

Numerical Simulation of Deformation / Motion of a Drop Suspended In Viscous Liquids Under Influence of Steady Electric Fields

Jinsong Hua^{1*}, Liang Kuang Lim², and Chi-Hwa Wang²

¹ Institute of High Performance Computing, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632

² Department of Chemical and Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore, 117576, Singapore.

Keyword: Electrohydrodynamics; Computational fluid dynamics; Front tracking / finite volume method; Droplet deformation.

Abstract

The deformation / motion of a droplet suspended in a viscous liquid under the influence of an applied external electrical field are investigated through numerical simulations. The two-phase flow field of the drop suspension system is simulated using a front tracking / finite volume method for solving the full Navier-Stokes equations. Three different electric field models are applied in order to take into account the effects of the electric field, electric charge, and electrical properties of liquids. Drops with no net charge but finite electrical conductivity are simulated using a leaky dielectric model. Perfect dielectric model is used for the drops of electrically isolating fluid. To take into account the presence of a net charge on drop surface, we proposed a simplified constant surface charge model. In addition, the simulation code using the leaky dielectric model and perfect dielectric model is validated systematically against the results of theoretical analysis, the available experimental data, and the simulations by other researchers. It shows that the proposed numerical method (front tracking / finite volume method coupled with various electric field models) can make reasonable prediction on droplet deformation / motion under externally applied electrical field. Under different combinations of liquid properties, the droplets may deform into either prolate or oblate shape, and induce different inner and outer circulating flow patterns. When a net charge presents on the droplet surface and an electrical field is applied, both droplet deformation and motion can be reasonably predicted by the constant charge model. The simulation results demonstrate that the current numerical method may provide an effective approach to quantitatively analyze the complex electrohydrodynamic problems.

Introduction

Under the influence of an externally applied electric field, a drop suspended in a viscous liquid may experience complex behaviors¹⁻⁵ (e.g. deformation, motion, electrorotation, and burst) depending upon the electric field strengths and the fluid

properties (e.g. viscosity, surface tension, electrical conductivity, and permittivity). Electric field has been used extensively to produce and manipulate the liquid drops in many industries^{3, 6, 7} for atomization, inkjet printing, enhanced coalescence, emulsion breaking, etc

Mathematical Formulations

Fig. 1 illustrates a schematic 2D axisymmetric model for the problems to be analyzed in the present study. We consider an axisymmetric fluid drop of volume $\frac{4}{3}\pi R_d^3$ (effective radius R_d), density ρ_i , viscosity μ_i , permittivity ε_i , and electrical conductivity σ_i , suspended in an immiscible fluid of density ρ_o , viscosity μ_o , permittivity ε_o , and electrical conductivity σ_o . The drop suspension system consists of two immiscible liquid phases, the inner liquid phase (represented by subscript i) and the outer liquid phase (represented by subscript o). At the initial stage, the shape of the drop is assumed to be spherical, and the centre of drop is located at the middle of a parallel-plate capacitor with a separation distance of $8R_d$. After applying different electric potentials to the parallel plates (ϕ_-, ϕ_+), a steady and uniform electric field (\mathbf{E}) is generated along the axial direction (Z) of the drop. Under the influence of electric field, the drop may start to deform depending upon the operating conditions. In this study, the densities of the drop and the surrounding fluid are assumed to be identical so that the drop is under neutrally buoyant conditions and the effect of gravitational force can be neglected. The interface separating the two fluids is assumed to have a constant interfacial tension coefficient γ . To easily characterize the two-phase fluid system, we define the following fluid property ratios: $M = \rho_i / \rho_o$, $\lambda = \mu_i / \mu_o$, $Q = \varepsilon_i / \varepsilon_o$, $R = \sigma_i / \sigma_o$. Here, the density ratio and viscosity ratio are fixed at the value of one ($\lambda = 1, M = 1$) so that our attention can focus on studying the influence of electric field on the drop deformation and motion.

Governing equations for two-phase flow

The flow field simulation is formulated by solving the governing equations of mass and momentum conservation. Assuming the system to be isothermal, both phases can be considered incompressible. Hence, the mass conservation over the whole simulation domain, including both fluid phases and their interface, can be expressed as

$$\nabla \cdot \mathbf{U} = 0, \quad (1)$$

where \mathbf{U} is the fluid velocity.

In addition, the two-phase flow system studied here is coupled with the applied electric field and electric charges on the interface. To take into account the surface tension on liquid-liquid interface (\mathbf{F}_{ST}) and the electric stress (\mathbf{F}_{ES}), the Navier-Stokes equations would need to include the additional terms for these forces and can be re-written as

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot \rho \mathbf{U} \mathbf{U} = -\nabla p + \nabla \cdot [\mu (\nabla \mathbf{U} + \nabla \mathbf{U}^T)] + \mathbf{F}_{ST} + \mathbf{F}_{ES}, \quad (2)$$

where ρ is the density of the fluid, p is the pressure, μ is the viscosity of the fluid. \mathbf{F}_{ST} is the body force due to the surface tension, while \mathbf{F}_{ES} is the body force due to the electric field.

The surface tension force on the interface can be calculated as follows

$$\mathbf{F}_{ST} = \int_f \gamma \kappa_f \mathbf{n}_f \delta(\mathbf{x} - \mathbf{x}_f) dS_f, \quad (3)$$

where γ is the surface tension coefficient, κ_f is the curvature of the interface, S_f denotes the line element on the interface, and $\delta(\mathbf{x} - \mathbf{x}_f)$ is a Dirac-delta function. Subscript f refers to the front or interface. The use of a Dirac-delta function will ideally create a sharp interface in the mathematical formulation. However, to implement this in the numerical simulation, the Dirac-delta function should be expressed in a discretised form, and an approximation will be described in a latter section.

Following the previous works by Melcher and Taylor¹⁰ and Saville¹¹, the electric stress can be calculated by taking the divergence of the Maxwell stress tensor ($\boldsymbol{\tau}^M$) while assuming that the fluid is incompressible. The final results in terms of the force per unit volume is given as

$$\mathbf{F}_{ES} = \nabla \cdot \boldsymbol{\tau}^M = -\frac{1}{2} \mathbf{E} \cdot \mathbf{E} \nabla \varepsilon + q^v \mathbf{E} + \nabla \cdot \left(\frac{1}{2} \mathbf{E} \cdot \mathbf{E} \frac{\partial \varepsilon}{\partial \rho} \boldsymbol{\rho} \right), \quad (4)$$

where \mathbf{E} is electric field strength, ε is the permittivity of fluid and q^v is the volume charge density near the interface. The first term on the right-hand side of Eq. (4) is due to the polarization stress, and it acts along the normal direction of the interface as a result of the term $\nabla \varepsilon$. The second term is due to the interaction of the electric charges with the electric field, acting along the direction of the electric field. The last term results from the changes in material density, usually called electrorestriction force density. This term is neglected in this study as the fluid is assumed to be incompressible. As the electric charges are located on the interface, both the polarization electric stress and the charge-field interaction electric stress would thus be exerted on the interface. In order to calculate the electric force, the electric field strength (\mathbf{E}) and volume charge density (q^v) in Eq. (4) are estimated using the various electric field models discussed in the following section.

Governing equations for electric field

The electrohydrodynamics in two-phase flows has been reviewed by several authors including Melcher and Taylor⁸ and Saville⁹. In electrohydrodynamics, the dynamic currents are small, and hence the magnetic induction effects can be ignored. Therefore, the electric field intensity is irrotational ($\nabla \times \mathbf{E} = 0$). The Gauss law in a dielectric material with permittivity (ε) can be written in terms of the electric displacement ($\mathbf{D} = \varepsilon \mathbf{E}$) as

$$\nabla \cdot \mathbf{D} = \nabla \cdot (\varepsilon \mathbf{E}) = q^v, \quad (5)$$

where q^v is the volume density of local free charges. And the charge conservation can be expressed as follows,

$$\frac{Dq^v}{Dt} = \frac{\partial q^v}{\partial t} + \mathbf{U} \cdot \nabla q^v = -\nabla \cdot (\sigma \mathbf{E}), \quad (6)$$

where $D()/Dt$ is the material derivative, σ denotes the electrical conductivity, and \mathbf{U} represents the velocity of the fluid. In a homogeneous incompressible fluid where ε and σ are constants and $\nabla \cdot \mathbf{U} = 0$, we can make far-reaching conclusions about the distribution of the free-charge density q^v . Combining Eqs. (5) and (6), we obtain the following equation about the free charges,

$$\left[\frac{\partial}{\partial t} + \mathbf{U} \cdot \nabla \right] q^v = -\frac{\sigma}{\varepsilon} q^v \text{ and } q^v = q_o^v e^{-\sigma/\varepsilon t}. \quad (7)$$

From Eq. (7), it can be estimated that the free-charge density in the neighborhood of a given fluid particle decays from the initial charge density q_o^v with the electric relaxation time $t^E = \varepsilon/\sigma$. The viscous time scale of the fluid motion is given by $t^v = \rho L^2/\mu$, where ρ and μ are the density and viscosity of the fluid, and L is the characteristic length scale. If the fluid is electrically conductive and satisfies the relation $t^E \ll t^v$, the charge may accumulate at the interface almost instantaneously as compared to the time scale of fluid motion. On the other hand, for the weakly conducting fluid, it may behave as a perfect dielectric material when $t^E \gg t^v$. There is no free electric charge in the perfect dielectric fluid system.

1. Leaky dielectric model

When both liquids in a two-fluid system are electrically conductive and satisfy the condition $t^E \ll t^v$, the charge conservation in the bulk of an inhomogeneous continuous medium can attain steady state much faster than the time scale of the fluid motion. The charge conservation equation (Eq. (6)) can be simplified with an quasi-static assumption, and expressed by the divergence of the current density due to the electrical conduction

$$\nabla \cdot (\sigma \mathbf{E}) = 0. \quad (8)$$

In the absence of any time-varying magnetic field, the curl of the electric field is zero ($\nabla \times \mathbf{E} = 0$). The electric field can be re-expressed in terms of electric potential (ϕ) by $\mathbf{E} = -\nabla \phi$. This would then mean that the charge conservation equation in the liquid can be written as

$$\nabla \cdot (\sigma \nabla \phi) = 0. \quad (9)$$

In a two-fluid system, the electrical conductivity is constant within each fluid, and Eq. (9) for electric potential (ϕ) can be reduced to Laplace equation ($\nabla^2 \phi = 0$) in each medium. At the interface between the two fluid mediums, the continuities of electric potential and electric current are preserved

$$\|\phi\| = 0, \text{ and } \|\sigma \nabla \phi \cdot \mathbf{n}\| = 0, \quad (10)$$

where $\|\ \|\$ represents a jump across the interface and \mathbf{n} the unit normal vector at the interface. It is understood that the above boundary conditions at the interface between two fluids can be embedded in the governing equation (Eq. (9)) for electric potential with variable electric conductivity σ in the different fluid regions of the system. The electric potentials on the physical boundaries can normally be determined according to the experimental condition. With the solution of Eq. (9), the electric potential can be

obtained, and then the electric field strength is calculated by $\mathbf{E} = -\nabla\phi$. Based on Eq. (5), we can obtain the distribution of volume charge density,

$$q^v = \nabla \cdot (\varepsilon \mathbf{E}). \quad (11)$$

With the calculated distributions of electric charge density and electric field strength, the electric stress within the liquid bulk in the vicinity of interface can then be determined through Eq. (4) for incompressible fluid by

$$\mathbf{F}_{ES} = \nabla \cdot \boldsymbol{\tau}^M = -\frac{1}{2} \mathbf{E} \cdot \mathbf{E} \nabla \varepsilon + q^v \mathbf{E}. \quad (12)$$

It can be clearly seen from Eqs. (11) and (12) that both the polarity and the magnitude of the electric charge density are dependent on the change of permittivity and electric field along the span of the interface. For the case of a spherical or near spherical droplet, there is no net free electric charges on the drop due to the fact that the positive charge density on one side of the drop will be balanced out by the negative charge density on the opposite side of the drop.

2. Perfect dielectric model

When both liquids in a two-fluid system have low electrical conductivities and satisfy the condition $t^E \gg t^v$, they can be considered as dielectric materials. An externally applied electric field polarizes the molecules of the dielectric material. The formed molecular dipoles will also modify the electric field, which again change the polarization field. The results of this infinite regress can be obtained directly by solving for the electric displacement from the free-charge configuration using Eq. (5). As a perfect dielectric medium has inhomogeneous isotropic polarizability and no free charge is presenting in the medium ($q^v = 0$), the governing equation for the electric field can be written as

$$\nabla \cdot (\varepsilon \mathbf{E}) = 0. \quad (13)$$

In the absence of any time-varying magnetic field, the curl of the electric field is zero ($\nabla \times \mathbf{E} = 0$). The electric field can be expressed as the gradient of electric potential, $\mathbf{E} = -\nabla\phi$. Hence, equation (13) can be re-written in terms of electric potential ϕ as

$$\nabla \cdot (\varepsilon \nabla \phi) = 0. \quad (14)$$

In the current study, we are interested in the situation where there are two dielectric fluids in the system and they are separated by a sharp interface. Within each fluid, the permittivity is constant, and the governing equation for electric potential (Eq. (14)) is reduced to a Laplace equation ($\nabla^2\phi = 0$). Since there is no free charge at the interface between the two fluids with different permittivities, the conditions of continuity of the normal component of electric displacement across the interface and the continuity of electric potential are applicable,

$$\|\phi\| = 0, \text{ and } \|\varepsilon \nabla \phi \cdot \mathbf{n}\| = 0. \quad (15)$$

In fact, the above boundary conditions at the interface between two fluids can be embedded in the governing equation (Eq. (14)) for electric potential with variable permittivity ε in the different fluid regions of the system. The electric potentials on the physical boundaries normally can be determined by the test conditions of the applied electric field.

In this case, the electric field can be determined by the calculated electric potential distribution using the relation $\mathbf{E} = -\nabla\phi$. Therefore, with the conditions of no existence of free charge ($q^v = 0$) and incompressible fluid, the electric stress on the interface between two dielectric fluid mediums can be determined from Eq. (4) as

$$\mathbf{F}_{ES} = -\frac{1}{2}\mathbf{E} \cdot \nabla \varepsilon \quad (16)$$

The direction of the electric force for a perfect dielectric drop is in the normal direction of the interface, since this direction is determined by the gradient of the electrical permittivity $\nabla\varepsilon$, pointing from the medium with high permittivity to the one with low permittivity. Furthermore, the electric stress acts only on the interface since the electrical permittivity gradient exists only across the interface.

Results and Discussion

Leaky dielectric drop

To examine whether the numerical method proposed in the present study (front tracking / finite volume method coupled with various electric field models for different fluid systems) are able to produce accurate prediction on the droplet deformation under influence of external electric field, numerical simulations are compared with the available experimental results under the same operation conditions. The experimental data by Torza et al.¹ are chosen as the basic case for the validation study. The fluid inside the drop is silicon oil and the outside fluid is oxidized castor oil. Since the fluids used in the experiment are conductive, the leaky dielectric model is used to simulate the electrical effect. Based on the fluid properties (Class C, system 16) provided in Torza et al.¹, we can obtain the following dimensionless number to characterize the problem: $Oh = 144.3$, $R < 0.033$, $Q = 0.44$, $\varepsilon_o / \varepsilon_a = 6.3$ and Ca_E is varied at 0.137, 0.380 and 0.745 respectively. Here, ε_a stands for the permittivity of vacuum/air, having a value of 8.854×10^{-12} F/m. With the initial assumption of spherical drop suspending in the stationary liquid, transient simulation is performed until a steady drop shape is obtained.

To characterize the droplet deformation, the drop deformation factor D is calculated using the following definition,

$$D = \frac{L - B}{L + B} \quad (17)$$

where L is the end-to-end length of the droplet measured along the axis of symmetry and B is the maximum breadth in the traverse direction. A positive D represents a deformation of the droplet that has an increased length in the axial (axis-symmetric) direction (prolate), while a negative D represents a deformation of the droplet that has an increased length in the radial direction (oblate).

Fig. 2 shows the comparison of droplet deformation between the experimental observations (top) and the simulation results (bottom). The drop deforms into an oblate shape. The deformation increases when the electric field strength becomes stronger. The measured drop deformations in the experiment are $D = -0.020$ for $Ca_E = 0.137$, $D = -0.062$ for $Ca_E = 0.380$ and $D = -0.139$ for $Ca_E = 0.745$. The simulation results on the drop deformation are $D = -0.020$, $D = -0.058$ and $D = -0.133$ for conditions of

respective electric strengths. The comparison indicates that the deformation factors predicted by the numerical simulations agree well with experimental data.

The early work of Taylor¹⁰ presented a theoretical analysis on the drop deformation under external electric field. Expressed in term of Taylor's asymptotic results, an explicit relationship between droplet deformation D and electric field strength Ca_E as well as the fluid properties such as the electrical conductivity, permittivity and viscosity, turns out to be

$$D = \frac{9}{8} \frac{f_d(R, Q, \lambda)}{(2 + R)^2} Ca_E, \quad (18)$$

where, f_d represents the discriminating function and is given by

$$f_d(Q, R, \lambda) = R^2 + 1 - 2Q + \frac{3}{5}(R - Q) \frac{(2 + 3\lambda)}{(1 + \lambda)}, \quad (19)$$

where the viscosity ratio (λ) is always set to be one in the current study. When $f_d > 0$, the drop will deform into a prolate shape, while when $f_d < 0$, the drop will deform into an oblate shape.

Based on the Taylor theory, the droplet deformations for the experimental cases by Torza et al.¹ are $D = -0.0195$ for $Ca_E = 0.137$, $D = -0.0543$ for $Ca_E = 0.380$ and $D = -0.1064$ for $Ca_E = 0.745$ as shown in Fig. 2. If we compare the theoretical predictions on the drop deformation with those obtained from experiments and simulation, it is easy to find that they all agree very well when the electric field strength is low or the drop deformation is small. However, the Taylor's theoretical prediction deviates from the results of experiments and simulation significantly when the droplet has a large deformation ($|D| > 0.05$). This is because the Taylor's theoretical analysis is based on the assumption of small drop deformation.

Due to the limited availability of experimental data on drop deformation under the influence of uniform external electric field, it is difficult to validate the current model against experimental results over a wide range of operation conditions. Fortunately, the accuracy of Taylor's theory for small drop deformation has been proven by the previous research works of Feng & Scott¹¹ and Lac & Homsy¹². Therefore, a series of simulations are conducted in this study to investigate the effects of electric field strength, electrical conductivity ratio and permittivity ratios on drop deformation. The simulation results are compared with the prediction by Taylor's theory for validation. In the following simulations, we assume that the drop fluid and the surrounding fluid have the same density ($M = 1$) and viscosity ($\lambda = 1$), and a constant Ohnsorge number $Oh = 0.289$ which is based on the fluid system with $\rho = 800 \text{ kg/m}^3$, $\mu = 0.1 \text{ Pa S}$, $R_0 = 0.005 \text{ m}$ and $\gamma = 0.03 \text{ N/m}$. These parameters are fixed in all other simulations reported in the present study unless they are explicitly specified otherwise.

Fig. 3 shows the simulation for the effect of electric field strength on the drop deformation. The electrical capillary number Ca_E is increased from 0.1 to 2.5, while other parameters are kept constant ($R = 2.5$ and $Q = 2.0$). It is clearly shown that the drop deformation increases with the increasing strength of electric field. When the drop deformation is small, the deformation almost increases linearly with the electrical capillary number, which agrees well with the prediction by Taylor's theory (Eq. 18).

Conclusions

The front tracking/finite volume method for two-phase flows, coupled with various electric models (leaky dielectric model, perfect dielectric model and constant charge model) has been utilized to simulate the deformation / motion of a drop in viscous liquid under the influence of an externally applied electrical field. To take into account the coupling of electric field and charge, drop deformation and surface tension, and flow field inside and outside drop, the full Navier-Stokes equations, including the additional source terms of electric force and surface tension on the drop surface, are solved for the flow field. Subsequently the front tracking method is used to the tracking the position of drop interface while deformation is taking place, as well as the distribution of fluid properties and electric charge distribution. The proposed numerical method has been applied to investigate the deformation / motion of a drop of various fluids under the influence of a steady electric field. The simulation predicted the drop deformation under the variations in electric field strength, permittivity ratio, and electrical conductivity ratio. The fluid flow behavior inside and outside the drop is also predicted. The simulation results of both leaky dielectric model and perfect dielectric model have been validated with the theoretical results and available experimental data. We also use the current method to simulate the deformation and motion of a charged drop in an electric field. It is found that the current model can give reasonable predictions on the drop deformation / motion in an electric field under a wide range of operating conditions.

The present study of the drop deformation /motion under a steady electric field demonstrates that the current numerical method is robust and accurate. It has high potential to be further extended to study other more complex and interesting electrohydrodynamic problems.

Acknowledgement

This research was supported by Agency of Science, Technology and Research (A*STAR) and National University of Singapore (NUS) under the grant number R279-000-208-305.

References

- ¹ S. Torza, R. G. Cox and S. G. Mason, "Electrohydrodynamic deformation and burst of liquid drops," *Philos. Trans. R. Soc. London, Ser.A* **269**, 295 (1971).
- ² J. W. Ha and S. M. Yang, "Electrohydrodynamics and electrorotation of a drop with fluid less conductive than that of the ambient fluid," *Phys. Fluids* **12**, 764 (2000).
- ³ J. S. Eow and M. Ghadiri, "Motion, deformation and break-up of aqueous drops in oils under high electric field strengths," *Chem. Eng. Processing* **42**, 259 (2003).
- ⁴ O. Visika and D. A. Saville, "The electrohydrodynamic deformation of drops suspended in liquids in steady and oscillatory electric fields," *J. Fluid Mech.* **239**, 1 (1992).
- ⁵ E. Giglio, B. Gervais, J. Rangama, B. Manil, B. A. Huber, D. Duft, R. Muller, T. Leisner and C. Guet, "Shape deformation of surface-charge microdroplets," *Phys. Rev. E* **77**, 036319 (2008).

- ⁶ S. W. J. Welch and G. Biswas, "Direction simulation of film boiling including electrohydrodynamic forces," *Phys. Fluids* **19**, 012106 (2007).
- ⁷ J. W. Xie, L. K. Lim, Y. Y. Phua, J. S. Hua and C. H. Wang, "Electrohydrodynamic atomization for biodegradable polymeric particle production," *J. Colloid Interface Sci.* **302**, 103 (2006).
- ⁸ J. R. Melcher and G. I. Taylor, "Electrohydrodynamics: A review of the role of interfacial shear stresses," *Annu. Rev. Fluid Mech.* **1**, 111 (1969).
- ⁹ D. A. Saville, "Electrohydrodynamics: The Taylor-Melcher leaky dielectric model," *Annu. Rev. Fluid Mech.* **29**, 27 (1997).
- ¹⁰ G. Taylor, "Studies in electrohydrodynamics. I. The circulation produced in a drop by electrical field," *Proc. R. Soc. London A* **291**, 159 (1966).
- ¹¹ 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**, 289 (1996).
- ¹² E. Lac and G. M. Homsy, "Axisymmetric deformation and stability of viscous drop in a steady electric field," *J. Fluid Mech.* **590**, 239 (2007).

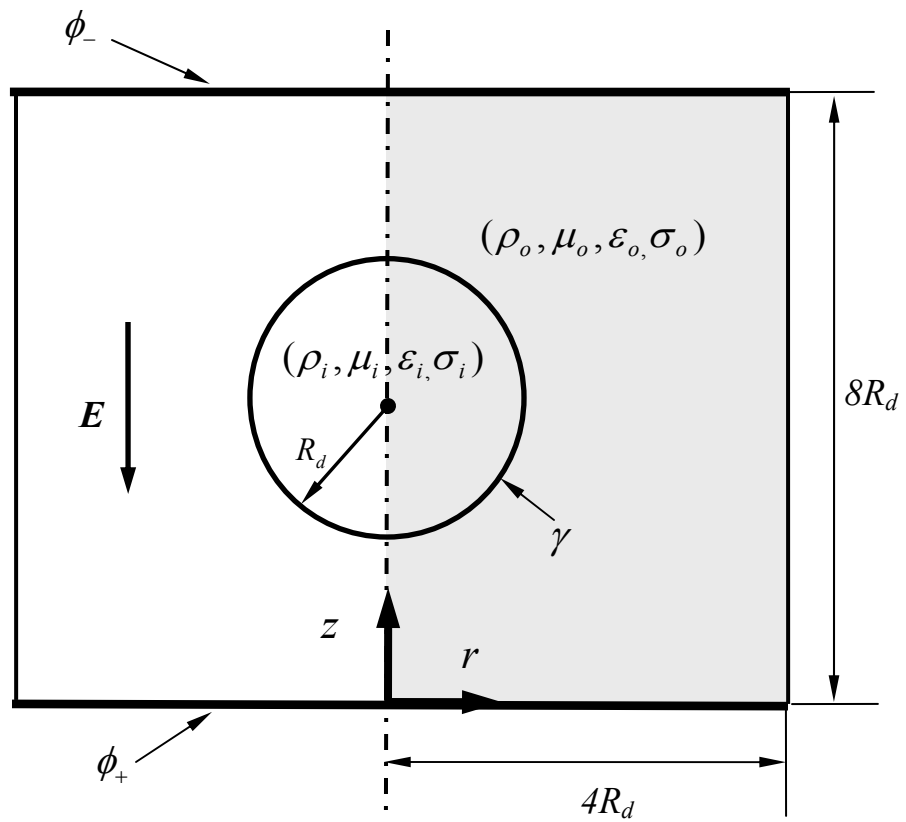


FIG. 1. Schematic of the axisymmetric model of a droplet suspending in another immiscible liquid under an external electric field.

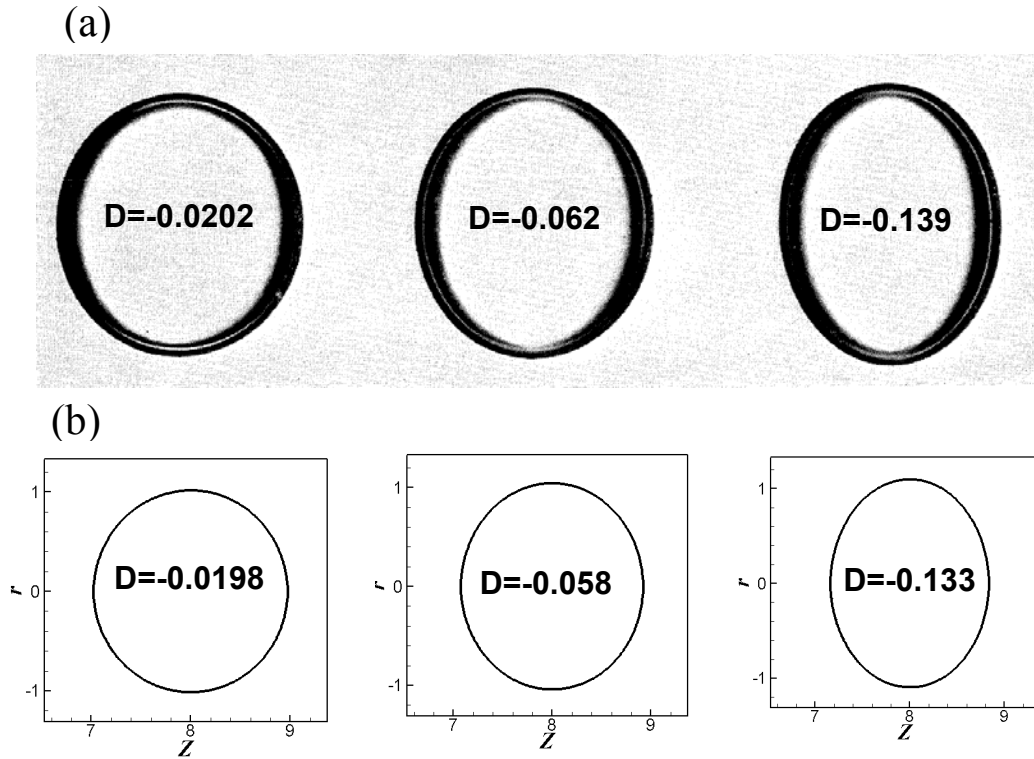


FIG. 2. Comparison of the droplet deformation (a) observed in the experiments of Torza et al. (1971) and (b) predicted in the simulation using the leaky dielectric model. D is the deformation factor. The test condition is as follows: $R < 0.033 < 0.33$, $Q = 0.44$, and Ca_E is changed from left to right at 0.136, 0.38 and 0.745, respectively. The predicted droplet deformations by Taylor's theory are $D = -0.0195$, $D = -0.0543$, and $D = -0.1064$, respectively.

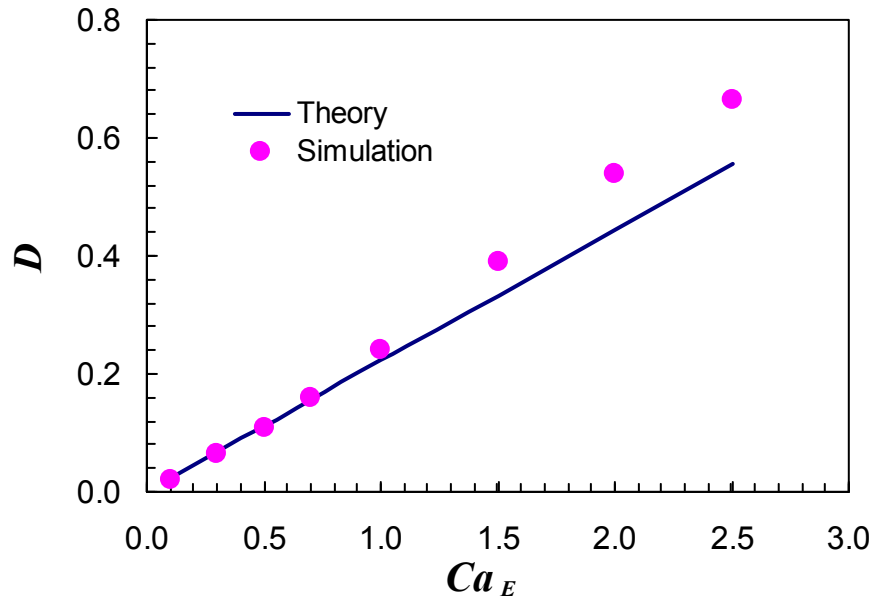


FIG. 3. Effect of electric field strength on droplet deformation as predicted by Taylor's theory and the present numerical simulation (leaky dielectric model). Other parameters are kept constant: $R = 2.5$, $Q = 2.0$.