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Simulation of electro-osmotic flow in microchannel with lattice Boltzmann method

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Abstract

In this Letter, an incompressible lattice Boltzmann model without compressible effect for simulating flow field and a new lattice Boltzmann model for correctly solving the Poisson–Boltzmann equation are introduced. The proposed models can be used to eliminate some unexpected errors in lattice Boltzmann method that has been applied to simulate electro-osmotic flow in microchannel. Transient behavior of electro-osmotic transport and effects due to the variations of the ionic concentration, channel height, external electric field and zeta (ζ) potential on the velocity profile were investigated with present models. Detailed numerical results are in good agreement with the corresponding analytical solutions or numerical results in existing literature.

Keywords: Lattice Boltzmann method; Electro-osmotic flow; Electric double layer; Zeta potential

1. Introduction

Electro-osmotic flow (EOF) is created when an electric field is applied through a liquid-filled microchannel where an electrical double layer (EDL) is formed due to the interaction between an electrolyte solution and a solid surface [1]. Due to the important applications of this type of flow in various biomedical lab-on-a-chip devices to transport and manipulate liquids for different purposes, such as sample injection, chemical reactions, and species separation, EOF in microchannels has received increasing attention in recent years [1,2].

Historically, many studies have been carried out on electro-osmotic flow in microchannels. Burgreen and Nakache [3] established a mathematical model in ultrafine capillary slits. Later, the same problem was studied by Rice and Whitehead [4] in narrow cylindrical capillary. Qu and Li [5] also formulated a mathematical model for overlapped EDL fields. Due to the constraints of the experimental conditions and the theoretical analysis, many numerical methods were developed for simulating electro-osmotic flow in microchannel in the past several years. Patankar and Hu [6] developed a numerical scheme to simulate the electro-osmotic flow in the intersection of channel. Bianchi et al. [7] developed a finite element formulation for simulating electro-osmotic flow in microscale channel networks. Mitchell et al. [8] simulated electro-osmotic flow in three typically encountered geometries with finite cloud method. Jin and Luo [9] also simulated the electro-osmotic flow at the cross region in microfluidic chips and compared their simulated results with the experimental images. Tan and Ng [10] studied 3D developing flow in microchannel with numerical method. Zhao and Liao [11] studied thermal effects on electro-osmotic pumping of liquids in microchannels with finite difference method. Xuan et al. [12] investigated thermal end effects on electro-osmotic flow in a capillary using finite element method.

As reported by Fan and Harrison [13], the duration of electro-osmotic injection affects the separation efficiency. Therefore, investigation of transient behavior can provide more insights

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into the characters of electro-osmotic flow and is also important for the Biochip operation [15]. A theoretical framework for describing the transient phenomena was built by Söderman and Jönsson [14], and then further developed by many researchers [15–17]. However, the encountered geometries analyzed with analytical theory are very simple, and there are many difficulties for researchers to extend the analytical theory to the complex geometries. To address this problem, the numerical analysis may be used as an alternative tool to analyze the transient phenomena in complex geometries. For example, Qiao and Aluru [18] have applied a reduced-order modelling approach to analyze the transient behavior of electro-osmotic flow in four different geometries.

In addition, many factors, including the ionic concentration of the electrolyte, channel height, ζ potential and external electric field, may have important impacts on the velocity profile. The relations between them are studied in detail in the present work.

In the past decades, several approaches were developed for simulating EOF in microchannels, including finite element [7], finite difference [19], molecular dynamics (MD) [20] and so on. However, there are many difficulties in simulating such phenomena with the methods mentioned above due to the presence of an electric double layer [21].

As a new mesoscopic numerical approach, the lattice Boltzmann method (LBM), has received more and more attention in simulating complex fluid flows and transport phenomena based on kinetic theory and statistic physics. Because of its distinctive advantages over conventional numerical methods, the LBM has achieved great success in a variety of fields since its emergence [22–24]. Furthermore, many efforts have been made to apply the LBM to simulate electrokinetic phenomena [21,25–29]. However, two problems arise when existing lattice Boltzmann models are applied to simulate electrokinetic phenomena. Firstly, as the compressible schemes is applied to simulate incompressible fluid flows, the compressible effect might lead to some undesirable errors in numerical simulations [30]. Secondly, the existing models applied to solve Poisson–Boltzmann equation provide approximate solutions by solving steady diffusion equation, this is because the term $\partial/\partial t$ exists in their final recovered equation [25,28,29]. Therefore, some unexpected errors may be induced by this term in numerical experiments.

To address the problems listed above, an incompressible lattice Boltzmann model without compressible effect and a new lattice Boltzmann model for correctly solving Poisson–Boltzmann equation are proposed in this Letter. Subsequently, transient behavior of electro-osmotic transport and the effects of the variations of the ionic concentration, channel height, external electric field and ζ potential on the velocity profile are studied in detail with proposed models.

The rest of the Letter is organized as follows. In following section, the macroscopic governing equations for EOF are introduced. In Section 3, the lattice Boltzmann models for solving macroscopic governing equations are proposed. Numerical experiments are performed in Section 4, and finally, a brief summary and conclusion are presented in Section 5.

2. Macroscopic hydrodynamic equations for EOF

The general equations for governing EOF are incompressible Navier–Stokes equations, including continuity equation and momentum equation adapted electrical external force

$$\nabla \cdot \mathbf{u} = 0, \tag{1a}$$

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla P + \mu\nabla^2\mathbf{u} + \rho_e\mathbf{E}, \tag{1b}$$

where $\mathbf{u}$ is the velocity vector, ρ is the density of solution, P is the pressure, μ is the dynamic viscosity of the flow, ρ_e is the net charge density, and $\mathbf{E}$ is the external electric field.

In the incompressible limit, the change of the density can be neglected, Eq. (1) reduce to following equation

$$\nabla \cdot \mathbf{u} = 0, \tag{2a}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla P' + \nu\nabla^2\mathbf{u} + G, \tag{2b}$$

where $P' = P/\rho$, $G = \rho_e\mathbf{E}/\rho$ is the acceleration due to external force, ν is kinetic viscosity.

As the sample is usually a dilute solution, the same properties are assumed in the whole bulk solution in microchannel. The physical parameters such as the viscosity are assumed to be equal to the solvent characteristics. According to the EDL theory [31], the induced electric potential of ions satisfies the Poisson equation

$$\nabla^2\psi = -\frac{\rho_e}{\varepsilon\varepsilon_0}, \tag{3}$$

where ψ is the electrical potential, ρ_e is the net charge density, ε and ε_0 are the dimensionless dielectric constant and permittivity of vacuum, respectively.

For the flows over a non-conducting stationary surface, the ion distribution can be well approximated by the Boltzmann distribution [31],

$$n_i = n_{i\infty}\exp\left(-\frac{z_i e}{k_b T}\psi\right),$$

where n_i is the ionic number concentration of ith species, z_i is the valence of type-i ions, n_∞ is the ionic number concentration in the bulk solution, e is the fundamental electric charge, k_b is the Boltzmann constant, and T is the temperature. For a symmetric electrolyte ($z_i = z$ and $n_{i\infty} = n_\infty$) considered in the present work, the net charge density can be defined as

$$\rho_e = -2n_\infty ze\sinh\left(\frac{z_i e}{k_b T}\psi\right). \tag{4}$$

Substituting Eq. (4) into Eq. (3) leads to the following Poisson–Boltzmann equation

$$\nabla^2\psi = \frac{2n_\infty ze}{\varepsilon\varepsilon_0}\sinh\left(\frac{ze}{k_b T}\psi\right). \tag{5}$$

If the term $\frac{z_i e}{k_b T}\psi$ is small enough (for example, $|\psi| < 25$ mV), $\sinh(\frac{z_i e}{k_b T}\psi) \approx \frac{z_i e}{k_b T}\psi$ [21], which is known as Debye–Hückel approximation. With the aid of this approximation, Eq. (5) can