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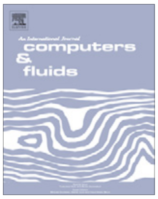

Numerical modeling of electrowetting processes in digital microfluidic devices

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We use a three-dimensional multiphase lattice-Boltzmann model to study basic operations such as transport, merging and splitting of nanoliter water droplets actuated by electrowetting in digital microfluidic devices. In a first step, numerical and analytical predictions for the droplet transport velocity are compared and very good agreement is obtained for a wide range of contact angles. The same algorithm is employed then to study the dynamics of the splitting processes at different contact angles and different geometries of the cell. The configuration of the liquid droplet involved in a splitting process and the dependence of the splitting time on the transport velocity are also investigated and phenomenological laws describing these processes are also proposed.

1. Introduction

Digital microfluidics [1] emerged as a second-generation architecture for lab-on-chip devices that is based upon the manipulation of discrete nanoliter volume droplets between two parallel plates (Hele-Shaw cells [2]). By applying a force locally on each individual droplet, digital microfluidic devices allow unit-sized packets of fluid to be transported, merged, mixed, split or stored in a discrete manner by using programmable external controllers [1]. Among the various mechanisms capable of manipulating discrete droplets on a surface (dielectrophoresis [3], thermocapillarity [4] and surface acoustic wave transport [5]), the electrowetting effect [6], defined as the change in the solid–liquid contact angle due to an electric potential difference between the solid and the liquid, offers the distinct advantage of being highly suitable for large scale integration on lab-on-chip devices. In such devices, the potential difference is applied between an array of individually controllable electrodes patterned on the bottom plate and a ground plane placed on the top plate. A microfluidic device consisting of a Hele-Shaw cell and an array of patterned electrodes on the bottom plate is usually referred to as an electrowetting-on-dielectric (EWOD) or digital microfluidic device.

In digital microfluidic devices, the droplets experience very complex geometrical changes, rapid displacements, and complicated internal recirculation of fluid when submitted to the electrowetting forces. To improve the reliability and accuracy of these devices, it is thus critically important to achieve a complete understanding of the fundamental processes involved in the manipulation of the droplets. Both analytical [7,2,8–10] and numerical [11–14] methods have been proposed in the past for this purpose. However, most of these studies have considered either (i) that the droplets are in static equilibrium [9,10,15,12], (ii) very simplified droplet geometries [15], or (iii) have involved some purely empirical parameters [8]. New methods are thus required before the complex processes occurring during the manipulation of the droplets can be fully understood.

The fundamental challenge in modeling such kind of processes consists mainly of the mesoscopic nature of the physical systems usually considered in digital microfluidics and nanofluidics. Classical approaches to computational fluidics based on discretizations of macroscopic continuum equations (like Navier–Stokes) present several difficulties [8,11] in dealing with wetting processes and contact line dynamics. On the other hand, molecular dynamics approaches, although successful for modeling wetting effects at the atomistic level (carbon nanotubes for example [16]), cannot be used for the sub-millimeter sized liquid droplets found in digital microfluidic devices as the number of atoms (molecules) is then simply too large for the actual computers. A relatively new numerical tool, designed to fill the gap between the microscopic (atomistic) level and the classical macroscopic methods is the lattice Boltzmann (*LB*) approach [17,18]. This new method, which is a numerical version of the continuous (full) Boltzmann equation, consists of simplified kinetic models incorporating the essential physics of microscopic or mesoscopic processes so that the macroscopic averaged properties obey the desired macroscopic equations [17]. The main strength of the *LB* method is that it behaves like a classical Navier–Stokes solver in the bulk liquid whereas its mesoscopic nature becomes important at the interfaces [19]. This advantage allows to easily address physical processes involving multicomponent or multiphase systems and complicated phenomena like contact line dynamics on complex boundaries.

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In this paper, we apply a 3D *LB* numerical algorithm in order to study basic operations in electroweting induced processes in digital microfluidic devices. The numerical results are compared to analytical models and simple phenomenological laws for the total splitting time of liquid droplets are given.

2. Numerical model

Several *LB* numerical schemes for addressing multiphase and multicomponent fluid flows are available in the literature. One of the first *LB*-based multicomponent model has been developed by Gunstensen and Rothman [20] and was based on the lattice gas model of Rothman and Keller [21]. Multiphase flows and phase separation have successfully been simulated by using the method of Shan and Chen [22,23], based on the use of an interaction pseudopotential between different phases (or components) of the system. Free-energy [24–26] and mean-field [27] *LB* approaches based on the themodynamics of two-component fluids and the free-energy thermodynamic functional can also be used for modeling multiphase and interfacial dynamics.

We numerically implemented a multiphase *LB* algorithm as described by Shan and Chen [22] and Shan and Doolen [23] by considering a three-dimensional lattice with 19 speeds (well known in the literature as the D3Q19 scheme [28]) denoted as $\vec{e}_i$, where i goes from 0 (particles at rest) to 18 (for the other predefined directions). The fluid particles at the nodes $\vec{x}$ of the lattice are interacting with their first-order neighbors (located at $\vec{x}+\vec{e}_i$) via an attractive short-range force of the form

$$\vec{F}(\vec{x}) = -G_{LL}\Psi(\vec{x})\sum_i w_i \Psi(\vec{x}+\vec{e}_i) \tag{1}$$

where G_{LL} is a negative quantity equivalent to the thermodynamic temperature and it is responsible for the liquid to vapor density ratio as well as the surface tension coefficient. Ψ is an interaction potential responsible for the equation of state (EOS) and equilibrium densities of the considered physical system (liquid and vapor) [29]. However, the choice of the interaction potential has to be made according to the relevant dimensionless number of the physical problem under investigation. In case of sub-millimeter sized droplets actuated by electrowetting, the surface tension and viscosity effects are dominant [30]. Thus, the capillary number

$$Ca = \frac{\eta U}{\gamma} \tag{2}$$

has to be considered. η and γ in the expression above are respectively the dynamic viscosity and the surface tension coefficient, whereas U is the droplet velocity. We have chosen an interaction potential that leads to one of the most stable EOS [31] that is

$$\Psi[\rho] = \Psi_0 \exp\left(-\frac{\rho_0}{\rho}\right) \tag{3}$$

where ρ stands for the fluid density whereas Ψ_0 and ρ_0 are constant parameters responsible for the equilibrium vapor and liquid densities. In our implementation, $G_{LL} = -120$, $\Psi_0 = 4$ and $\rho_0 = 200$ give a surface tension coefficient $\gamma^{LB} = 14.1$.

This value has been obtained by simulating liquid droplets of different radii and applying the Laplace law for the pressure difference across the free surface (Fig. 1a). The dynamic viscosities η^{LB} in the simulation are related to the collision time τ through the kinematic viscosity $\nu^{LB} = (\tau - 0.5)/3$ and the density ρ of the fluid (since $\eta^{LB} = \nu^{LB}/\rho$). In this paper, we consider the default value of the collision time $\tau = 1$ in the BGK collision term [32] therefore the two phases (equivalent liquid and gas) will present identical kinematic viscosities but different dynamic viscosities since different densities are obtained after the phase separation.

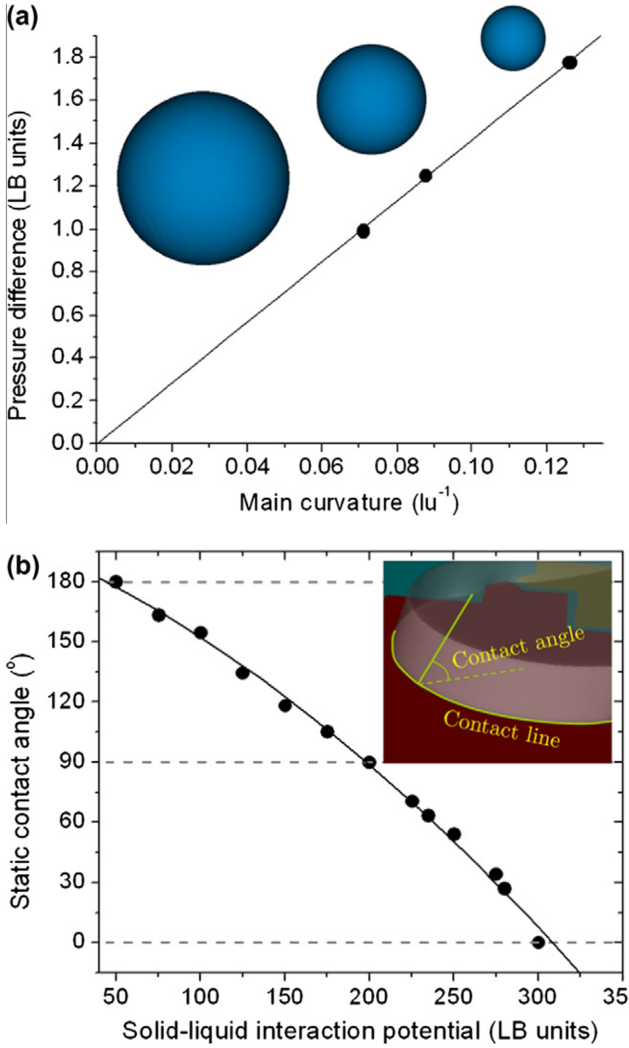

Fig. 1. (a) Linear fit with the Laplace's law of the pressure difference across spherical droplets of different radii; (b) simulated contact angles at the solid plates obtained by adjusting the interaction potential with the solid nodes.

The wettability of solid obstacles in the simulation (plates, electrodes and walls) is modeled by assuming a default value of the interaction potential Ψ (for example 1.0) at all the nodes inside these obstacles. Then the interaction constant G_{LL} in Eq. (1) is replaced with another constant G_{LS} (also negative) able to reproduce any desired contact angle of the liquid relative to the solid walls. As shown in Fig. 1b, a full range of contact angles from 0° to 180° can be obtained by appropriately tailoring the solid–liquid interaction potential. Note that the numerical values on the abscissa of this graph correspond to absolute (positive) values of the G_{LS} constant. It is worth mentioning that the quantity G_{LS} is not strictly related to the electrical voltage applied in a real electrowetting device. However, if necessary, such dependence can be obtained by correlating well known experimental electrical voltage dependencies of the liquid–solid contact angle to the numerical simulations presented in Fig. 1b. That is, the electrowetting equation as well as the problem of contact angle saturation in electrowetting [33] can be accounted for in a phenomenological manner. As for the actuation mechanism, by changing the contact angle at a certain region of the droplet, a change in the macroscopic curvature of the liquid free surface and consequently a difference in the internal pressure of the liquid droplet will be induced. Finally this difference in the internal pressure will eventually induce a displacement of the liquid against the