Effect of Interfacial Charge on the Drop Deformation under the Application of Oscillatory Electric Field.

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Introduction

Study of interaction of drops and bubbles with electric field is important for understanding the physics involved in various physical phenomenas and industrial processes. Important applications arise in colloidal systems (Miller and Scriven, 1970), meteorology and cloud physics (Sartor, 1969), electrostatic spraying of liquids (Balachandran and Bailey, 1981), power engineering applications (Krasucki, 1962), nuclear physics (Bohr and Wheeler, 1939), aerosol science (Whitby and Liu, 1966), and in oil and petroleum industries. The phenomena involved in such processes fall in the ambit of multiphysics because of interaction of hydrodynamics, electrodynamics, mass transport and interfacial phenomena. The geometry can also become complex due to deformation of interfaces. The multiphysics software such as COMSOL is ideally suited to couple these physical phenomena and simulate the process.

In the present work, deformation of a spherical droplet of salt solution, suspended in viscous hydrocarbon oil, under the influence of an applied oscillating electric field, is investigated through numerical simulation. The results of simulations are verified using experiments. Due to the ions of the salts, the interface is electrically charged. Due to the

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oscillatory nature of the electric field, the interfacial charge also alternates with time. The transport of ions from the bulk of the drop to the interface is also important in deciding the charge density at the interface. In the presence of the electric field, the interface is subjected to both electrostatic and dielectrostatic Maxwell stresses. These stresses not only deform the interface, but also induce the flows in contiguous phases, which further modify the deformation of the interface. The aim of the present study is to predict this oscillatory deformation of the interface. The COMSOL Multiphysics software version 3.5a is used for the simulation.

The experimental verification is obtained by conducting experiments in a parallel electrode cell. Silicone oil of different viscosities is used as the continuous phase. A drop of aqueous NaCl solution is suspended between the electrodes. The oscillatory electric field is then applied and the drop is photographed using a high speed camera. The images of the drop are analyzed using image analysis software to determine the deformation at various locations. The size of the drop is varied in the range of 100-300 μm. The concentration of NaCl is varied in the range of 0.1 to 10 mM. The distance between two electrodes is kept at 5mm. The potential difference between the two electrodes is varied from 1 kV to 5 kV. The results of the simulation are compared with those

Problem Formulation

We consider axisymmetric cylindrical geometry as shown in the figure 1. The boundary of the drop is indicated by GEC. FD and AB represent electrodes. The boundary of the curved cylindrical surface is denoted by DB. This surface is considered as the electrically insulated boundary. The continuous phase is enclosed in the region

GFDBACEG. The domain occupied by the drop is denoted by domain-1 and that by the continuous phase by domain-2.
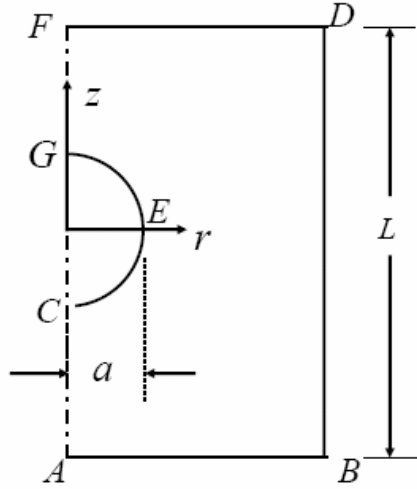
Figure 1: Two dimensional axisymmetric domains for simulation.

In domain-1 we use Poisson equation to describe the potential distribution.

$$\nabla^2 \phi_1 = -\frac{F}{\varepsilon \varepsilon_0} \sum z_i c_i \tag{1}$$

Here ϕ_1 is the electric potential inside the drop, i represents ionic species in the solution (Na^+ and Cl^-), c_i is its concentration and z_i, the valency. F is the Faraday constant, ε_0, permittivity of free space and ε is the dielectric constant of the solution.

The concentration of species i is obtained by solving the Nernst-Planck equation for that species.

$$\frac{\partial c_i}{\partial t} = \overline{\nabla} \cdot \overline{N}_i \tag{2}$$

$$\overline{N}_i = -D_i \overline{\nabla} c_i - F z_i u_i c_i \overline{\nabla} \phi_1 + c_i \overline{v}_1 \tag{3}$$

where $\overline{N}_i$ is the flux of species i, D_i is its diffusivity, and u_i the mobility. $\overline{v}_1$ is the fluid velocity. The fluid velocity is obtained by solving the equations of continuity and motion.

$$\overline{\nabla} \cdot \overline{v}_1 = 0 \tag{4}$$

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$$\rho_1 \frac{\partial \overline{v}_1}{\partial t} + \rho_1 \left(\overline{v}_1 \cdot \overline{\nabla} \right) \overline{v}_1 = \overline{\nabla} \cdot \left[p_1 \overline{\overline{I}} + \eta_1 \left(\overline{\nabla} \overline{v}_1 + \left(\overline{\nabla} \overline{v}_1 \right)^T \right) \right] + \overline{f}_{E1} + \rho_1 \overline{g} + \sigma \kappa \hat{n} \delta \qquad (5)$$

In the equation above, ρ_1 denotes the density of the fluid, η_1 represents the viscosity, p the pressure, σ the surface tension, $\hat{n}$ the unit normal to the interface, $\kappa = -\overline{\nabla} \cdot \hat{n}$ is the curvature of the fluid interface, δ is a Dirac-delta function which is concentrated at the interface. The term $\sigma \kappa \hat{n} \delta$ defines the surface tension force. $\overline{g}$ is the gravity vector. $\overline{f}_{E1}$ is the electrical force due to stress (Maxwell stress) and is given by

$$\overline{f}_{E1} = \overline{\nabla} \cdot \overline{\overline{\tau}}_{E1} - \left(\sum z_i c_i \right) \overline{\nabla} \phi_1 \qquad (6)$$

In the equation above, $\overline{\overline{\tau}}_E$ is the Maxwell stress tensor and is given by

$$\overline{\overline{\tau}}_{E1} = \varepsilon_1 \varepsilon_0 \left[\overline{\nabla} \phi_1 \overline{\nabla} \phi_1 - \frac{1}{2} \left(\overline{\nabla} \phi_1 \cdot \overline{\nabla} \phi_1 \right) \overline{\overline{I}} \right] \qquad (7)$$

Domain-2 is assumed to be electrically neutral. The electric potential is therefore governed by the Laplace equation.

$$\overline{\nabla}^2 \phi_2 = 0 \qquad (8)$$

The equations of continuity and that of motion are given by

$$\overline{\overline{\nabla}} \cdot \overline{v}_2 = 0 \qquad (9)$$

$$\rho_2 \frac{\partial \overline{v}_2}{\partial t} + \rho_2 \left(\overline{v}_2 \cdot \overline{\nabla} \right) \overline{v}_2 = \overline{\nabla} \cdot \left[p_2 \overline{\overline{I}} + \eta_2 \left(\overline{\nabla} \overline{v}_2 + \left(\overline{\nabla} \overline{v}_2 \right)^T \right) \right] + \overline{f}_{E2} + \rho_2 \overline{g} + \sigma \kappa \hat{n} \delta \qquad (10)$$

In the continuous phase, the electric force due to stress is given by

$$\overline{f}_{E2} = \overline{\nabla} \cdot \overline{\overline{\tau}}_{E2} \qquad (11)$$

$$\overline{\overline{\tau}}_{E2} = \varepsilon_2 \varepsilon_0 \left[\overline{\nabla} \phi_2 \overline{\nabla} \phi_2 - \frac{1}{2} \left(\overline{\nabla} \phi_2 \cdot \overline{\nabla} \phi_2 \right) \overline{\overline{I}} \right] \qquad (12)$$

The following are the boundary conditions:

1. On the boundary CG, we have axisymmetry with respect to potential, velocity, concentrations and pressure.

2. On the boundary FD, the potential is sinusoidal with amplitude $\phi_0 / 2$ and angular velocity ω.

$$\phi_2 = \frac{1}{2}\phi_0 \sin(\omega t) \tag{13}$$

The no-slip condition for the fluid velocity gives

$$\bar{v}_2 = 0 \tag{14}$$

3. On the boundary AB, the potential is sinusoidal with amplitude $-\phi_0/2$ and angular velocity ω.

$$\phi_2 = -\frac{1}{2}\phi_0 \sin(\omega t) \tag{15}$$

The no-slip condition for the velocity is also valid here.

$$\bar{v}_2 = 0 \tag{16}$$

4. The boundary BD is electrically insulated. Also no-slip condition for the fluid velocity is valid.

5. On the boundary CEG, velocity continuity yields

$$\bar{v}_1 = \bar{v}_2 \tag{17}$$

The stress continuity is given by

$$n\left[\eta_1\left(\overline{\nabla}\bar{v}_1 + \left(\overline{\nabla}\bar{v}_1\right)^T\right) - P_1\bar{\bar{I}} - \eta_2\left(\overline{\nabla}\bar{v}_2 + \left(\overline{\nabla}\bar{v}_2\right)^T\right) + P_2\bar{\bar{I}}\right] = 0 \tag{18}$$

The Gauss law yields

$$\hat{n} \cdot \left[\varepsilon_1\overline{\nabla}\phi_1 - \varepsilon_2\overline{\nabla}\phi_2\right] = -\frac{q}{\varepsilon_0} \tag{19}$$

Where q is the charge density at the interface.

The charge balance equation can be written as

$$\frac{\partial q}{\partial t} = \hat{n} \cdot \sum_i z_i\left(\overline{N}_i - c_i\bar{v}_1\right) - \kappa_2\overline{\nabla}\phi \tag{20}$$

where κ_2 is the conductivity of the oil.

6. The following initial conditions are used, At $t = 0$:

$$c_i = c_i^0, \quad \phi_1 = 0 \ \phi_2 = 0 \tag{21}$$

Use of Comsol Multiphysics

The present problem is formulated using combination of Chemical Engineering and Multiphysics Modules. The following application modes are used

1. **Chemical Engineering Module-Momentum Transport-Multiphase Flow-Two-Phase Flow, Laminar-Level Set, Transient Analysis.** Using this application mode, we have obtained the velocity field as well interface profile as functions of time and location. The electrical forces are incorporated in the Navier-Stokes equation as a source term.

2. **Chemical Engineering Module-Mass Transport-Nernst Planck, Transient Analysis.** Using this application mode, we have obtained the concentration fields of the ionic species as well as the charge distribution as a function of time.

3. **Multiphysics Module-Heat Transfer-Conduction and Convection- Steady State Analysis.** Using this application mode, we have obtained the potential distribution in both the domains. In domain-1 we solve the Poisson equation and in domain-2 we solve the Laplace equation.

The major difficulty in this problem is to incorporate the transient interfacial charge balance equation in the COMSOL formalism. The present COMSOL module does not allow incorporating transient boundary conditions similar to those occurring in the present problem. Our experience in solving this problem will help COMSOL community to attempt the problems of the similar nature.

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