lattice Boltzmann simulation of electrowetting-on-dielectric in a rough-wall channel

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A lattice Boltzmann model was proposed to simulate electrowetting-on-dielectric (EWOD). The insulative vapor and the electrolyte liquid droplet were simulated by the lattice Boltzmann method respectively, and the linear property between cosine of contact angle and the electric field force confirms the reliability of this model. In the simulation of electrolyte flowing in a rough-wall channel under an external electric field, we found that a narrow channel is more sensitive than a broad channel and the flux decreases monotonously as the electric field increase, but may suddenly increase if the electric field is strong enough.

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With the development and progress of nano-science and nano-technology, how to manipulate tiny amounts of liquids on surfaces becomes great challenge to nano-engineering. Gradients of both temperature and concentration of surfactants across droplets may produce forces to propel droplets\textsuperscript{[1]}, but compared to these methods, chemical and nonwetting surfaces may be used to enhance electrowetting effect\textsuperscript{[2]}. Recently, the experimental research on electrowetting has made great progress: electrowetting has been promoted to application of lab-on-a-chip\textsuperscript{[3]}; through an external voltage, adjusting hydrophobic nature of an oil droplet containing dissolved dye, an electrowetting-based reflective display has been invented\textsuperscript{[4]}; changing the contact angle of a sessile droplet via electrowetting, shape of the droplet, as well as the focal length of this droplet can be changed, and a flexible liquid lenses may be made\textsuperscript{[5]}. Theoretically, the contact angle should decrease rapidly as the external voltage increases, but in experiment, the contact angle has been found to be saturated when the external voltage is high enough\textsuperscript{[2]}. Because many factors may affect the contact angle of a droplet in experiment, the saturation mechanism of this angle keeps unknown\textsuperscript{[1]}, despite several various mechanisms have been proposed\textsuperscript{[1]}. In order to study the variation of contact angle on electrowetting as well as the electric effect on microchannel and microfluidics, it is desirable to propose a numeric method to study electrowetting of tiny electrolyte droplet on an insulative layer.

Since the lattice Boltzmann method (LBM)\textsuperscript{[6, 7]} has been proposed, it has succeeded in simulating complex fluid flows including multi-phase flow\textsuperscript{[10]} particle suspension flow\textsuperscript{[11, 12]}, binary mixture\textsuperscript{[10, 13]} and blood flow\textsuperscript{[14, 15, 16]}. Because of its intrinsically parallel and simpleness, it has been recognized as an alternate method for computational fluid dynamics\textsuperscript{[17]}. Through introducing intermolecular forces, the lattice Boltzmann method may be used to study microfluidics\textsuperscript{[18]}, microchannel and nanochannel flows\textsuperscript{[19]}.

In this Letter, base on the multiple phases lattice Boltzmann model\textsuperscript{[10]}, considering the electric force exerted on the electrolyte near an insulative layer, a lattice Boltzmann model was proposed to investigate two-dimensional electrolyte electrowetting on a smooth insulative layer and the effect of EWOD on the electrolyte flow in a rough-wall channel.

In two dimensions, the system of the D2Q9 lattice Boltzmann model\textsuperscript{[8]} is described by a single particle distribution function $f_\alpha(x, t)$, which can be thought as the number of fluid particles at site $x$, time $t$, and possessing one of the nine velocities $e_\alpha$ with $e_0 = (0, 0)$, $e_\alpha = (\cos \pi(\alpha - 1)/2, \sin \pi(\alpha - 1)/2)$, $\alpha = 1, 2, 3, 4$, and $e_\alpha = \sqrt{2}(\cos \pi(2\alpha - 1)/4, \sin \pi(2\alpha - 1)/4)$, for $\alpha = 5, 6, 7, 8$. The distribution function evolves according to a Boltzmann equation that is discrete in both space and time,

$$f_\alpha(x + e_\alpha, t + 1) - f_\alpha(x, t) = -\frac{1}{\tau}(f_\alpha - f_\alpha^{eq}). \quad (1)$$

The density $\rho$ and macroscopic velocity $\mathbf{u}$ are defined as

$$\rho = \sum_\alpha f_\alpha, \quad \rho \mathbf{u} = \sum_\alpha f_\alpha e_\alpha. \quad (2)$$

In order to reproduce the Navier-Stokes equation, the equilibrium distribution function $f_\alpha^{eq}$ may have the following form\textsuperscript{[8]}


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where \( w_0 = 4/9, w_a = 1/9 \), for \( \alpha = 1, 2, 3, 4 \), and \( w_a = 1/36 \), for \( \alpha = 5, 6, 7, 8 \).

Considering the intermolecular interaction, through an interaction potential among particles in the LBM, Shan and Chen improved the LBM to simulate multiple phases fluid [10]:

\[
V(X, X') = G_\alpha(X, X')\varphi(x)\phi(x'),
\]

where \( G_\alpha(X, X') \) is a Green function and \( G_\alpha(X, X') = \mathcal{G} \) for \( |X - X'| = \sqrt{2} \), \( G_\alpha(X, X') = 2\mathcal{G} \) for \( |X - X'| = 1 \) and \( G_\alpha(X, X') = 0 \) otherwise. Here we take \( \varphi(x) = \rho_0(1 - \exp(-\rho/\rho_0)) \) with \( \rho_0 \) of a constant. The resulting force is

\[
F_\alpha(x) = -\varphi(x) \sum_\alpha G_\alpha \varphi(x + e_\alpha)e_\alpha.
\]

If the node at \((x + e_\alpha)\) is a solid node, similar to a fluid node, the according resulting force can be written as [20]

\[
F_w(x) = -\varphi(x) \sum_\alpha W_\alpha S(x + e_\alpha)e_\alpha,
\]

where \( W_\alpha = w_\alpha \) for \(|e_\alpha| = \sqrt{2}\), \( W_\alpha = 2w_\alpha \) for \(|e_\alpha| = 1 \) and \( W_\alpha = 0 \) for \(|e_\alpha| = 0 \). If the node at \((x + e_\alpha)\) is a solid node, \( S = 1 \), else \( S = 0 \).

For an EWOD system, which consists of a conductive droplet and a metallic electrode insulated with an insulative layer, the double conductive layer has a fixed capacitance per unit area, \( c = \varepsilon_0\varepsilon_d/d \). \( d \) and \( \varepsilon_d \) are the thickness and dielectric constant of the insulative layer. \( \varepsilon_0 \) is the vacuum permittivity. The free energy of the system reads

\[
F^c = A_{lv}\sigma_{lv} + A_{sv}\sigma_{sv} + A_{sl}(\sigma_{sl} - \frac{\varepsilon_0\varepsilon_dU^2}{2d}) - \Delta p V,
\]

where \( A \) is the area of the interface and \( \sigma \) is the interfacial tension. The subscript \( lv, sv, \) and \( sl \) indicate the liquid-vapour, solid-vapour, and solid-liquid interfaces respectively. \( U \) is the potential difference between the conductive droplet and the metallic electrode. \( \Delta p \) describe the pressure drop across the liquid-vapour interface and \( V \) is the volume of the droplet. Through minimizing the free energy \( F^c \), we obtain the basic equation of EWOD [11]

\[
\cos(\theta) - \cos(\theta_0) = \frac{\varepsilon_0\varepsilon_dU^2}{2d\sigma_{lv}},
\]

where \( \theta \) is the contact angle of the droplet and \( \theta_0 \) is that without external electric field. The electric force exerted on the bottom layer of the conductive droplet per unit area is \( f = f/n = \frac{\varepsilon_0\varepsilon_dU^2}{2d}\sigma_{lv}n \) and \( n \) is the unit normal vector of the layer pointing to the metallic electrode. Thus equation (8) is simplified as

\[
\cos(\theta) - \cos(\theta_0) = \frac{f}{\sigma_{lv}}.
\]

Based on equation (9), through a force exerted on the single layer of the liquid near the insulative layer, we may simulate an electrolyte droplet electrowetting on an insulative layer by the LBM.

Fig. 1 is a droplet adopted on a smooth substrate simulated by the LBM. The single layer of fluid near the substrate is shown in Fig. 2. The fluids in the center with a high density \( \rho_l \) consist the liquid, the other fluids in the two sides with a low density \( \rho_v \) belong to the vapor. There is a transition part connect the liquid and the vapor. Because the liquid is conductive but the vapor is insulative, it is necessary to introduce a critical density \( \rho_c \) \( (\rho_c < \rho_v < \rho_l) \) to distinguish the fluid from conducter (with \( \rho \geq \rho_c \)) and insulator (with \( \rho < \rho_c \)). In Fig. 2, the fluids in the range between \( x_1 \) and \( x_2 \) in the single layer near the substrate are conductive. Fluids outside this range are regarded as insulative vapor.

Under the influence of such forces, the momentum at each fluid node is changed to

\[
\rho u' = \rho u + \tau(F_e + F_w + f),
\]

where \( u' \) is the new velocity used in equation (1).

FIG. 1: Shape of a droplet without external electric field.

We now present the simulation results on a box consisting of 100 x 50 lattice units. we fixed the fluid-fluid interaction strength \( G = 0.52 \), fluid-wall interaction strength \( w = -0.14 \) and the relaxation time \( \tau = 0.9 \). The constant \( \rho_0 \) in the expression of potential \( \varphi \) was chosen to be 1.0. At beginning, the fluid was homogenous and possessed a density of 0.85. An attractive force was assumed to push the fluids to condense into

FIG. 2: The density of the single layer of fluid near the substrate. \( \rho_l \) and \( \rho_v \) are the density of the conductive liquid and insulative vapor respectively. \( \rho_c \) is a critical density to distinguish whether the fluid is conductive \( (\rho \geq \rho_c) \) or insulative \( (\rho < \rho_c) \). The fluid in the range of \( x_1 \leq x \leq x_2 \) is regarded as conductive. Here we choice \( \rho_c = 1.0 \).
a droplet in the middle of the substrate. When the droplet had formed, the artificial attractive force was eliminated and a normal droplet formed in the middle of the substrate shown as in Fig. 4. Next, an electrostatic force of attraction $f$ was exerted on the single layer of fluids near the substrate to simulate EWOD. Fig. 3 shows the contact angle changes with the electric force. From this figure we can see that $\cos \theta - \cos \theta_0$ increases proportionally with electric force $f$, consistent with Eq. (9). Thus, this simple model can be used to simulate EWOD.

![FIG. 3: cos(θ) - cos(θ₀) versus electric force $f$. θ and θ₀ are the contact angle of the droplet with and without external electric field.](image)

![FIG. 4: Sketch of rough-wall channel.](image)

![FIG. 5: Rough-wall channel with width $w = 160$. The body force pointing right is $f_b = 8.0 \times 10^{-6}$. The electric force: (a) $f = 0.0$, (b) $f = 0.15$, (c) $f = 0.25$.](image)

![FIG. 6: Rough-wall channel with width $w = 80$. The body force pointing right is $f_b = 8.0 \times 10^{-6}$. The electric force: (a) $f = 0.0$, (b) $f = 0.15$, (c) $f = 0.25$.](image)

![FIG. 7: Average of fluid velocity along x-axis $\overline{u_x}$ in the rough-wall channel with width $w = 80$.](image)

For a nanochannel, as the channel size decreases, the surface-to-volume ratio increases. Therefore, various properties of the walls, such as surface charges and roughness, greatly affect the fluid motions in the nanochannels [21]. Recently, sufficient roughness effect on micro-flow has been widely studied from theory [22], molecular dynamic (MD) and other numeric methods [21, 23, 24] and experiment [25]. Here, we focus on the effect of EW on an electrolyte flow inside a rough-wall channel. Fig. 4 shows a sketch of rough-wall channel. The top and the bottom walls of the channel were both equipped with steps of width $a$ and height $b$. The centreline distance between two neighbouring steps was $p$. The
where the vapor layer makes the wall slip more (shown in Fig. 7 between the electrolyte and another wall (see Fig. 6 (b)) and electrolyte leans towards one wall and lives thick vapor layer be-
more rapidly than in a broad channel. When the electric field
dimensionless flux in a narrow rough-wall channel decreases
ging rightward, the contact points keep static, because of small
fields. The according dimensionless flux
fluid velocity along x-axis
external electric field or charges. Fig. 7 shows the average of
affect the flow very much, to an electrolyte flow, but also the
velocity of the flow.
with another rough-wall. Although the electrolyte keeps flow-
channel living only little parts of the electrolyte keep contacting
can not stay in the center of the channel. Fig. 6 (c) shows that
is obviously seen. For a more narrow rough-wall channel, as
shown in Fig. 8 when the electric force is strong enough, the balance of the system will be break down and the electrolyte can not stay in the center of the channel. Fig. 6 (c) shows that the electrolyte are absorbed into one rough-wall of the channel living only little parts of the electrolyte keep contacting with another rough-wall. Although the electrolyte keeps flowing rightward, the contact points keep static, because of small velocity of the flow.
For a narrow channel, not only the properties of the wall affect the flow very much, to an electrolyte flow, but also the external electric field or charges. Fig. 7 shows the average of fluid velocity along x-axis \( u_x \) under different external electric fields. The according dimensionless flux \( Q/Q_0 \) is shown in Fig. 8. \( Q \) is defined as:

\[
Q = \frac{1}{L} \int_0^L u_x \, dx \, dy, \tag{11}
\]

where \( L \) is length of the channel and \( Q_0 \) is the flux without external electric field. From this figure we can see that the dimensionless flux in a narrow rough-wall channel decreases more rapidly than in a broad channel. When the electric field is strong enough, for a narrow rough-wall channel, the electrolyte leans towards one wall and lives thick vapor layer between the electrolyte and another wall (see Fig. 6 (b)) and the vapor layer makes the wall slip more (shown in Fig. 7 for \( f = 0.25 \)). Thus the flux increases suddenly under such external electric field (see Fig. 8 for \( f = 0.25 \)).

In conclusion, we introduced a critical density \( \rho_c \) to distin-
guish conductive liquid from insulative vapor and an electric force exerted on the conductive liquid to improve the LBM to simulate EWOD. The linear property of contact angle confirmed the reliability of this moel. Further, we applied this model to simulate electrolyte flowing in a rough-wall channel and found that the external electric field affect the density distribution, velocity and flux greatly for a narrow rough-wall channel. For a narrow rough-wall channel, when the external electric field is strong enough, the electrolyte may be adopted into one rough-wall and departure another rough-wall, reducing the whole resistance and resulting a suddenly increasing of flux in the channel.

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Fig. 9