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The Lattice Boltzmann Modeling of Two-phase Electroosmotic Flow in Microchannels

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Abstract

In this paper, a numerical framework based on the lattice Boltzmann method is presented for modeling two-phase electroosmotic flow within microchannels. In the model, lattice Boltzmann schemes are designed for all the governing equations involved such as Navier-Stokes equations for momentum transport, Nernst-Planck equations for ion transport, the Cahn-Hilliard equation for the immiscible fluid interface motion, and Poisson equation for the electric potential referring the model proposed in Shao's work [6]. Related boundary schemes are also proposed to modeling the slip effect on the microchannel surfaces. The theoretical analysis shows that the model has second order accuracy.

Keyword: *lattice Boltzmann method, electrokinetic phenomena, two-phase flow*

1. Introduction

Electroosmotic flow in microchannels is an important phenomenon in many industry applications especially involving lab-on-a-chip. Owing to the scale effect, hydrodynamic slip boundary condition now usually cannot be neglected. In the meantime, the overlapped electric double layers (EDL) effect may appear and the widely used Poisson-Boltzmann model becomes invalid in describing the phenomenon. As in many applications, hydrophobic or hydrophilic wall surfaces will be used for special purposes such as accurate control on the flow rate in the channels. Thus two-phase or multiphase electroosmotic flow in the microchannels combined the boundary slip and overlapped electric double layers (EDL) effect poses an urgent task to find proper models to understand the underlying mechanism.

Up to now, few works has been to include all above effects [1-6]. Among these works, Shao [6] first proposed a continuum hydrodynamic model for two-phase immiscible flows which can include the hydrodynamic slip boundary, the overlapped electric double layers effect. However, the corresponding numerical framework is not discussed in detail and the advanced frameworks can investigate the problem are still rare.

As a popular mesoscopic method, lattice Boltzmann method has shown its ability in modeling the microfluidics and nanofluidics especially the electroosmotic flow[7-10]. However, no works have been done to investigate all above effect. In this paper, a lattice Boltzmann based numerical framework is presented to modeling the problem. The rest sections are organized as follows: In section 2, the governing equations and related boundary conditions are introduced. In section 3, the lattice Boltzmann model to solve the equations is proposed and some implementation details are presented. Finally, in section 4, some useful conclusions are summarized.

2. Governing equations

As mentioned in the introduction part, three kinds of effect are to be considered, which are overlapped EDL, hydrodynamic slip, two-phase flow. In order to include all these effects, the governing equations are to be solved as follows referring Shao's work [6]:

$$-\nabla \cdot (\epsilon \nabla \mathrm{V}) = \sum_\alpha e q_\alpha c_\alpha \tag{1}$$

$$\frac{\partial c_\alpha}{\partial t} + \boldsymbol{u} \cdot \nabla c_\alpha = \nabla \cdot (D_\alpha \nabla c_\alpha + e q_\alpha M_\alpha c_\alpha \nabla V + M_\alpha B_\alpha c_\alpha \nabla \phi) \tag{2}$$

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = \nabla \cdot \left(M_\phi \nabla \mu_\phi\right) \tag{3}$$

$$\nabla \cdot \boldsymbol{u} = 0 \tag{4}$$

$$\rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}\right) = \nabla \cdot \boldsymbol{\sigma} - \nabla p + \mu \nabla \phi - \frac{\tilde{\epsilon} \boldsymbol{E}^2}{2} \nabla \phi - k_B T \sum_\alpha \nabla c_\alpha + \rho_e \boldsymbol{E} \tag{5}$$

In the governing equations, Eq. (1) is the Poisson equation governing the relationship between the electric potential V and the net change density ρ_e (where $\rho_e = \sum_\alpha e q_\alpha c_\alpha$, $e q_\alpha$ and c_α are the corresponding charge and concentration of the αth ion species involved. Here e, q_α are the elementary charge and the valence of the αth ion species) in the electrolyte solution. In the equation, ϵ is the dielectric constant. It should be noted that in the single phase flow problem, ϵ in the whole region is a constant value indeed. However, ϵ in the phase interface region is not a constant any more because two-phase flow is introduced here. Therefore, if mean field theory is assumed, we can set

$$\epsilon(\phi) = \frac{\epsilon_1(1-\phi)}{2} + \frac{\epsilon_2(1+\phi)}{2} = \bar{\epsilon} + \tilde{\epsilon}\phi, \qquad \bar{\epsilon} = \frac{\epsilon_1 + \epsilon_2}{2}, \qquad \tilde{\epsilon} = \frac{\epsilon_2 - \epsilon_1}{2}$$

for simplicity, where ϕ is an order parameter determined by Eq. (3) in the phase field to distinguish between the two immiscible fluid components, ϵ_1, ϵ_2 are the dielectric constants of the two immiscible fluids respectively .

Eq. (2) is the Nernst-Planck equation governing the ion transportation for each ion species. In the equation, $\boldsymbol{u}$ is the velocity of the incompressible fluid in the microchannels. D_α is the diffusion coefficient of the αth ion species and M_α is the corresponding mobility which can be calculated by the Einstein relation $D_\alpha = M_\alpha k_B T$ from D_α. Here k_B, T are the Boltzmann constant and the reference temperature. The term $M_\alpha B_\alpha c_\alpha \nabla \phi$ here reflects the block effect of the fluid-fluid interface on the ion transport. In the term, B_α is a parameter to measure the phase field barrier height that keeps the ions within the electrolyte and keeps them from penetrating into the nonconductive fluid in the channels. Nernst-Planck equation here is solved instead of using the Boltzmann distribution to determine the ion distribution in the channel, therefore, the overlapped EDL effect can be described by this governing equation.

To include the two-phase fluid flow in the microchannels, a phase field based model is used. In the model, Eq.(3) , the Cahn-Hilliard equation is introduced to capture the immiscible fluid

interface motion; the Navier-Stokes equations (4)-(5) are introduced to model the fluid flow involved. Unlike the Cahn-Hilliard equation without considering the electric effect, here a general form of the diffusion term is used which reads

$$\mu_\phi = \mu + \sum_a B_\alpha c_\alpha - \frac{\tilde{\epsilon}}{2}(\nabla V)^2 \tag{6}$$

where

$$\mu = -\nabla \cdot (K\nabla\phi) - r\phi + u\phi^3$$

is the chemical potential in the bulk and the last two terms in the Eq. (6) model the electric effect on the interface motion of the two immiscible fluids. Here K, r, u are material parameters associated with the fluid–fluid interface, the relationship between these parameters and the interfacial thickness ξ and interfacial tension γ reads

$$\xi = \sqrt{K/r}, \qquad \gamma = \frac{2\sqrt{2}r^2\xi}{3u}$$

In the incompressible Navier-Stokes equation, Eq. (4) is the continuum equation and Eq.(5) is the momentum equation. In Eq. (5), p is the pressure, $\boldsymbol{\sigma} = \eta(\nabla\boldsymbol{u} + \boldsymbol{u}\nabla)$ is the viscous stress tensor, η here is the dynamic viscosity of fluid involved. Owing to the two-phase flow is considered, by assuming the mean field theory, we can also set η as a function of the order parameter ϕ for simplicity

$$\eta(\phi) = \frac{\eta_1(1-\phi)}{2} + \frac{\eta_2(1+\phi)}{2}$$

Similarly, the density of the fluid ρ can also read as

$$\rho(\phi) = \frac{\rho_1(1-\phi)}{2} + \frac{\rho_2(1+\phi)}{2}$$

where $\eta_1, \eta_2, \rho_1, \rho_2$ are dynamic viscosity and density of the two immiscible fluids respectively. To address the electric effect and two-phase flow effect, four last terms in right hand side of Eq.(5) are introduced, where $\mu\nabla\phi$ is for the capillary force, $-\frac{\tilde{\epsilon}\boldsymbol{E}^2}{2}\nabla\phi$ models the Maxwell stress and $-k_BT\sum_\alpha \nabla c_\alpha$ is due the osmotic pressure gradient, $\rho_e\boldsymbol{E}$ is the electric body force. Here $\boldsymbol{E} = -(\nabla V + \nabla\psi)$ is the strength of the total electrical field and ψ in the expression is the external applied electric potential.

The corresponding boundary conditions at the microchannel walls for the governing equations (1)-(5) uses in this work are as follows:

$$\partial_n V = \frac{\sigma}{\epsilon} \tag{7}$$

$$\partial_n \mu_\alpha = 0 \tag{8}$$

$$\frac{\partial \phi}{\partial t} + u_\tau \partial_\tau \phi = -\Gamma L_\phi \tag{9}$$

$$\partial_n \mu_\phi = 0 \tag{10}$$

$$\beta v_\tau^{slip} = -\eta(\partial_n u_\tau + \partial_\tau u_n) + L_\phi \partial_\tau \phi \tag{11}$$

$$u_n = 0 \tag{12}$$

Where Eq. (7) is for the Poisson equation (Eq. (1)), Eq. (8) is for the Nernst-Planck equations (Eq.(2)) for each ion species transport, Eq.(9-10) is for the Cahn-Hilliard equation (Eq.(3)) and Eq.(11-12) is for the Navier-Stokes equations (Eq.(4-5)). In the equations, σ is the surface charge density on the walls of the microchannels. Similarly, the density is a function of the order parameter ϕ, here the nonlinear interpolation method is used and the expression reads

$$\sigma(\phi) = \sigma_1\left(1 - \sin\frac{\pi\phi}{2}\right) + \sigma_2\left(1 + \sin\frac{\pi\phi}{2}\right) = \bar{\sigma} + \tilde{\sigma}\sin\frac{\pi\phi}{2}, \qquad \bar{\sigma} = \frac{\sigma_1 + \sigma_2}{2}, \;\; \tilde{\sigma} = \frac{\sigma_2 - \sigma_1}{2}$$

In Eq. (8), μ_α is defined as the chemical potential for c_α

$$\mu_\alpha = k_B T(\ln c_\alpha + 1) + eq_\alpha V + B_\alpha \phi$$

In Eq. (9), the relaxational boundary condition for the order parameter ϕ is used. Γ here is a positive rate coefficient and L_ϕ in the right hand side of the equation has the following form.

$$L_\phi = K\partial_n \phi + \left(V\tilde{\sigma} - \frac{\sqrt{2}}{3}\frac{r^2\xi}{u}\cos\theta_s\right)s_\gamma(\phi)$$

where $s_\gamma(\phi) = \frac{\pi}{2}\cos\frac{\pi\phi}{2}$ and θ_s is the static contact angle at the fluid-solid surface. Eq.(10) is the boundary condition for the effective chemical potential μ_ϕ at the fluid-solid surface. Eq. (11-12) describes the hydrodynamic slip boundary condition for tangential velocity at the fluid-solid surface and the boundary condition for normal velocity respectively. Here β is the slip coefficient and also a local composition of ϕ. Similarly, it reads

$$\beta(\phi) = \frac{\beta_1(1-\phi)}{2} + \frac{\beta_2(1+\phi)}{2}$$

If we denote,

$$\boldsymbol{x} = \boldsymbol{x}' L_{ref}, \qquad \boldsymbol{u} = \boldsymbol{u}' U_{ref}, \;\; t = t'\frac{L_{ref}}{U_{ref}},$$

$$p = p'\rho_{ref}U_{ref}^2, c_\alpha = c_\alpha' C_{ref}, \boldsymbol{E} = \boldsymbol{E}' E_{ref}, V = V' L_{ref}\, E_{ref}, \sigma = \sigma' e L_{ref} C_{ref}$$

Here L_{ref}, U_{ref}, ρ_{ref}, E_{ref} are the reference parameters for length, velocity, density and the

strength of the electrical field, we will have

$$\nabla = \frac{\nabla'}{L_{ref}}, \frac{\partial}{\partial t} = \frac{\partial}{\partial t'}\frac{U_{ref}}{L_{ref}}$$

Then we can get the dimensionless version of the above governing equations (the primes are dropped):

$$-\nabla \cdot (\mathcal{E}\nabla V) \ = \sum_\alpha q_\alpha c_\alpha \tag{13}$$

$$\frac{\partial c_\alpha}{\partial t} + \boldsymbol{u} \cdot \nabla c_\alpha = \nabla \cdot (\mathcal{D}_\alpha \nabla c_\alpha + \mathcal{P}_\alpha q_\alpha c_\alpha \nabla V + \mathcal{C}_\alpha c_\alpha \nabla \phi) \tag{14}$$

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = \mathcal{L}_d \nabla \cdot (\nabla \mu) + \ \nabla \cdot (\nabla \sum_a \mathcal{L}_\alpha c_\alpha) \ - \mathcal{L}_e \nabla \cdot (\nabla (\nabla V)^2) \tag{15}$$

$$\nabla \cdot \boldsymbol{u} = 0 \tag{16}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = \nabla \cdot (\nabla \boldsymbol{u} + \boldsymbol{u} \nabla) \ \frac{1}{Re} \ - \nabla p + \mathcal{B}\mu \nabla \phi - \mathcal{Q}\boldsymbol{E}^2 \ \nabla \phi - \mathcal{S} \sum_\alpha \nabla c_\alpha + \mathcal{F} \sum_\alpha q_\alpha c_\alpha \ \boldsymbol{E} \tag{17}$$

where

$$\mathcal{E} = \frac{\epsilon E_{ref}}{e L_{ref} C_{ref}}, \quad \mathcal{D}_\alpha = \frac{D_\alpha}{L_{ref} U_{ref}}, \quad \mathcal{P}_\alpha = \frac{e E_{ref} M_\alpha}{L_{ref} U_{ref}}, \quad \mathcal{C}_\alpha = \frac{B_\alpha M_\alpha}{L_{ref} U_{ref}}$$

$$\mathcal{L}_d = \frac{r M_\phi}{U_{ref} L_{ref}}, \qquad \mathcal{L}_\alpha = \frac{M_\phi C_{ref} B_\alpha}{U_{ref} L_{ref}}, \quad \mathcal{L}_e = \frac{M_\phi \tilde{\epsilon} E_{ref}^2}{2 U_{ref} L_{ref}}, \qquad Re = \frac{\rho L_{ref} U_{ref}}{\eta}$$

$$\mathcal{B} = \frac{r}{\rho U_{ref}^2}, \qquad \mathcal{Q} = \frac{1}{\rho U_{ref}^2} \frac{\tilde{\epsilon} E_{ref}^2}{2}, \quad \mathcal{S} = \frac{C_{ref}}{\rho U_{ref}^2} k_B T, \qquad \mathcal{F} = \frac{L_{ref}}{\rho U_{ref}^2} e C_{ref} E_{ref}$$

Here we assume $r = u$ in the derivation for simplicity and then μ reads as

$$\mu = -\frac{\xi^2}{L_{ref}^2} \nabla \cdot (\nabla \phi) - \phi + \phi^3$$

by using the expression $\xi = \sqrt{K/r}$.

The corresponding boundary conditions can also be derived as follows:

$$\partial_n V = \frac{\sigma}{\mathcal{E}} \tag{7}$$

$$\mathcal{D}_\alpha \ \partial_n c_\alpha + c_\alpha \ \mathcal{P}_\alpha q_\alpha \partial_n V + c_\alpha \ \mathcal{C}_\alpha \partial_n \phi = 0 \tag{8}$$

$$\frac{\partial \phi}{\partial t} + u_\tau \partial_\tau \phi = -\mathcal{V}_s L - \mathcal{V}_e V \tilde{\sigma} s_\gamma(\phi) \tag{9}$$

$$\partial_n (\mathcal{L}_d \mu + \sum_\alpha \mathcal{L}_\alpha c_\alpha - \mathcal{L}_e (\nabla V)^2) = 0 \tag{10}$$

$$u_\tau^{slip} = -\mathcal{L}_s \partial_n u_\tau + (\mathcal{B}\mathcal{L}_s L + \mathcal{F}V\tilde{\sigma}s_\gamma(\phi))\partial_\tau \phi \tag{11}$$

$$u_n = 0 \tag{12}$$

where $L = \frac{\xi^2}{L_{ref}^2}\partial_n \phi - \frac{\sqrt{2}}{3}\cos\theta_s\, s_\gamma(\phi)$

3. Lattice Boltzmann model

To solve the above governing equations (13-17), a lattice Boltzmann based numerical framework is presented in this work. Four lattice Boltzmann schemes are constructed to recover the equations, the Poisson equation, the Nernst-Planck equation, Cahn-Hilliard equation and Navier-Stokes equation. In this part, we will introduce them one by one. In addition, the schemes which deal with the boundary conditions are presented in the end.

As for the Poisson equation, many lattice Boltzmann models have been proposed in the literatures [9,10]. Here the model introduced by Chai [9] is used owing to its advantages in eliminating the transient term existing in the previous models. In the model, the traditional single relaxation time lattice Boltzmann model is used to solve Eq. (13). Thus the evolution equations of the corresponding density distribution functions read:

$$f_{V\,i}(\boldsymbol{x} + \boldsymbol{c}_i\delta t, t + \delta t) - f_{V\,i}(\boldsymbol{x}, t) = -\frac{1}{\tau_V}\left(f_{V\,i}(\boldsymbol{x}, t) - f_{V_i}^{eq}(\boldsymbol{x}, t)\right) - \delta t\, \overline{\omega_i} \sum_\alpha q_\alpha c_\alpha$$

Here τ_V is the dimensionless relaxation time and $\delta t\, \overline{\omega_i} \sum_\alpha q_\alpha c_\alpha$ is for the source term in the right hand side of the Poisson equation. $f_{V_i}^{eq}(\boldsymbol{x}, t)$ is the equilibrium distribution function associated with ith discrete velocity direction $\boldsymbol{c}_i$ at position $\boldsymbol{x}$ and time t, and can be written as

$$f_{V_i}^{eq}(\boldsymbol{x}, t) = \begin{cases} (1-\omega_0)V(\boldsymbol{x}, t), & i = 0 \\ \omega_i V(\boldsymbol{x}, t), & i = 1-8 \end{cases}$$

for D2Q9 model, and $\overline{\omega_i}$ and ω_i here are weighting coefficients involved and can be defined as,

$$\overline{\omega}_i = \begin{cases} 0, & i = 0 \\ \frac{1}{8}, & i = 1-8, \end{cases} \quad \omega_i = \frac{1}{9}, i = 0-8$$

The discrete velocity $\boldsymbol{c}_i$ here is defined as

$$\boldsymbol{c}_i = \begin{cases} (0,0)c, & i = 0 \\ \left(\cos\left[\frac{(i-1)\pi}{2}\right], \sin\left[\frac{(i-1)\pi}{2}\right]\right)c, & i = 1-4 \\ \sqrt{2}\left(\cos\left[\frac{(i-5)\pi}{2} + \frac{\pi}{4}\right], \sin\left[\frac{(i-5)\pi}{2} + \frac{\pi}{4}\right]\right)c, & i = 5-8 \end{cases}$$

where $c = \delta x/\delta t$ is the particle velocity and $\delta x, \delta t$ are the lattice spacing and time step. τ_V can be get by

$$\mathcal{E} = \frac{2}{3}\left(\tau_V - \frac{1}{2}\right)c^2\delta t$$

The macro parameter solved here, the electrical potential $V(x,t)$ can be calculated as

$$V(\boldsymbol{x}, t) = \frac{1}{1-\omega_0}\sum_{i=1} f_{V_i}^{eq}(\boldsymbol{x}, t)$$

As for the Nernst-Planck equation Eq.(14), the multiple relaxation time lattice Boltzmann model is used by referring the model proposed by Chai[11] for general convection-diffusion equations. In the model, the evolution equation of the corresponding density distribution function for αth ion transport,

$$f_{C_i}(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) - f_{C_i}(\boldsymbol{x},t) = -[M^{-1}S^c M]_{ij}\left(f_{C_j}(\boldsymbol{x},t) - f_{C_j}^{eq}(\boldsymbol{x},t)\right) + \delta t\left[M^{-1}\left(1-\frac{S^c}{2}\right)M\right]_{ij} R_{C_j}(\boldsymbol{x},t)$$

Here $f_{C_i}(\boldsymbol{x},t)$ is the density distribution function associated with ith discrete velocity $\boldsymbol{c}_i$ at position $\boldsymbol{x}$ and time t and $f_{C_j}^{eq}(\boldsymbol{x},t)$ is the corresponding equilibrium distribution function with form as

$$f_{C_i}^{eq}(\boldsymbol{x},t) = \omega_{c_i}c_\alpha\left(1+\frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2}+\frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c_s^4}-\frac{\boldsymbol{u}\cdot\boldsymbol{u}}{2c_s^2}\right)+\overline{\omega_{c_i}}\,\frac{c_\alpha p}{\rho c_s^2}$$

Where the related weighting coefficients for D2Q9 model can be read as

$$\overline{\omega_{c_i}} = \begin{cases} -\frac{5}{9}, & i=0 \\ \frac{1}{9}, & i=1-4, \\ \frac{1}{36}, & i=5-8 \end{cases} \quad \omega_{c_i} = \begin{cases} \frac{4}{9}, & i=0 \\ \frac{1}{9}, & i=1-4, \\ \frac{1}{36}, & i=5-8 \end{cases}$$

the transformation matrix M can be written as

$$M = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & 2 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix},$$

$S^c = diag(s_0^c, s_1^c, s_2^c, s_3^c, s_4^c, s_5^c, s_6^c, s_7^c, s_8^c)$ in the evolution equation is the non-negative diagonal relaxation matrix. If we set $s_3^c = s_5^c = \frac{1}{\tau_\alpha}$, the relaxation parameters can be obtained by

$$\mathcal{D}_\alpha = c_s^2\left(\tau_\alpha - \frac{1}{2}\right)\delta t$$

The values for other relaxation parameters are chosen as shown in Chai's work [4]. $R_{C_j}(\boldsymbol{x},t)$ in the discrete source term can be read as

$$R_{C_j}(x,t) = \omega_{c_j}\left[\left(1+\frac{\boldsymbol{c}_j\cdot\boldsymbol{u}}{c_s^2}\right)R + \frac{\boldsymbol{c}_j\cdot\left(\frac{p}{\rho}\nabla c_\alpha + \frac{c_\alpha(\boldsymbol{F}_a+\boldsymbol{F})}{\rho}\right)}{c_s^2}\right]$$

Here

$R = \nabla\cdot(\mathcal{P}_\alpha q_\alpha c_\alpha \nabla V + \mathcal{C}_\alpha c_\alpha \nabla\phi)$, $\boldsymbol{F} = \mathcal{B}\mu\nabla\phi - \mathcal{Q}\boldsymbol{E}^2\nabla\phi - \mathcal{S}\sum_\alpha \nabla c_\alpha + \mathcal{F}\sum_\alpha q_\alpha c_\alpha \boldsymbol{E}$, $\boldsymbol{F}_a =$

$\frac{\rho_A-\rho_B}{\phi_A-\phi_B}(\mathcal{L}_d\nabla\cdot(\nabla\mu)+\ \nabla\cdot(\nabla\sum_a\mathcal{L}_\alpha c_\alpha)\ -\mathcal{L}_e\nabla\cdot(\nabla(\nabla V)^2))\boldsymbol{u}$

The macro parameters c_α can be evaluated by

$$c_\alpha=\sum_i g_i+\frac{\delta t}{2}R$$

$\nabla V,\nabla c_\alpha$ involved in the equations can be calculated by

$$\nabla V=-\frac{1}{\frac{2}{3}c^2\tau_V\delta t}\sum_j \boldsymbol{c}_j\ \left(f_{V\,j}-f_{V_j}^{eq}\right)$$

$$\nabla c_\alpha=-\frac{\sum_i \boldsymbol{c}_i\left[f_{C\,i}-f_{C_i}^{eq}\right]+\frac{\delta t}{2}\left(\frac{c_\alpha(\boldsymbol{F}_a+\boldsymbol{F})}{\rho}+\boldsymbol{u}R\right)}{\delta t\left(\tau_\alpha c_s^2+\frac{p}{2\rho}\right)}$$

As for the Cahn-Hilliard equation, another multiple relaxation time lattice Boltzmann model is used referring the work by Liang [12]. In the model, the evolution equation for the corresponding density distribution is presented as

$$h_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t,t+\delta t)-h_i(\boldsymbol{x},t)=-\Lambda_{ij}^h\left[h_j(\boldsymbol{x},t)-h_j^{eq}(\boldsymbol{x},t)\right]+\delta t R_i(\boldsymbol{x},t)$$

where $h_i(\boldsymbol{x},t)$ is the density distribution function for the order parameter ϕ and $h_i^{eq}(\boldsymbol{x},t)$ is the corresponding equilibrium distribution function,

$$h_i^{eq}(\boldsymbol{x},t)=\begin{cases}\phi+\left(\omega_0^h-1\right)\eta\mu_\phi, & i=0\\ \omega_i^h\eta\mu_\phi+\omega_i^h\frac{c_i\cdot\phi\boldsymbol{u}}{c_s^2}, & i\neq 0\end{cases}$$

where the weighting coefficients ω_i^h read

$$\omega_i^h=\begin{cases}\frac{4}{9}, & i=0\\ \frac{1}{9}, & i=1-4,\\ \frac{1}{36}, & i=5-8\end{cases}$$

Here $c_s^2=\frac{1}{3}c^2$ and μ_ϕ in $h_i^{eq}(\boldsymbol{x},t)$ has the following expression

$$\mu_\phi=\mu+\sum_a\frac{\mathcal{L}_\alpha}{\mathcal{L}_d}c_\alpha+\frac{\mathcal{L}_e}{\mathcal{L}_d}(\nabla V)^2$$

$\Lambda_{ij}^h=M^{-1}S^hM$ is the collision operator, the transformation matrix M has the same form as in previous models, the relaxation matrix S^h here is

$$S^h=diag(s_0^h,s_1^h,s_2^h,s_3^h,s_4^h,s_5^h,s_6^h,s_7^h,s_8^h)$$

If we set $\tau_h=\frac{1}{s_3^h}=\frac{1}{s_5^h}$, the relaxation parameters can be calculated by $\mathcal{L}_d=\eta c_s^2\left(\tau_h-\frac{1}{2}\right)\delta t$.

The discrete source term here reads as

$$R_i = \left(M^{-1}\left(I - \frac{S^h}{2}\right)M\right)_{ij} \bar{R}_j$$

where

$$\bar{R}_j = \frac{\omega_j c_j \cdot \partial_t \phi \boldsymbol{u}}{c_s^2},$$

The macro parameter ϕ can be got by

$$\phi = \sum_i h_i$$

In this model, we need calculate the time derivate and one or second order spacial derivatives for certain functions such as $\partial_t \phi \boldsymbol{u}$ or $\nabla \cdot (\nabla \phi)$. Here the explicit difference scheme is used for time derivate and second-order isotropic central schemes [13] are recommended for calculate one or second order spacial derivatives of certain functions. The schemes are as follows:

$$\partial_t \chi(\boldsymbol{x}, t) = (\chi(\boldsymbol{x}, t) - \chi(\boldsymbol{x}, t - \delta t))/\delta t$$

$$\nabla \chi(\boldsymbol{x}, t) = \sum_{i \neq 0} \frac{\omega_i^h c_i \chi(\boldsymbol{x} + \boldsymbol{c}_i \delta t, t)}{c_s^2 \delta t}$$

$$\nabla^2 \chi(\boldsymbol{x}, t) = \sum_{i \neq 0} \frac{2\omega_i^h [\chi(\boldsymbol{x} + \boldsymbol{c}_i \delta t, t) - \chi(\boldsymbol{x}, t)]}{c_s^2 \delta t^2}$$

Here $\chi(\boldsymbol{x}, t)$ is an arbitrary function.

As for the Navier-Stokes equation, multiple relaxation time lattice Boltzmann model again is used referring the work by Liang [12]. In the model, the evolution equation for the corresponding density distribution is

$$g_i(\boldsymbol{x} + \boldsymbol{c}_i \delta t, t + \delta t) - g_i(\boldsymbol{x}, t) = -[M^{-1} S^g M]_{ij}\left[g_j(\boldsymbol{x}, t) - g_j^{eq}(\boldsymbol{x}, t)\right] + \delta t \left[M^{-1}\left(1 - \frac{S^g}{2}\right)M\right]_{ij} F_j(\boldsymbol{x}, t)$$

where the equilibrium distribution function $g_i^{eq}(\boldsymbol{x}, t)$ is defined as

$$g_i^{eq}(\boldsymbol{x}, t) = \begin{cases} \rho s_i(\boldsymbol{u}) + \dfrac{(\omega_i^g - 1)p}{c_s^2}, & i = 0 \\ \rho s_i(\boldsymbol{u}) + \omega_i^g \dfrac{p}{c_s^2}, & i \neq 0 \end{cases}$$

In the expression $\omega_i^g = \omega_i^h$, $s_i(\boldsymbol{u}) = \omega_i^g \left(\frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u} \cdot \boldsymbol{u}}{2c_s^2}\right)$, M has the same form as the transformation matrix in the previous models. The relaxation matrix is defined as

$$S^g = diag(s_0^g, s_1^g s_2^g, s_3^g, s_4^g, s_5^g, s_6^g, s_7^g, s_8^g)$$

If we set $\tau_g = \frac{1}{s_7^g} = \frac{1}{s_8^g}$, we can calculate the relaxation parameter by

$$\frac{1}{Re} = c_s^2 \left(\tau_g - \frac{1}{2}\right)\delta t,$$

As for the discrete force term F_j, we can define it as

$$F_j = \frac{(\boldsymbol{c}_j - \boldsymbol{u})}{c_s^2} \cdot \{[\Gamma_j(\boldsymbol{u}) - \Gamma_j(0)]\nabla(\rho c_s^2) + (\boldsymbol{F}_a + \boldsymbol{F})\Gamma_j(\boldsymbol{u})\},$$

where $\Gamma_j(\boldsymbol{u}) = \frac{f_i^{eq}}{\rho}$ and $f_i^{eq} = \omega_i \rho + \rho s_i(\boldsymbol{u})$

The macro parameters $\boldsymbol{u}$ and p can be got by

$$\boldsymbol{u} = \frac{\left[\sum_i c_i g_i + \frac{1}{2}\delta t \boldsymbol{F}\right]}{\left[\rho - \frac{1}{2}\delta t(\rho_A - \rho_B)\nabla \cdot \frac{M_\phi \nabla \mu_\phi}{\phi_A - \phi_B}\right]}$$

$$p = \frac{c_s^2}{1 - \omega_0^g}[\sum_{i \neq 0} g_i + \frac{1}{2}\delta t \boldsymbol{u} \cdot \nabla \rho + \rho s_0(\boldsymbol{u})]$$

As for the boundary condition implementation scheme, the non-equilibrium extrapolation method is used which is proposed by Guo [14]. As an example, we present here the implementation procedure of the method for Eq.(9-10). In the method, the density distribution function $h_i(\boldsymbol{x_B}, t)$ at certain wall node is first decomposed into its equilibrium and non-equilibrium parts

$$h_i(\boldsymbol{x_B}, t) = h_i^{eq}(\boldsymbol{x_B}, t) + h_i^{neq}(\boldsymbol{x_B}, t)$$

As for the non-equilibrium part, we can approximate it by the corresponding non-equilibrium parts at the nearest fluid node $\boldsymbol{x_F}$

$$h_i^{neq}(\boldsymbol{x_B}, t) \approx h_i(\boldsymbol{x_F}, t) - h_i^{eq}(\boldsymbol{x_F}, t)$$

As for the equilibrium part, we only need to get approximate values of the macro parameters ϕ, μ_ϕ on the wall node by applying certain finite difference schemes on Eq.(9-10). Once the values is obtained, we can calculate the $h_i^{eq}(\boldsymbol{x_B}, t)$.

Through Chapman-Enskog expansion analysis and Taylor approximation method, Eq. (13)-(17) can finally be recovered with second order accuracy by the lattice Boltzmann based numerical framework proposed referring the similar procedures used in the literatures [9,10,11,12].

4. Conclusions

In this work, a numerical framework based on the lattice Boltzmann method is proposed to simulating two-phase electroosmotic flow in microchannels with hydrodynamic slip boundary conditions. In the framework, a single relaxation time lattice Boltzmann model is presented for the Poisson equation which governing the electrical potential in the channels, and multiphase relaxation time lattice Boltzmann models are introduced for the Nernst-Planck equation which describes the ion transportation, the Cahn-Hilliard equation which models the interface motion between two immiscible phases, and Navier-Stokes equations which models the fluid flow transportation. By using this model, all three effects mentioned in the introduction part, the overlapped EDL, two-phase flow, hydrodynamic slip effect can be investigated. Theoretical analysis can show that the numerical framework can recover the governing equations involved with second order numerical accuracy.

5. References

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