Micro Droplets Merging by Electrowetting: Lattice Boltzmann Study

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Abstract

In this paper, the Free Energy Based Lattice Boltzmann (FEB-LB) method which has been recently extended by the author for modeling and simulation of Electrowetting (EW) phenomenon is applied to another application of EW, i.e., droplets merging. The obtained results ware compared against experimental data and the results show good accuracy of the numerical simulation.

Keywords: Optimization, Electrowetting, Lattice Boltzmann, Micro droplets, Merging

1. Introduction

When there is an interface between two materials, there is a specific energy, the so-called interfacial energy, which is proportional to the surface area of the interface and the constant of proportionality is called the surface tension. As a result liquid drops are spherical when they are in air, to minimize the surface energy. Since there are typically a liquid, a solid, and a surrounding gas interacting in wetting phenomena, one can consider three types of surface tensions: the liquid-gas, the gas-solid, and the liquid-solid surface tensions. When liquid drops are in contact with a solid substrate, the liquid-gas interface maintains a spherical cap profile and the angle at which the liquid drop joins the solid substrate is called the Young contact angle. If the surface upon which the drop is supported has an embedded electrode, then upon applying a voltage to the electrode, an electric double-layer builds up spontaneously at the solid-liquid interface consisting of charges on the metal surface on the one hand and a cloud of oppositely charged counter-ions on the liquid side of the interface on the other. This leads to reduction in the surface energy of the liquid-solid interface. In accordance with the Young's equation, this reduction in surface energy leads to a decrease in the equilibrium contact angle between the liquid and the solid, causing the drop to further wet the surface. This phenomenon is called EW and has seen resurgence in modern applications in the area of Micro-Electro-Mechanical Systems (MEMS) [1].

Nowadays, EW has been proposed as a mechanism for transporting, mixing, and dispensing droplets with volumes in the range of nano-liters or less [2], "Lab-on-a-Chip" systems for applications such as DNA and protein analysis, and biomedical diagnostics [3].

The FEB-LB approach, which first introduced by Swift et al. [4], has advantages for wetting problems. Of course, the original version of the method suffered, however, from the lack of Galilean invariance, a serious drawback, when hydrodynamic transport becomes a relevant issue. This problem was solved by Holdych et al. [5] who proposed a modified expression for the relation between the pressure tensor and the second moments of the population densities in the lattice Boltzmann model.

Recently this method successfully developed by author to model and simulation of the Electrowetting phenomena [6,7]. Mixing is an important process in microfluidic devices for chemical and biological applications. However, as is well known, mixing is more difficult at small scales than at large scales because of the weak advection at low Reynolds numbers. In this paper simulation of droplets merging one of another EW operation, using FEB-LB method has been presented.

2. Lattice Boltzmann Method

In LB algorithm, the Navier-Stokes equations are solved via following the evolution of a set of distribution functions $f_i(r,t)$. Here, $f_i(r,t)$ represents the mass density at time t and position r with velocity c_i. In the present study, a 3D lattice which has fifteen velocity vectors, so-called D3Q15, is employed. Physical quantities are defined as moments of $f_i(r,t)$. Thus, the particle density and momentum are obtained by

$$\rho = \sum f_i \quad ; \quad \rho u_\alpha = \sum f_i c_i \tag{1}$$

where i indicates the velocity directions and α is used to denote Cartesian directions. LB collisions and particle displacements are governed by the LB equation, with BGK collision operator for the time evaluation of distribution functions

$$f_i(r + c_i\Delta t, t + \Delta t) - f_i(r,t) = -\frac{1}{\tau}[f_i(r,t) - f_i^{eq}(r,t)] \tag{2}$$

In the above equation, Δt is the time step of the simulation, f_i^{eq} is the equilibrium distribution function (is calculated from the power series proposed by Swift et al. [2]) and is depended on local fluid properties and τ is the relaxation parameter which is related to the kinematic viscosity in D3Q15 for hydrodynamic simulations as follows [10]

$$\upsilon = (\frac{2\tau - 1}{6})\frac{\Delta r^2}{\Delta t} \tag{3}$$

3. Free Energy Definition

To study the electric double-layer from the free energy point of view, four elements have to be considered [7]: (1) The electrostatic energy of the surface charges and the bulk charges, (2) The entropy involved in the uneven distribution of the ions, (3) The chemical preference of the ions forming the surface charges for the surface over the bulk or the tendency to electrolytic dissociation of groups in the surface, and (4) Mechanical free energy of the system. When a constant potential is applied to the substrate, the total free energy of the mentioned electrowetting system can be represented as follows

$$\Psi_\varphi^t = \int_\Gamma \phi(\rho,\varphi)\,d\Gamma + \int_\Omega \{W + \frac{\kappa}{2}(\partial_\alpha \rho)^2 - [\frac{\varepsilon}{2}(\partial_\alpha \varphi)^2 + \Pi]\}\,d\Omega \tag{4}$$

If one minimizes the above total free energy relation, one can conclude that

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$$\sigma_{gl} = \int_{\rho_g}^{\rho_l} \sqrt{2\kappa W}\, d\rho + \int_{\varphi_g}^{\varphi_l} \sqrt{2\varepsilon\Pi}\, d\varphi$$

$$\sigma_{sg} = \int_{\rho_s}^{\rho_g} \sqrt{2\kappa W}\, d\rho + \int_{\varphi_s}^{\varphi_g} \sqrt{2\varepsilon\Pi}\, d\varphi \qquad (5)$$

$$\sigma_{sl} = \int_{\rho_s}^{\rho_l} \sqrt{2\kappa W}\, d\rho + \int_{\varphi_s}^{\varphi_l} \sqrt{2\varepsilon\Pi}\, d\varphi + \phi_0 - \phi_1\rho_s \cdot$$

For more details on the derivation of Eq.(5) the reader is referred to [6].

4. Results and Discussion

Figure 1 shows the top views of sequential frames of droplets merging simulation. The results have been compared with Cooney et al. [9] experimental ones, i.e., Fig. 2. It should be noted that in the experimental results of Cooney et al., there is a 50 μm gaps between gold ground lines and underlying transparent electrodes and the droplet in this state does not contact the underlying surface and the mentioned initial contact angle is the contact angle of droplet with golden lines. Therefore times predicted by the simulation time are slightly more than the experimental ones.

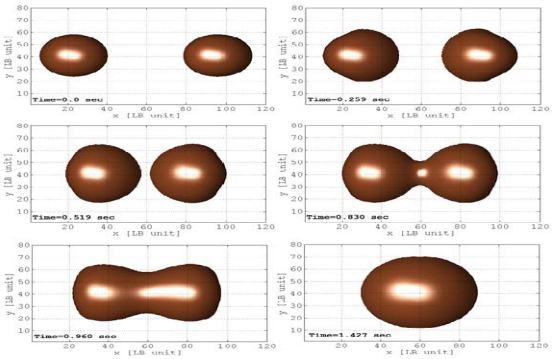

Figure 1: Top views of the simulation of the droplets merging by Electrowetting.

Also, it should be mentioned that in Fig. 2, the nature of droplet times, 1.2 and 3.7 seconds are different. As can see in times 1.2 second the obtained droplet colour has been not stabilized yet. After 2.5 seconds (i.e. in times 3.7 sec) the colour of produced droplet is stabilized. In fact in this time the internal velocities are equilibrated. This issue is also observed in the simulation results.

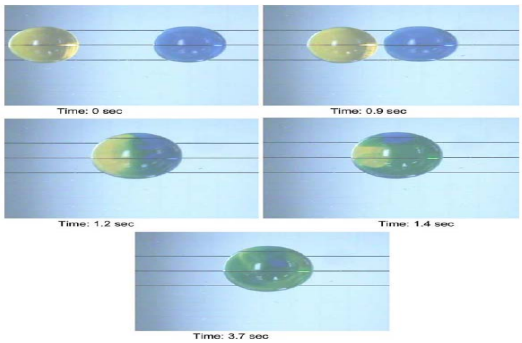

Figure 2: Top views of experimental results for droplets merging $\theta : 113^\circ \rightarrow 71^\circ$.

Figure 3 presents that although droplet has been reached to its final shape but there are still internal velocities. Of course, after 1.5 seconds (i.e., in times 2.854 sec) the internal velocities are vanished. One can relate the difference between simulation results and experimental ones, due to the presence of a wall in the simulations (i.e., underlying plate). However, the presence of the wall initially causes to increase the time of merging, but in the following it causes to reduce the time required to reach the internal stabilization.

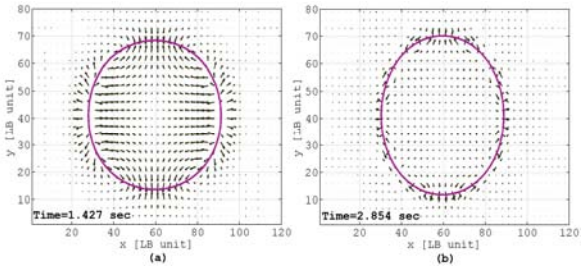

Figure 3: Velocity fields in two times: a) exactly after merging, b) after reaching to equilibrium.

5. Conclusion

In this paper the free energy based LB method which has been recently extended by the author for modeling and simulation of electrowetting phenomenon used to study the merging two micro size droplets using electrowetting. Comparison of the time scale of merging shows good agreements.

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