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Three-dimensional modeling of dynamics of liquid dielectric droplets on a wettable surface in the electric field

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Abstract. Three-dimensional non-stationary modeling of liquid dielectric droplets on a wettable surface in an electric field is performed. The distribution of the electric field is calculated by solving the equation for the electric field potential. The lattice Boltzmann method is employed to describe the hydrodynamic processes with gravitational, electrostatic, and capillary forces. A hemispherical droplet is placed on the surface of the lower electrode. Two variants of the droplet behaviour are observed. The droplet can acquire its equilibrium shape after several oscillations or elongate unlimitedly up to its destruction.

1. Introduction

It is well known that the electric field changes not only the shape of the droplet lying on a solid surface, but can lead to unlimited lengthening of the droplet up to its destruction [1,2].

In this work, three-dimensional modeling of the behavior of dielectric droplets in the electric field is carried out. Such a multiphysical process of the action of gravitation, capillary forces, and electric field is modeled by the method of lattice Boltzmann equations (LBE, LBM). A droplet in the form of a spherical segment is placed on a flat wettable surface. One of the dimensionless parameters is the Bond number $\mathrm{Bo} = \rho g R^2 / \sigma$ that determines the ratio of gravity forces and surface tension, where σ is the surface tension, and R is the characteristic size of the droplet. The second dimensionless parameter is the electric Bond number $\mathrm{Bo}_E = \varepsilon_0 (\varepsilon_{\mathrm{liq}} - 1) E^2 R / \sigma$, where $\varepsilon_{\mathrm{liq}}$ is the dielectric constant of the liquid.

2. Hydrodynamic model with electric field forces

To describe the hydrodynamics of dielectric fluid the LBE method is very appropriate. We use the D3Q19 variant of this method described in detail in works [3,4], where it was considerably improved compared to the classical LBM with phase transitions. The Helmholtz electrostatic forces

$$\mathbf{F} = -\frac{\varepsilon_0 E^2}{2} \nabla \varepsilon + \frac{\varepsilon_0}{2} \nabla \left[E^2 \rho \left(\frac{\partial \varepsilon}{\partial \rho} \right)_T \right], \tag{1}$$

acting in the bulk of the dielectric and the forces of interaction of a fluid with a wettable solid surface can be easily incorporated into the LBM. For this purpose, the Exact Difference Method is used [4]. The potential of the electric field is determined at every time step at the conventional boundary conditions at electrodes. The non-uniform distribution of the dielectric constant is also taken into account as $\varepsilon = 1 + 3\alpha\rho/(1-\alpha\rho)$ in accordance with the Clausius–Mossotti formula for non-polar dielectric. Here, α is the polarizability. Then the distribution of electric field is calculated.

The interaction forces between the node $\mathbf{x}$ belonging to fluid and five nearest nodes $(\mathbf{x}+\mathbf{e}_i)$ of solid surface are taken into account as it was done in work [5]

$$\mathbf{F}(\mathbf{x}) = B\Phi(\mathbf{x})\sum_{i=1}^{5} w(\mathbf{e}_i)\Phi_{\text{solid}}(\mathbf{x}+\mathbf{e}_i)\cdot\mathbf{e}_i \, , \tag{2}$$

where $\Phi = \sqrt{\rho/3 - P(\rho,T)}$ [3]. The van der Waals equation of state for a fluid is used in the form written in the dimensionless variables

$$\tilde{P}(\tilde{\rho},\tilde{T}) = \frac{8\tilde{\rho}\tilde{T}}{(3-\tilde{\rho})} - 3\tilde{\rho}^2 \, . \tag{3}$$

Here, B is the interaction coefficient (adhesion level). It determines the value of the contact angle (figure 1) and allows varying it in a wide range. The theoretical value of 90º at $B = 1.00$ is shown by point 2. The linear approximation of data obtained in our simulations has the form (figure 1, line 1)

$$\theta = 596.458 - 506.964 \cdot B \, . \tag{4}$$

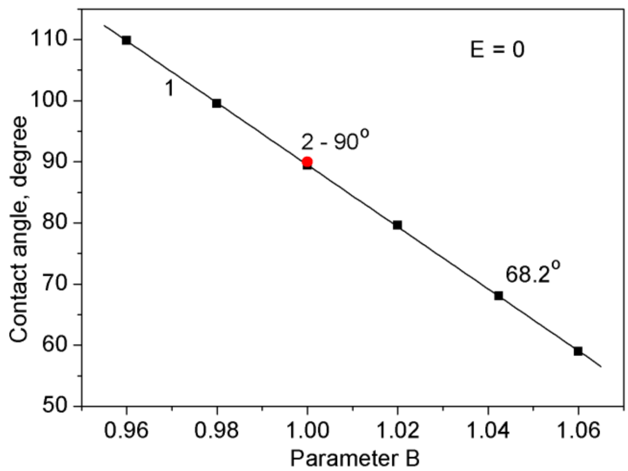

Figure 1. The values of contact angle (line 1) obtained in our simulations (■) without electric field. Point 2(●) is related to the theoretical value of 90º at $B = 1.00$.

We use two Titan-Xp multiprocessor graphics cards (GPUs) to speed up simulations. For massively parallel computing on all cores of GPUs, the CUDA technology is used for parallel programming.

3. Results of modelling

Three-dimensional modeling of the behavior of dielectric droplets in the electric field is performed. Initially, a hemispherical droplet is placed on the surface of lower electrode (figure 2a). Then constant DC voltage is applied to the interelectrode gap. There are two possible variants of evolution of a droplet shape. If the electric field strength is less than a certain critical value, the profile of droplet acquires its equilibrium shape after several oscillations. The duration of oscillations depends on the kinematic viscosity of liquid ν (the Ohnesorge number $\mathrm{Oh} = \nu\sqrt{\rho/(\sigma R_0)}$).

In another case, the droplet elongates unlimitedly (figures 2 and 3). For this simulation, the value of the electric Bond number is slightly greater than the critical one. The first stage is the establishing of approximate equilibrium for gravity, electric and surface tension forces for a given contact angle ($t \approx$ 7000 time steps, figure 3). If the electric Bond number exceeds the critical value, the droplet begins to lengthen slowly along the electric field maintaining a convex shape (the second stage, up to $t \approx 50000$, figures 2c,d and 3). The last stage is unlimited elongation of the droplet apex and its destruction. The growth of droplet apex at the last stage is a phenomenon very similar to explosive growth of perturbations on initially flat free surface described in [6]. Note that the contact line is practically motionless in our calculations (figure 2).

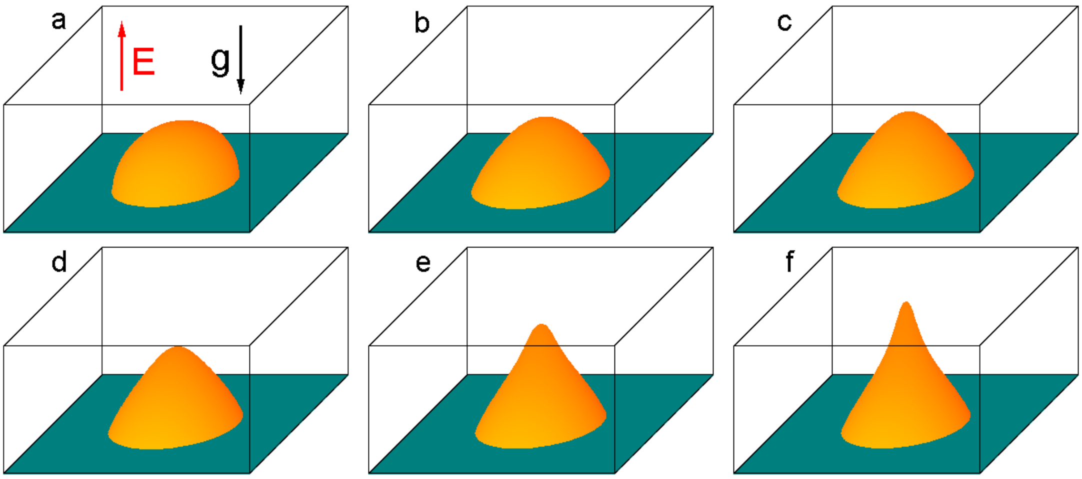

Figure 2. Evolution of droplet in an electric field. $t =$ 400 (a), 5000 (b), 30000 (c), 50000 (d), 60000 (e), 62400 (f). R_0 = 105, Bo = 2.3, $B =$ 1.0417 ($\theta \approx 68.5°$). $\varepsilon_{\text{liq}} = 13.3$, $\text{Bo}_E = 14.6$, Oh = 0.17. Lattice 432×432×224.

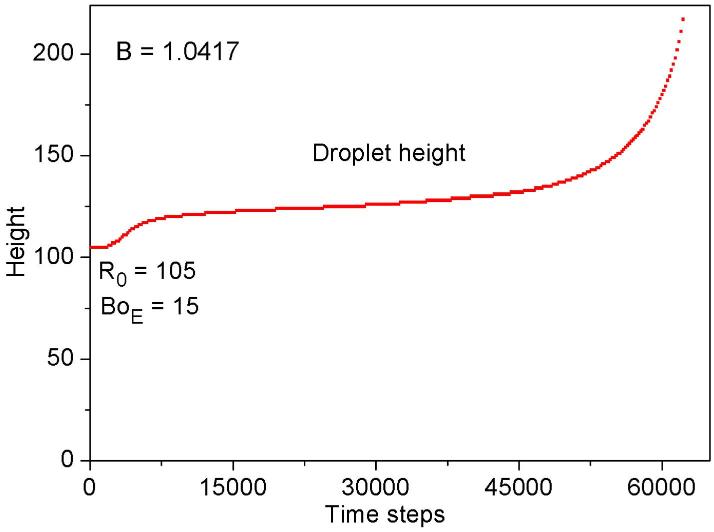

Figure 3. The elongation of a droplet in the direction of the electric field. $\text{Bo}_E = 14.6$, $B =$ 1.0417 ($\theta \approx 68.5°$).

The critical value of the electric Bond number depends on the contact angle [2], as well as on the ratio of the droplet height and the interelectrode gap. Moreover, the electric field at the tip of the droplet increases as the droplet elongates. The simplest estimation can be made, if we consider the droplet as a flat dielectric layer of thickness h. In this case, the electric field above the dielectric layer can be calculated by the following formula (plot in figure 4)

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$$E = \frac{V}{d\,(1-\beta+\beta/\varepsilon_{\rm liq})}, \qquad (5)$$

where $\beta = h/d$ is the dimensionless thickness of a dielectric layer, d is the distance between electrodes, and V is the applied DC voltage. Therefore, the local electric Bond number also increases as the droplet elongates, despite the decrease in the radius of curvature at the droplet tip (figure 2d,e,f).

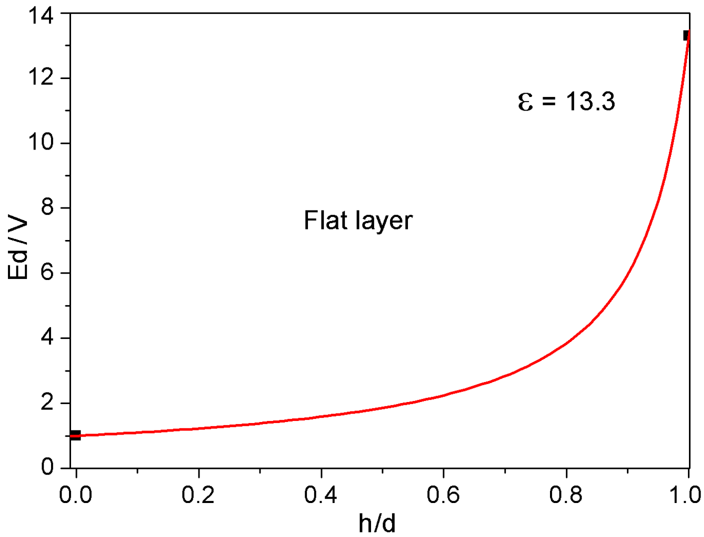

Figure 4. The value of the dimensionless electric field strength above a flat layer of a dielectric placed on the lower electrode. $\varepsilon_{\rm liq} = 13.3$.

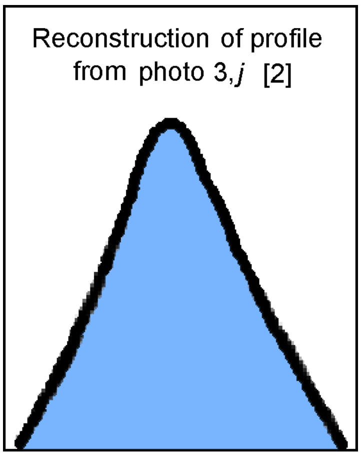

Figure 5. The surface profile of the droplet reconstructed from the photograph presented in [2]. t = 756.5 ms, V = 13.5 kV, d = 5 cm. Volume is about 10 μl.

All stages for sessile droplet were experimentally observed in work [2]. The droplet size was from 2 to 3 mm. The DC voltage V = 13.5 kV was applied to parallel electrodes with distance between them d = 5 cm. The surface profile of the droplet at the last stage (figure 5) is reconstructed from the photo presented in [2]. The results of our simulation (figure 2e,f) are in qualitative agreement with the reconstructed profile.

Conclusion

Three-dimensional non-stationary modeling of liquid dielectric droplets on a wettable surface in an electric field has been performed. There are two variants for the droplet behavior. A droplet can acquire its equilibrium shape after several oscillations or elongate unlimitedly up to its destruction if the electric Bond number exceeds the critical value. In the latter case, there are three stages of growth. The first stage is the establishing of approximate equilibrium for gravity, electric and surface tension forces for a given contact angle. Then, the droplet begins to lengthen slowly along the electric field, maintaining a convex shape (second stage). The last stage is the unlimited elongation of the top of the droplet and its destruction.

Acknowledgements

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