A Convection-Conduction Model for Electrohydrodynamic Simulations

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An electrohydrodynamic model for the simulation of droplet formation, detachment and motion in an electrically driven droplet generator is introduced. The numerical approach is based on the coupled solution of the multiphase flow problem with the charge continuity equation. For the latter, a modified convection-conduction model is applied, taking into account conductive, capacitive as well as convective electrical currents in the fluid. This allows for a proper description of charge relaxation phenomena in the moving fluid. A diffuse interface model on a static grid, based on the Volume of Fluid method, is used to describe motion of the phase boundaries, providing efficient handling of topology changes. The contact line motion at the solid boundaries is furthermore taken into account using a dynamic model including pinning effects, in order to accurately describe droplet motion on solid surfaces.

Index Terms-Electrohydrodynamics, electromagnetic forces, fluid flow control, finite volume methods

I. INTRODUCTION

Dynamic droplet processes under the influence of strong electric fields play an important role in many technical applications. The perhaps best known example is electrospraying [1], [2]. Electric fields can furthermore be used for controlled droplet generation. In electrically driven drop-on-demand generators, reliable injection of liquid samples into a test chamber even under extreme atmospheric conditions is achieved by applying strong electric pulses on the liquid [3].

The dynamics of liquid droplets in such a generator defines an elecrohydrodynamically coupled and strongly nonlinear problem, which can be described accurately only by means of numerical simulation. Several aspects should be taken into account in the simulation of such processes. Firstly, the numerical scheme must be able to handle the sudden event associated with a modification of the phase boundary topology which occurs at an extremely thin liquid thread. Using an explicit interface tracking technique with sharp geometry boundaries in this case becomes numerically extremely cumbersome [4]. Secondly, liquid droplets produced by breakup or detachment may carry a net electric charge [5]. This effect is due to the finite charge relaxation time of conductive liquids. The numerical model must be able to describe such charging phenomena accurately since the behavior of liquid droplets under various experimental conditions depends substantially from their electric charge. Thirdly, the charge relaxation time, depending on the fluid conductivity, and the fluid dynamical time scales may be comparable. In this case, the electric field solution depends not only on the instantaneous droplet shape but also on the convection flow associated with droplet motion [6].

In this work, we introduce a conduction-convection model for the simulation of droplet dripping process under the influence of low frequency electric fields, involving dynamic charging effects. This model is applied in the simulation of an electrically driven droplet generator. First simulation results for acetone droplet generation show an excellent agreement with the experimental data.

II. NUMERICAL MODEL

A. Interface representation

In order to efficiently account for topology changes in the phase boundary, the interface between fluids is represented using the Volume of Fluid (VoF) method [7]. In the VoF method, the material properties in the fluid mixture are calculated using the volume fraction α of either liquid in each cell of the computational grid. The volume fraction field defines material properties of the liquid mixture by weighted averaging, e.g. $\rho = \alpha \rho_{\text{liq}} + (1 - \alpha) \rho_{\text{gas}}$. The resulting diffuse interface is passively transported at each time step by the velocity field of the fluid mixture and implicitly tracks topology changes.

B. Fluid flow problem

The fluid flows considered in this work are described by the incompressible Navier-Stokes equations,

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) - \mu \nabla \cdot (\nabla \vec{u} + \nabla \vec{u}^{\mathrm{T}}) = -\nabla p + \rho \vec{g} + \vec{f_{\mathrm{s}}} + \vec{f_{\mathrm{e}}}, \qquad (1)$$

$$\nabla \cdot \vec{u} = 0, \qquad (2)$$

where ρ is the fluid density, μ is the dynamic viscosity, \vec{u} the velocity, p the pressure. $\vec{f_e}$ and $\vec{f_s}$ are, respectively, the electric force density and the surface tension force density acting at the interface between different fluid phases.

The surface tension contributions at the contact line where the two fluid phases meet a solid wall are described in terms of an apparent contact angle, θ . The model used for describing its dynamics is based on the Kistler correlation [8]

$$\theta = f_{\rm H} \left(\frac{\mu_{\rm liq} u_{\rm cl}}{\gamma} + f_{\rm H}^{-1} \left(\theta_{\rm adv/rec} \right) \right) \,, \tag{3}$$

with
$$f_{\rm H}(x) = \arccos\left(1 - 2 \tanh\left[5.16\left(\frac{x}{1+1.31x^{0.99}}\right)^{0.706}\right]\right)$$
. (4)

In (3), γ is the surface tension and u_{cl} the signed velocity of the contact line. It is considered positive when the contact line is advancing, and negative otherwise. The two angles $\theta_{adv}/\theta_{rec}$ denote the limiting advancing or receding contact angle, respectively.

C. Electric field problem

The model is based on the solution of the charge conservation equation

$$\frac{\partial \rho_e}{\partial t} + \nabla \cdot \vec{J} = 0, \qquad (5)$$

where $\rho_{\rm e}$ is the free electric charge density in the fluids, and \vec{J} the current density. For incompressible conductive fluids, this density consists of a conduction and convection term, $\vec{J} = \rho_{\rm e}\vec{u} - \kappa\nabla\Phi$, where Φ is the electric potential and κ the electrical conductivity. The electric potential is, furthermore, related to the free charge density by Gauss' law:

$$\nabla \cdot \varepsilon \nabla \Phi = -\rho_{\rm e} \,. \tag{6}$$

Equations (5) and (6) define the electric field problem, including conductive, capacitive and convective currents in the fluids.

For the numerical solution of (5) and (6), electric properties at the diffuse interface between fluids is defined by harmonic averages of the dielectric permittivity and electric conductivity, respectively, as

$$\frac{1}{\varepsilon} = \frac{\alpha}{\varepsilon_{\text{liq}}} + \frac{1-\alpha}{\varepsilon_{\text{gas}}}, \quad \frac{1}{\kappa} = \frac{\alpha}{\kappa_{\text{liq}}} + \frac{1-\alpha}{\kappa_{\text{gas}}}.$$
 (7)

The choice of harmonic averaging, leads to faster numerical convergence of the discrete boundary value problems (5) and (6), in the case of fully charged interfaces, where the electric field is essentially normal to the phase boundary [9].

III. RESULTS

The model is illustrated through the example of an electrically driven droplet generator, shown in Fig. 1. A metallic capillary, surrounded by electrodes, slowly introduces liquid in a pressure chamber, producing a pendant droplet. As the droplet reaches a specified size, the electrode voltage is switched on, producing an electric force accelerating the droplet downwards, causing it to eventually detach. A comparison between experimental and simulated axisymmetric dynamics of the detachment process for an acetone droplet, (cf. Fig. 2), shows excellent agreement. Additional results on the detachment

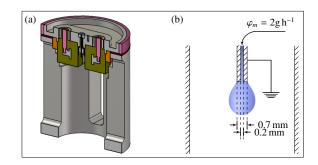


Fig. 1. (a) Model of the droplet generator including capillary, electrodes and test chamber (cf. [3]). (b) Schematic view and main parameters of the simulation model.

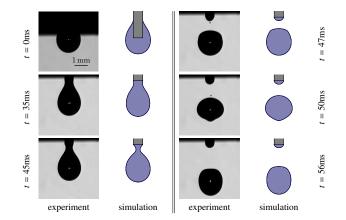


Fig. 2. Comparison between simulation and experiment for an acetone droplet shape in the generator at different time instants during the detachment process.

dynamics of test liquids with lower conductivity and effects of the applied voltage on the detachment time and oscillations of free falling droplets will be included in the full paper.

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