Analytical and Numerical Investigation of Micro Droplets Stability

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Abstract

In this paper, the stability of a droplet in a finite system was studied analytically and numerically using free energy based lattice Boltzmann method has been studied. It was shown that the droplet stability is a function of the system size and droplet contact angle. The simulation results were in good agreement with analytical solution and it has been concluded that in the finite systems an unstable droplet can be stabilized by applying a voltage (i.e., using Electrowetting). Based on this observation, a new method for merging droplets in the finite systems has been proposed.

Keywords: Evaporation, Condensation, Electrowetting, Lattice Boltzmann method, Micro droplets

1. Introduction

In the past 10-15 years, the LBM has been successfully applied to simulate fluid flows and transport phenomena. Unlike the conventional computational fluid dynamics (CFD) methods, the LBM has an intrinsic kinetic nature which leads to the some advantages: reduction from second order to first order partial differential equations, simplification of nonlinear modeling, computational efficiency and accuracy, simple fluid interface boundary conditions, and a mathematical framework allowing molecular level modeling; therefore it is effective for problems in which both mesoscopic and microscopic statistics become important [1].

Recently, the free energy based LBM has been successfully employed to modeling and simulation of some of EW operations, i.e., droplet spreading, motion, and splitting in three dimensions [2,3]. In this paper in addition to simulation of droplets merging one of another EW operations, also the same method is applied to study of interesting issues such as instability (evaporation) of droplets in a system with finite size (i.e., the finite systems) [4]. In last few years the vapor liquid equilibrium in the finite systems has received more attention [5-7]. The stabilization of the droplets using a voltage in the finite systems as a new application of the EW phenomenon has been investigated in this paper for first time.

2. Thermodynamics

The thermodynamic of one component stable heterogeneous system (i.e., a liquid drop in equilibrium with its vapor according Fig. 1) and including a solid substrate (s) is determined by [8]

$$\Psi^{in\hom} = \int\left[W(T,\rho) + \frac{\kappa}{2}(\nabla\rho)^2\right]\mathrm{dV} + \int\psi_s(\rho_s)\,\mathrm{dS} \tag{1}$$

In the above equation, the surface integral term represents the contribution of solid-fluid interactions and W is the effective free energy and expressed as follows [20]

$$W(T,\rho) = \psi_b(T,\rho) - \mu_b(T)\rho - p_b(T) \tag{2}$$

where, ψ_b is the free energy density of the bulk liquid, μ_b and p_b are the chemical potential and pressure in the bulk respectively. It should be noted that W is a non-negative function of ρ that vanishes, along with $\frac{\partial W}{\partial \rho}$, when ρ is equal to the liquid bulk density or to the gas bulk density. Optimizing the volume integral term in Eq.(1) [8]

$$W(\rho) = \frac{\kappa}{2}(\nabla\rho)^2. \tag{3}$$

κ is a positive constant which is related to the surface tension and tunes interface width. If one considers an unstable inhomogeneous finite system (i.e., two phases), the system becomes stable homogeneous system via forming the supersaturated vapor [6] (i.e., one phase), because Eq. (1) cannot be applied to study of the stable inhomogeneous systems, the free energy functional of these systems are expressed as follows

$$\Psi^{\hom} = \int\left[W(\overline{\rho})\right]\mathrm{dV} + \int\psi_s(\overline{\rho})\,\mathrm{dS} \tag{4}$$

where $\overline{\rho}$ is the average density and determined by the following relations

$$\overline{\rho} = \rho_g + \delta\rho;\ \ \delta\rho = (\rho_l - \rho_g)\frac{V_l}{V}. \tag{5}$$

The surface free energy ψ_s, it is commonly approximated as

$$\psi_s(\rho_s) = \phi_0 - \phi_1\rho_s. \tag{6}$$

The constant ϕ_1, called wetting potential, determines interaction between fluid and substrate. In the critical state $\Delta\Psi = 0$, therefore one can conclude

$$\begin{aligned}&\rightarrow \pi R^2(1-\sin(\alpha))\left[2\sigma_{lv} + [1+\sin(\alpha)]\phi_1(\rho_g - \rho_l)\right]\\ &-\left[\frac{1}{2}W''(\rho_g)(\rho_l-\rho_g)^2\left(\frac{\pi}{3}R^3\left[2-3\sin(\alpha)+\sin^3(\alpha)\right]\right)^2/\mathrm{V}\right]\\ &+2L^2\phi_1(\rho_l-\rho_g)\frac{\pi}{3}R^3\left[2-3\sin(\alpha)+\sin^3(\alpha)\right]/\mathrm{V} = 0.\end{aligned} \tag{7}$$

The above equation was solved using the simple Newton–Raphson algorithm. The radius which satisfies the above relation is called the critical radius. That is for each unstable inhomogeneous system with the prescribed size, there is a critical radius and droplets with radii less than it, are evaporated and a one phase stable homogeneous system (i.e., supersaturated vapor) is produced.

3. Lattice Boltzmann Implementation

In order to study a two-phase liquid-vapor system a free-energy based lattice Boltzmann method that was introduced by Swift et al. [9]. In LB algorithm, the Navier-Stokes equations

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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

$$\rho = \sum f_i \quad ; \quad \rho u_\alpha = \sum f_i c_i \tag{8}$$

where *i* indicates the velocity directions and α is used to denote Cartesian directions. For more details about free energy based lattice Boltzmann method the reader is referred to [9].

4. Results and Discussion

Figure 1 represents the critical radius curve changes in a cubic system with system size (in a cubic system Lx=Ly=Lz) based on the analytical solution in Section 2. As seen with increasing of the cubic system length, the critical radius is also increased. That is a droplet which was stable in the system before increasing its length, it will be unstable. The simulation results have been compared with analytical ones in Fig. 1, which shows good agreement between them.

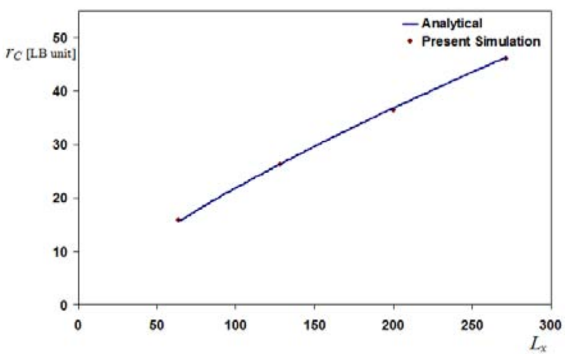

Figure 1: Comparison of the variation of critical radius with analytical ones.

Figure 2 presents the critical radius of droplet versus the contact angle. As it can be seen droplet stability increases when the contact angle is reduced and the results are in good agreement with the analytical solution.

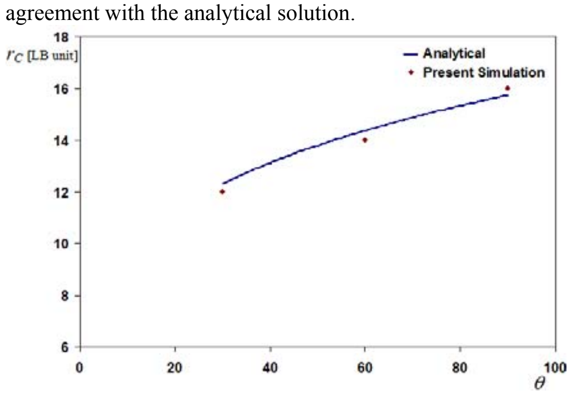

Figure 2: Comparison of the variation of the contact angle with analytical ones.

In Fig. 3, two micro droplets on the unstable state have been presented. The voltage is applied on the right side of the substrate. Figure 3a shows the droplets shape at start time (i.e., time=0) and for a time after starting (i.e., time>0) the droplet shape have been presented in Fig. 3b As seen, applying the electric field causes to stabilize the right side droplet, while the left side droplet starts to evaporate inside the system. Since the right side droplet is stable, it starts to grow because of condensation of the evaporated droplet at the right side.

5. Conclusion

In this paper the free energy based LB method has been used to investigate the influence of electrowetting on the droplet evaporation and condensation, as a new aspect of this phenomenon. The stability of one component system, i.e., a liquid drop with its vapor, was studied in three dimensions. It has been concluded that the stability of the droplet in the cubic system depends on the system size and contact angle. Comparison of the results with analytical solution show good agreements. It should be emphasized that the presented method in this paper also can be applied to study of the stability of multicomponent heterogeneous systems.

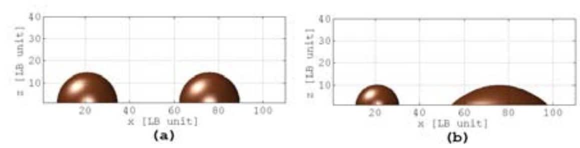

Figure 3: the simulation of the electric field effect on the unstable droplet evaporation process: a) at time=0 and without electric field, b) For a time≠ 0 and with electric field only at the right side.

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