude. This requires different treatments of the flow in these two regions and application of an appropriate matching between them. The computational modelling will greatly benefit from the experimental study for validation purposes and will provide feed back to experiments by reducing the parameter space.

2.2 Formulation

In Figure 2 we have three layers of media, liquid I, liquid II, and air, from the axis to the outside. The liquid I is modelled as a leaky dielectric material with constant electric permittivity ϵ^1, and similarly to liquid II with ϵ^2. The air is considered as a vacuum, that is, material with ϵ_0. Further, we assume there is no net charge. Electric effects of a leaky dielectric material come from two different mechanisms, conduction and polarization. A conductive material is a special case of leaky dielectric material with no polarization; while a perfect dielectric material has no mobile charges, consequently no accumulated charges on surfaces or boundaries of the material. Once the permittivity of a material is specified, polarization has been taken care of.

For materials with constant permittivity and zero net volume charge, the equation governing electrostatics is

$$\partial_i \partial_i \phi = 0, \tag{1}$$

where ∂_i is a shorthand for $\frac{\partial}{\partial x_i}$ and $E_i = -\partial_i \phi$. The corresponding boundary conditions for equation (1) are the continuity of tangent component of electric field and jump condition of electric displacement ϵE_i, and they are equivalent to

$$\|\phi\| = 0, \tag{2}$$

$$\|\epsilon \partial_i \phi\| n_i = q, \tag{3}$$

where q stands for surface (boundary) charge density and $\|\cdot\|$ stands for the jump of some quantity in a outside-inside convention. Equations (1)-(3) should be applied to all three materials.

Liquid I and II satisfy continuity equation

$$\partial_i u_i = 0 \tag{4}$$

For momentum equation we first derive the general form then reduce it to the form for materials with constant permittivity and zero net charge. The body force consists of the contribution due to free charges and polarization

$$\rho^e E_i + (\epsilon - \epsilon_0) E_j \ \partial_i E_j = \partial_j T^e_{ij},$$

where T^e_{ij} denotes Maxwell stress tensor, which can be derived to show

$$T^e_{ij} = \epsilon E_i E_j - \frac{1}{2} \delta_{ij} \epsilon_0 E_k E_k \tag{5}$$

Navier-Stokes equations in an electric field read

$$\rho[\partial_t u_i + \partial_j (u_j u_i)] = \partial_j T^e_{ij} + \partial_j T_{ij} + \rho f_i, \tag{6}$$

where $T_{ij} = -p\delta_{ij} + \mu(\partial_j u_i + \partial_i u_j)$. Under assumptions of material with constant permittivity and zero net charge, equation (6) simply reduces to regular Navier-Stokes equation for liquid I and liquid II

$$\partial_t u_i + \partial_j (u_j u_i) = -\partial_i p + \frac{1}{Re} \partial_j \partial_j u_i + f_i \tag{7}$$

According to a combination of [9, 6, 18], boundary conditions for equation (7) look like

$$\|T_{ij} + T^e_{ij}\| n_j n_i = \kappa, \tag{8}$$

$$\|T_{ij}\| n_j \tau_i = q E_i \tau_i, \tag{9}$$

where κ stands for principal mean curvature and τ_i is the surface tangent.

Equations (1)-(3), (4), and (7)-(9) require charge density on interfaces to make the system closed. According to [18] the following equation evaluated on interface can be used to evolve surface charge density

$$\partial_t q + u_j \partial_j q - q n_i n_j \partial_j u_i = \| - \sigma E_i \| n_i, \tag{10}$$

where σ denotes conductivity of materials. Equation (10) should be applied to the interface between liquid I and II, and the interface between liquid II and the air. The kinematic boundary conditions for two interfaces are simply

$$(u_i - v_i)n_i = 0, \tag{11}$$

where v_i represents velocity of moving boundaries.

References

[1] A. Castellanos. *Electrohydrodynamics.* CISM Courses and Lectures. Springer-Verlag, 1998.

[2] J. J. Feng. The stretching of an electrified non-newtonian jet: a model for electrospinning. *Phys. Fluids*, 14(11):3912–3926, 2001.

[3] J. Q. Feng. Electrohydrodynamic behaviour of a drop subjected to a steady uniform electric field at finite electric reynolds number. *Proc. R. Soc. Lond. A*, 455:2245–2269, 1999.

[4] J. Q. Feng. Electrohydrodynamic flow associated with unipolar charge curent due to corona discharge from a wire enclosed in a rectangular shield. *J. Appl. Phys.*, 86(5):2412–2418, 1999.

[5] J. Q. Feng. Application of galerkin finite-element computations in studying electrohydrodynamics. *Journal of Electrostatics*, 51:590–596, 2001.

[6] J. Q. Feng and T. C. Scott. A computational analysis of electrohydrodynamics of a leaky dielectric drop in an electric field. *J. Fluid Mech.*, 311:590–596, 1996.

[7] J. Q. Feng and T. C. Scott. Dielectrophoresis of a deformable fluid particle in a nonuniform electric field. *Phys. Rev. E*, 54:4438–4441, 1996.

[8] C. H. Hertz and B. Hermanrud. A liquid compound jet. *J. Fluid Mech.*, 131:271–287, 1983.

[9] F. J. Higuera. Flow rate and electric current emitted by a taylor conde. *J. Fluid Mech.*, 484:303–327, 2003.

[10] I. G. Loscertales, A. Barrero, R. Cortijo, M. Marquez, and A. M. Ganan-Calvo. Micro/nano encapsulation via electrified coaxial liquid jets. *Science*, 295:1695–1698, 2002.

[11] J. A. Masliyah. *Electrokinetic transport phenomena.* Alberta Oil Sands Technology and Research Authority, 1994.

[12] J. R. Melcher and G. I. Taylor. Electrohydrdynamics: a review of the role of interfacial shear stresses. *Annu. Rev. Fluid Mech.*, 1:111–146, 1969.

[13] James R. Melcher. *Continum Electromechanics.* MIT Press, 1981.

[14] M. J. Miksis. Shape of a drop in an electric field. *Phys. Fluids*, 24(11):1967–1972, 1981.

[15] P. K. Notz and O. A. Basaran. Dynamics of drop formation in an electric field. *Journal of Colloid and Interface Science*, 213:218–237, 1999.

[16] R. F. Probstein. *Physicochemical Hydrodynamics.* Wiley, 2nd edition, 1994.

[17] L. Rayleigh. On the equilibrium of liquid conducting masses charged with electricity. *Phil. Mag. Ser.*, 5(14):184–186, 1882.

[18] D. A. Saville. Electrohydrodynamics: the taylor-melcher leaky dielectric model. *Annu. Rev. Fluid Mech.*, 29:27–64, 1997.

[19] G. I. Taylor. Studies in electrohydrdynamics, i. the circulation produced in a drop by an electric field. *Proc. R. Soc. Lond. A*, 291:159–166, 1966.

[20] S. Torza, R. G. Cox, and S. G. Mason. Electrohydrodynamic deformation and burst of liquid drops. *Proc. R. Soc. Lond. A*, 401:67–88, 1971.

[21] O. Vizika and D. A. Saville. The electrohydrodynamic deformation of drops suspended in liquids in steady and oscillatory electric fields. *J. Fluid Mech.*, 239:1–21, 1992.