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Electroviscous effect on non-Newtonian fluid flow in microchannels

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ABSTRACT

Understanding non-Newtonian flow in microchannels is of both fundamental and practical significance for various microfluidic devices. A numerical study of non-Newtonian flow in microchannels combined with electroviscous effect has been conducted. The electric potential in the electroviscous force term is calculated by solving a lattice Boltzmann equation. And another lattice Boltzmann equation without derivations of the velocity when calculating the shear is employed to obtain flow field. The simulation of commonly used power-law non-Newtonian flow shows that the electroviscous effect on the flow depends significantly on the fluid rheological behavior. For the shear thinning fluid of the power-law exponent n < 1, the fluid viscosity near the wall is smaller and the electroviscous effect plays a more important role. And its effect on the flow increases as the ratio of the Debye length to the channel height increases and the exponent n decreases. While the shear thickening fluid of n > 1 is less affected by the electroviscous force, it can be neglected in practical applications.

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1. Introduction

The application of micro-electro-mechanical-systems has been recently increasing in various fields. Devices with dimensions of the order of microns are being developed for a range of miniaturized fluidic systems in advanced detecting processes and propulsion systems [1]. Such microfluidic devices are not simply scale-down version of conventional ones and this motivates research toward a better understanding of microscale fluidic transport phenomena such as electrokinetic effect or surface effects to optimize the device design and operation.

It is known that most solid surfaces carry electrostatic charges or electrostatic surface potential. The electrostatic charges on the solid surface will attract the counterions in the liquid when the liquid contains certain amount of ions. The rearrangement of the charges on the solid surface and the balancing charges in the liquid are called the electrical double layer (EDL) [2,3], composing of the immobile compact layer and the mobile diffuse layer. When liquid flows through a microchannel under a hydrostatic pressure, the nonzero electrical charges in the mobile part of the EDL are carried downstream, building a balance between the streaming current flowing in the streamwise direction and the conductance current flowing back in the opposite direction. When the ions are moved in the diffuse layer, they pull the liquid along with them in the opposite direction to the pressure-driven flow, leading to a reduced flow rate compared with the conventional theory pre-

diction. Such electrokinetic effect of the presence of the EDL on the flow behavior is similar to that of a liquid having a higher apparent viscosity, referred to the electroviscous effect [2]. Some researches have shown that the electroviscous effect is significant in microflows and it causes an obvious flow resistance increase compared to conventional theory [3–5]. However, some literature [6,7], including our previous experimental and numerical study [8] has argued that the electroviscous effect is not so obvious in microchannel flow under moderate electrical conductivity of the liquid and conductivity of the walls. To the authors' best knowledge, most of the existing studies are limited to Newtonian fluid. However, the flow behavior of non-Newtonian fluid is of high interest in practical applications such as sample collection, dispensing, reaction, detection, mixing, and separation of various biological and chemical species on a micro-chip integrated with fluidic pumps and valves. The fluid rheological behavior combined with the microscale effects usually plays a more important and complex role. Fundamental understanding of the non-Newtonian role in liquid transport through microchannels is significant to correctly predict and control the characteristics and performance of such microfluidic devices. In this article, we numerically study the flow characteristics of non-Newtonian fluids combined with the electroviscous effect in microchannels by using the lattice Boltzmann method (LBM).

The LBM originates from mesoscopic kinetic equations and intrinsically possesses some essential microscopic physics ingredients, which makes the LBM of great potential to capture the non-continuum effects including non-equilibrium and electrokinetic phenomena in microfluidic devices. For the non-Newtonian fluid, its viscosity is related to the local rate of strain through the

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constitutive equation for the stress tensor. The kinetic essence of the LBM makes it capable of calculating the local components of the stress tensor without a need to estimate velocity gradients, while the Navier–Stokes solvers need to get the derivatives of obtained velocity profiles. This feature makes the LBM retain second-order accuracy and high efficiency for shear-dependent non-Newtonian flow simulations [9–15].

In the next section, the lattice Boltzmann equations for the velocity field of non-Newtonian fluid and for the electric potential distribution are introduced with their boundary conditions. In Section 3, the LBM equations are used to analyze the velocity profiles for non-Newtonian flow combined with the electroviscous effect under external pressure gradient. The distribution of the electroviscous force across the channel is also presented and discussed. This article is concluded in Section 4.

2. Numerical methods

2.1. The lattice Boltzmann equation for non-Newtonian fluid flow field

The LBM tracks the evolution of the local distribution functions, *f* of the computational particles to describe the conserved fields. The discrete evolution equation with the Bhatnagar–Gross–Krook (BGK) collision approximation is [16]:

$$f_i(\mathbf{r}+\mathbf{c}_i\delta_t,t+\delta_t)$$

$$= f_i(\mathbf{r}, t) - \frac{\delta_t}{\tau_u} [f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t)] + \delta_t \frac{\mathbf{F} \cdot (\mathbf{c}_i - \mathbf{u})}{RT} f_i^{\text{eq}}(\mathbf{r}, t), \tag{1}$$

where τ_v is the relaxation time, \mathbf{c}_i is the particle discrete velocity and \mathbf{F} is an external force term. For a D2Q9 square lattice, $\mathbf{c}_0 = 0$, $\mathbf{c}_i = (\cos[(i-1)\pi/2], \sin[(i-1)\pi/2])$ for i=1, 2, 3, 4 and $\mathbf{c}_i = (\cos[(i-5)\pi/2 + \pi/4], \sin[(i-5)\pi/2 + \pi/4])\sqrt{2}c$ for i=5, 6, 7, 8 where $c = \delta_x/\delta_t$ is the particle streaming speed $(\delta_x, \delta_t$ are the lattice spacing and time step, respectively). The equilibrium density distribution function, $f_i^{\text{eq}}(i=0, 1, ..., 8)$ for a D2Q9 lattice [17]:

$$f_i^{\text{eq}} = \rho \omega_i \left[1 + \frac{3(\mathbf{c}_i \cdot \mathbf{u})}{c^2} + \frac{9(\mathbf{c}_i \cdot \mathbf{u})^2}{2c^4} - \frac{3(\mathbf{u} \cdot \mathbf{u})}{2c^2} \right], \tag{2}$$

where $\omega_0 = 4/9$, $\omega_i = 1/9$ for i = 1, 2, 3, 4 and $\omega_i = 1/36$ for i = 5, 6, 7, 8. The relaxation time τ_v is linked to the kinematic viscosity ν through:

$$\tau_{\nu} = 3\nu \frac{\delta_t^2}{\delta_z^2} + 0.5\delta_t. \tag{3}$$

The mass density and momentum density can be obtained by summing over the distribution functions, $f_i(\mathbf{r},t)$:

$$\rho = \sum_{i} f_{i} \text{ and } \rho \mathbf{u} = \sum_{i} f_{i} \mathbf{c}_{i}. \tag{4}$$

We know that the stress tensor for an incompressible fluid with pressure p is given by:

$$\sigma_{\alpha\beta} = -p\delta_{\alpha\beta} + \eta \left(\frac{\partial u_{\alpha}}{\partial x_{\beta}} + \frac{\partial u_{\beta}}{\partial x_{\alpha}} \right) = -p\delta_{\alpha\beta} + 2\eta S_{\alpha\beta}, \tag{5}$$

where η is the dynamic viscosity, $\delta_{\alpha\beta}$ is the Kronecker delta, and $S_{\alpha\beta} = 1/2((\partial u_{\alpha}/\partial u_{\beta}) + (\partial u_{\beta}/\partial u_{\alpha}))$ is the shear strain rate tensor. We calculate $S_{\alpha\beta}$ at each node in the LBM as [18]:

$$S_{\alpha\beta} = -\frac{3}{2\rho c^2 \tau_{\nu}} \sum_{i=0} f_i^{(1)} \mathbf{c}_{i\alpha} \mathbf{c}_{i\beta}, \tag{6}$$

where $f_i^{(1)}$ is the non-equilibrium part of the distribution function. In the commonly used power-law model for non-Newtonian fluid,

the viscosity is given by:

$$\eta = \eta_0 \dot{\gamma}^{n-1} = \eta_0 (S_{\alpha\beta} S_{\alpha\beta})^{(n-1)/2},$$
(7)

where the shear rate-related $\dot{\gamma}$ is $\dot{\gamma} = \sqrt{S_{\alpha\beta}S_{\alpha\beta}}$ and the parameter n is the power-law exponent which determines the response of the fluid to changes in shear rate. The fluid is classified as shear thinning for n < 1 and shear thickening for n > 1. The fluid recovers the Newtonian behavior with shear-independent viscosity η_0 at n = 1.

Coupling Eqs. (3), (6) and (7), together with $\eta = \rho \nu$, we can derive a shear-dependent relaxation time τ_{ν} at each node in the lattice Boltzmann evolution Eq. (1).

Note that the quantity $f_i^{(1)} \mathbf{c}_{i\alpha} \mathbf{c}_{i\beta}$ in Eq. (6) is usually computed with second-order accuracy during the collision process in the LBM evolution. Therefore, the stress tensor components and the corresponding shear-dependent viscosity of non-Newtonian fluid can be obtained independent of the velocity fields, in contrast to most traditional CFD methods which estimate the stress tensor components from the obtained velocity field. This benefit without a need to get the derivatives of velocity profiles in computing the stress tensor and non-Newtonian viscosity is clear when dealing with flow in complex geometry of irregular cross-sections or flows characterized by large velocity gradients [18].

We can demonstrate that Eq. (1) recovers the Navier–Stokes equation by using the Chapman–Enskog approximation:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \rho \nu \nabla^2 \mathbf{u} + \rho \mathbf{F}, \tag{8}$$

The force term under external pressure gradient ∇p can be expressed as:

$$\rho \mathbf{F} = -\nabla p - \rho_{\rho} \mathbf{E},\tag{9}$$

where ρ_e is the net charge density per unit volume at any point in the liquid, **E** is the stream electric field caused by the ion movement in the solution, and ρ_e **E** presents the electro-viscosity term. The stream electric field can be obtained through a balance between streaming current and electrical conductance current at steady state.

$$\mathbf{E} = -\frac{\rho_e \mathbf{u}}{\lambda},\tag{10}$$

here λ is the electrical conductivity of the liquid layer. A solution conductivity law originally devised by Friedrich Kohlrausch (see Ref. [19] for details), which states that the conductivity of a dilute solution is the sum of independent values: the molar conductivity of the cations and the molar conductivity of the anion. The law is based on the independent migration of ions and then λ can be written as:

$$\lambda = n_+ \Lambda_+ + n_- \Lambda_-,\tag{11}$$

where Λ is the molar conductivity.

2.2. The lattice Boltzmann equation for electric potential

Note that the net charge density per unit volume, ρ_e , must be obtained before solving the velocity field from Eq. (9). The relationship between the electric potential in the liquid, ψ , and the net charge density per unit volume, ρ_e , at any point in the liquid is described by the Poisson equation:

$$\nabla^2 \psi = -\frac{\rho_e}{\varepsilon \varepsilon_0},\tag{12}$$

where ε_0 is the permittivity of free space and ε is the relative dielectric constant of the solution. Assuming that the equilibrium

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