CAPILLARY PENETRATION VIA A MEAN-FIELD LATTICE BOLTZMANN MODEL FOR MULTIPHASE FLOW

Gang Wan*, Baoming Li*[a)], Junfeng Zhang** & Daniel Y. Kwok***[b)]
*National Key Laboratory of Transient Physics, Nanjing University of Science and Technology, Nanjing, Jiangshu, China
**Department of Mechanical Engineering, Laurantian University, Sudbury, Ontario, Canada
***Nanoscale Technology and Engineering Laboratory, Department of Mechanical Engineering, Schulich School of Engineering, University of Calgary, Calgary, Alberta, T2N 1N4, Canada

Summary We studied liquid-vapor capillary penetration through a Mean-Field Free Energy Lattice Boltzmann Method. Static contact angles were first obtained and their effects on capillary penetration were examined within the context of the Washburn equation.

INTRODUCTION

Wettability of a liquid in contact with a solid surface is of utmost importance in pure and applied science. One physical phenomenon that contact angle (wettability) governs is the capillary penetration (filling) problem [1, 2], where the meniscus advancs as a result of the well-known Laplace pressure. In this paper, a Multiphase Mean-Field Lattice Boltzmann Method [6] was employed to examine the motion and dynamics of a capillary interface. In the literature, there exist several versions of the Lattice Boltzman models for multiphases. Chin *et al*. [3] described a squared-gradient free energy model [4] as a *top-down* model as it imposes a macroscopic free energy functional without considering its molecular origin. The Shan-Chen interparticle potential model [5], however, was said to be a *bottom-up* model, since the force term relates to pairwise interparticle interactions but cannot satisfy continuum thermodynamics in general. The mean-field free-energy lattice Boltzmann method can be considered as a method between the above two, which can recover macroscopic free energy functional as well as represent microscopic interactions.

WASHBURN EQUATION

A well-known equation to describe the displacement of a capillary front as a result of the Laplace pressure and hence wettability is that from Washburn [1]. In a single capillary, the Washburn equation describes the motion of a liquid in the capillary as

$$dz = \frac{H\gamma_{lv}\cos\theta}{8\eta z}dt \quad , \tag{1}$$

where z is the liquid displacement in the capillary, H is the channel height, γ_{lv} is the liquid-vapor surface tension, θ is the static contact angle and η is liquid viscosity. After integration, Eq.(1) can be written as

$$z^2 = \frac{H\gamma_{lv}\cos\theta}{4\eta}t \quad . \tag{2}$$

If we define

$$K = \sqrt{\frac{H\gamma_{lv}\cos\theta}{4\eta}} \quad , \tag{3}$$

where K is a constant when the liquid properties and capillary geometry are fixed, the Washburn equation (2) is

$$z = K\sqrt{t} \tag{4}$$

With the exception of the initial capillary motion where inertia dominates, the Washbrun equation clearly predicts that liquid displacement z will grow linearly with $\sqrt{t}$.

RESULTS AND DISCUSSION

Figure 1(a) shows our $D2Q9$ lattice Boltzmann model employed in the simulations, where Fig. 1(b) depicts the geometry for a tube with multiple capillaries. Suppose the length of all capillaries are the same and the geometry in Fig. 1(c) can be simplified to simulate the capillary penetration problem. Our system consists of 2600×20 lattice units. The capillary length was set to 1000 lattice units.

An independent LBM simulation was employed to determine the equilibrium contact angle as a result of the specified solid-liquid interaction K_w. Figure 2(a) shows the resulting contact angles when we change the solid-liquid interaction strength K_w. As K_w decreases from 0.075 to 0.025, the resulting contact angle changes from 0° to 180°, as expected because of the weaker solid-liquid interactions. As we decrease K_w further, the contact angle remains at 180°. It should be

[a)]Corresponding author. E-mail: baomingli@mail.njust.edu.cn [b)]Corresponding author. E-mail: daniel.kwok@ucalgary.ca

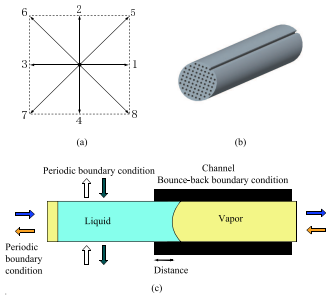
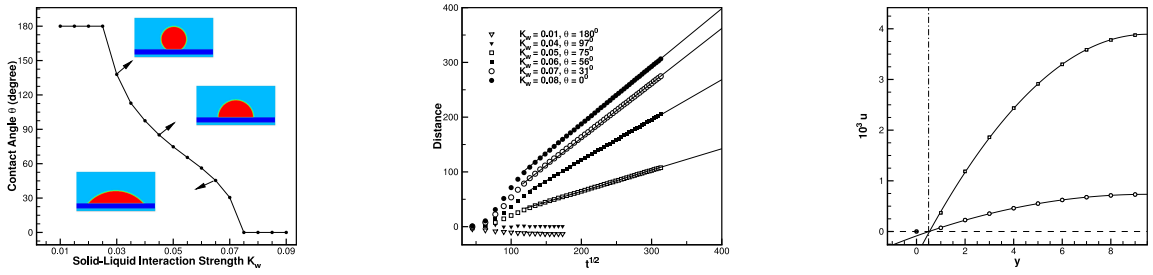


Figure 1. Our LBM simulation models: (a) lattice velocities for a $D2Q9$ lattice; (b) a 3D capillary geometry; (c) 2D capillary geometry in our simulation with the boundary conditions.



(a) (b) (c)

Figure 2. (a) Contact angles calcuated by a $D2Q9$ Mean-Field Lattice Boltzmann Method with different solid-liquid interaction strengths K_w . (b) Liquid displacement as a function of $\sqrt{t}$ for different contact angles θ. (c) Velocity profiles for different interaction strengths K_w. The cuts are located at X = 50 far away from the capillary entrance.

pointed out that these contact angle results were obtained directly from our LBM simulation without further "adjustment" on other parameters and, as a result, we can examine what our Mean-Field Lattice Boltzmann model predicts when the contact angle changes from 0° to 180°.

We should point out that capillary penetration is manifested by the presence of a Laplace pressure across the liquid-vapor interface and hence any contact angle larger than 90° will cause the meniscus to depress (capillary depression) without penentration. This can be employed as a simple check on the validity of our model in predicting this interesting phenomenon. In the capillary penetration simulation, vapor (ρ_v = 1.4) was set to fill in the capillary and liquid (ρ_v = 5.6) was placed outside the capillary. Figure 2(b) shows the liquid displacement distance in the capillary as a function of $\sqrt{t}$ for different solid-liquid interaction strengths K_w. For $K_w = 0.1$ and $K_w = 0.4$, their contact angles are, respectively, $\theta = 180^\circ$ (open gradient symbols) and $\theta = 97^\circ$ (filled gradient symbols); our LBM results show that capillary depression occurs and liquid cannot penetrate into the channel. As K_w increases further, causing the contact angle to decrease, liquid starts penetrating into the capillary due to the pressure of a Laplace pressure across the liquid-vapor interface. Figure 2(c) shows the velocity profiles of the liquid where solid lines present the parabolic Poiseuille flow. The displacement distance from our LBM simulation was found to increase linerly with $t^{\frac{1}{2}}$ for different solid-liquid interactions and contact angles ($< 90^\circ$). These results are in agreement with the Washburn equation but in contradiction with other LBM models that found their LBMs could not predict the linear relationship in Fig. 2(b).

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