Chemical Physics xxx (2018) xxx–xxx

Contents lists available at ScienceDirect

Chemical Physics

journal homepage: www.elsevier.com/locate/chemphys

Numerical simulation of electroosmotic flow in rough microchannels using the lattice Poisson-Nernst-Planck methods

Reza Kamali *, Mohsen Nasiri Soloklou, Hooman Hadidi

Department of Mechanical Engineering, Shiraz University 1, Shiraz, Fars 71348-51154, Iran

ARTICLE INFO

Article history:
Received 9 October 2017
In final form 12 April 2018
Available online xxxx

Keywords:
Microchannel
Electroosmotic flow
Electric double layer
Lattice Boltzmann method
Dynamic model
Roughness

ABSTRACT

In this study, coupled Lattice Boltzmann method is applied to solve the dynamic model for an electroosmotic flow and investigate the effects of roughness in a 2-D flat microchannel. In the present model, the Poisson equation is solved for the electrical potential, the Nernst– Planck equation is solved for the ion concentration. In the analysis of electroosmotic flows, when the electric double layers fully overlap or the convective effects are not negligible, the Nernst-Planck equation must be used to find the ionic distribution throughout the microchannel. The effects of surface roughness height, roughness interval spacing and roughness surface potential on flow conditions are investigated for two different configurations of the roughness, when the EDL layers fully overlap through the microchannel. The results show that in both arrangements of roughness in homogeneously charged rough channels, the flow rate decreases by increasing the roughness height. A discrepancy in the mass flow rate is observed when the roughness height is about 0.15 of the channel width, which its average is higher for the asymmetric configuration and this difference grows by increasing the roughness height. In the symmetric roughness arrangement, the mass flow rate increases until the roughness interval space is almost 1.5 times the roughness width and it decreases for higher values of the roughness interval space. For the heterogeneously charged rough channel, when the roughness surface potential ψ_r is less than channel surface potential ψ_s, the net charge density increases by getting far from the roughness surface, while in the opposite situation, when ψ_s is more than ψ_r, the net charge density decreases from roughness surface to the microchannel middle center. Increasing the roughness surface potential induces stronger electric driving force on the fluid which results in larger velocities in the flow.

1. Introduction

Increasing applications of the micro and nano systems, in the fields of biology, chemistry and pharmacy has attracted the attention of many researchers in recent years. Fluid transport in the micro and nano channels has become one of the most important subjects in this field. Recently, numerous numerical studies have been done in the field of electroosmotic flow in microfluidics and nanofluidics [1–3]. One of the most important advantages of the electroosmosis-based microfluidic systems is that they do not require any moving components compared with other mechanical microfluidic systems. This simplifies the design and fabrication of these microfluidic systems and enhances their applicability remarkably. Surface charges on the walls of the microchannels cause changes in the arrangement of the ions in the electrolyte and development of the electric double layer near the surface. Therefore, a thin and charged liquid layer forms near the solid wall which is called the EDL [5]. The EDL has a thickness in the order of (10–300) nm. The ion concentration in the EDL is inhomogeneous [6–8] and an externally applied electric field can create a net flow of charge within this layer. As a result, in the electroosmotic flow under the influence of an external electric force, the electrolyte between electrically charged plates begins to move [9,10]. Some of the applications of the electroosmotic flow include transportation and manipulation of liquids in various biomedical lab-on-a-chip devices for sample injection, chemical reactions and species separation [1,4]. Based on the observations, channel walls indicate some degree of roughness depending on the channel fabrication process. Since this surface roughness can affect the flow characteristics, it is important to consider roughness effects especially in the micro and nano-channel studies. Up to now, many studies have been carried out on electroosmotic flow in the microchannels and nanochannels [11–16]. However, most of the previous studies have concentrated on microchannels with smooth and homogeneous walls, and the fluid flow behavior in rough and

* Corresponding author.
E-mail address: rkamali@shirazu.ac.ir (R. Kamali).

https://doi.org/10.1016/j.chemphys.2018.04.008
0301-0104/© 2018 Published by Elsevier B.V.

heterogeneous micro and nano-channels are less understood. Hu et al. in a study, investigated the effect of three-dimensional roughness on electroosmotic flow through microchannels [17,18]. Wang et al. studied the effects of roughness and cavitation on electroosmotic flows in rough microchannels applying the lattice Poisson-Boltzmann methods [19]. Their results showed that by changing the roughness height and the interval space, electroosmotic flow rate varies non-uniformly. Wang and Kang modeled the electroosmotic flow in microchannels with random roughness. They generated a rough channel with a three-dimensional microstructure [20]. In most analyses of electroosmotic flows, the Poisson–Boltzmann (PB) model is used which solves the Navier–Stokes equation for fluid flow and PB equation for electric potential distribution [21–23]. However, this model's applicability is limited. For instance for the electroosmotic flows through a microchannel whose surface is heterogeneously charged, or in the case that the electric double layers fully overlap, the Poisson–Boltzmann model fails [24]. Therefore a more general model should be used, which utilizes the Nernst–Planck equation for ions transport instead of the Boltzmann distribution [24,25]. There are several efforts in the literature for simulating electroosmotic flow (EOF) in microchannels, including finite element [26], finite difference [27], molecular dynamics (MD) [14], etc.

As a numerical approach, the lattice Boltzmann method (LBM) has become a favorite method for the researchers for simulating complex fluid flows.

The LBM was firstly developed to simulate the flow instead of solving the Navier–Stokes equations and has been extended to solve the convection–diffusion-type equations. Although there are a large number of numerical schemes for solving these equations associated with the finite element and finite-difference methods, the LBM has received much attention because of its compatibility with parallel computing and its simplicity in programming.

LBM has a molecular basis, which makes it a suitable method for the simulation of fluid flow at micro and nano-scale [28–30].

Many efforts have been made to utilize the LBM for analyzing electroosmotic flows [13,19,31,32]. However, most of these studies are based on the PB equation, and there are limited studies in the field of electroosmotic flows with Lattice Boltzmann method (LBM) that models the Nernst-Planck equation as well.

More recently, Moran and Kang investigated electroosmotic flow using Lattice-Boltzmann method to solve the dynamic model for electroosmotic flows in microchannels. They studied the applicability of the PB model for electroosmotic flows in microchannels. Their results showed that the PB model is accurate for predicting electric potential distributions until the electric double layers fully overlap, and for flow modeling, the PB model is applicable until the thickness of the EDL is 10 times of the channel width [19].

In the present paper, we use a numerical framework to solve the model for electroosmotic flows through microchannels with surface roughness, under the conditions that the EDL layers fully overlap, which has not been considered in the previous studies. The Nernst-Planck equation has to be solved instead of PB equations. The remainder of the present paper is organized as follows. In Section 2, the governing equations for the electrical potential, ionic transports, and flows of electrolyte solutions are introduced. The numerical scheme based on the LBM is presented in Section 3, including the detailed numerical procedure. In Section 4, the validation of the code is presented. In Section 5, two specific patterns for roughness considered and investigated numerically using the present LBM. In addition, some studies on the effects of surface roughness height, roughness interval spacing and roughness surface potential on flow conditions are investigated for two patterns of the roughness, when the EDL layers fully overlap through the microchannel.

2. Mathematical models

2.1. Governing equations

The flow is assumed incompressible, laminar and single-phase. The governing equations for constant-property Newtonian electrolyte fluid flowing in the microchannel shown in Fig. 1, consist of, conservation of mass, conservation of momentum, laplace equation for external electric field, poisson and Nernst-planck for electric potential and ionic concentration distribution.

Displacement of the species in the flow is given by the following equation.

$$\frac{\partial C_k}{\partial t} + \mathbf{u}.\nabla C_k = D_k \nabla^2 C_k + \frac{eZ_k D_k}{KT} \nabla.(C_k \nabla \psi) \tag{1}$$

Here z, D and C are the valence capacity, the diffusivity and molar concentration of the kth species respectively; other parameters are: e, the absolute value of one proton charge, K the Boltzmann constant and T the absolute temperature. The quantity ψ denotes the local electrical potential caused by the ionic distribution. Electric double layer (EDL) theory relates this potential and the net electrical charge density per unit volume ρ_e by the Poisson equation as follows [33,34]:

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

Where ε is the dimensionless dielectric constant of the solution and ε_0 is the permittivity of a vacuum.

ρ_e indicates net charge of the ions expressed by $\rho_e = F\sum Z_k C_k$ (F and C are the Faraday constant and molar concentration respectively).

Electric field E is related to the gradient of the external electric field by:

$$\mathbf{E} = -\nabla \psi_{ext} \tag{3}$$

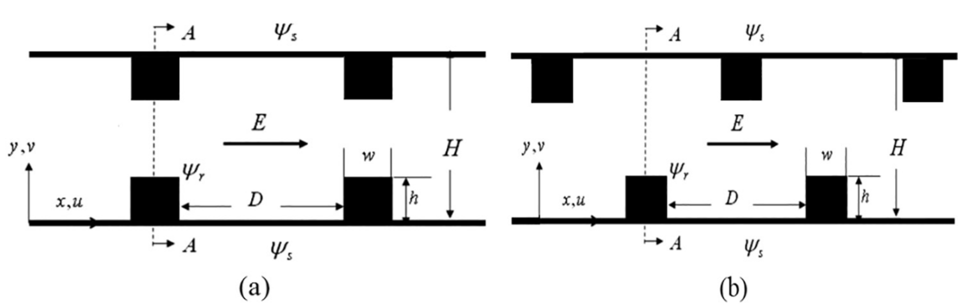

Fig. 1. Geometries and boundary conditions for the microchannel with roughness in two configurations: (a) symmetrical. (b) asymmetrical.

Please cite this article in press as: R. Kamali et al., Chem. Phys. (2018), https://doi.org/10.1016/j.chemphys.2018.04.008