

Analysis of electro-osmotic flow in a microchannel with undulated surfaces



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ABSTRACT

The electro-osmotic flow through a channel between two undulated surfaces induced by an external electric field is investigated. The gap of the channel is very small and comparable to the thickness of the electrical double layers. A lattice Boltzmann simulation is carried out on the model consisting of the Poisson equation for electrical potential, the Nernst–Planck equation for ion concentration, and the Navier–Stokes equations for flows of the electrolyte solution. An analytical model that predicts the flow rate is also derived under the assumption that the channel width is very small compared with the characteristic length of the variation along the channel. The analytical results are compared with the numerical results obtained by using the lattice Boltzmann method. In the case of a constant surface charge density along the channel, the variation of the channel width reduces the electro-osmotic flow, and the flow rate is smaller than that of a straight channel. In the case of a surface charge density distributed inhomogeneously, one-way flow occurs even under the restriction of a zero net surface charge along the channel.

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1. Introduction

Adjacent to the interface between an electrolyte solution and a charged solid surface, an electrical double layer is formed. The thickness of the double layer ranges from a few nanometers to hundreds of nanometers, depending on the salt concentration. Since the ion concentration in the electrical double layer is highly inhomogeneous and the local charge neutrality is broken, interaction with an externally applied electric field can cause a driving force acting on the electrolyte solution. The driving force is the main factor for electrokinetic effects, such as the electro-migration of colloid particles and the electro-osmotic flow inside microchannels [1,2], which are especially conspicuous in small-scale systems.

Micro- and nano-fabrication techniques have developed greatly in recent years, and so researchers have been able to control and use electrokinetic phenomena in engineering applications. For example, an electro-osmotic pump without moving parts [3,4] and an energy-harvesting device using the driving force induced by the salt-concentration gradient [5] have been proposed very recently. Along with the expectations for engineering applications, fundamental research relevant to electrokinetic phenomena in

small-scale systems, ranging from nano- to micrometers, has also attracted attention [6–15]. Particularly, the advances in observing and processing techniques have prompted research focusing on surface properties such as roughness and structure [16–23].

In the present study, to clarify the effects of surface properties on electrokinetic phenomena, we investigate electro-osmotic flows between two surfaces, which have a periodic structure and a non-uniform charge distribution, by means of both numerical and analytical approaches. The numerical analysis is based on the coupled lattice Boltzmann method for solving the Navier–Stokes equations, the Nernst–Planck equation, and the Poisson equation [24]. The numerical solutions to these equations, i.e., the electrolyte flow, the ion concentrations, and the electrical field, are directly obtained. In the analytical approach, the lubrication approximation theory [25–27] is applied to the system with electrical double layers of finite thickness, to derive a model equation that predicts the flow rate under the assumption of moderate variation of the surface structure along the channel. With these approaches, we investigate the electro-osmotic flow in microchannels formed by the surfaces that are undulated and (a) charged negatively at a constant surface charge density or (b) charged non-uniformly along the channel such that the net surface charge vanishes. For both cases, the electro-osmotic flow rate is evaluated and the dependency on geometrical parameters, such as the amplitude of the surface shape, is discussed.

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2. Problem and basic equations

2.1. Channel with undulated surfaces

Let us consider a channel between two walls, each of which has a periodic structure of period L in the x direction. The positions of the interfaces are expressed as $y = \pm h(x)$ (Fig. 1). The surface charge density on the channel walls is assumed to be a given function $\sigma(x)$. The two-dimensional domain between the surfaces ($-h(x) < y < h(x)$) is filled with a 1:1 electrolyte solution, and the electrical double layer is formed near the interfaces. We investigate the electro-osmotic flow caused by an electrical field applied in the x direction by applying the governing equations described in the next subsection.

2.2. Governing equations

We assume a Newtonian fluid for the electrolyte solution, and then the flow is described by the Navier–Stokes equations:

$$\frac{\partial u_j}{\partial x_j} = 0, \quad (1)$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2} + \frac{F_i}{\rho_0}, \quad (2)$$

where t is the time and \mathbf{x} is the spatial coordinate. In the present paper, we use either boldface letters or assign indexes i and j to designate vector elements. The summation convention is assumed for repeated indexes. The functions $\mathbf{u}(t, \mathbf{x})$ and $p(t, \mathbf{x})$ are the flow velocity and the pressure of the electrolyte solution, respectively, and $\mathbf{F}(t, \mathbf{x})$ is the body force per unit volume. The density ρ_0 and the kinematic viscosity ν of the electrolyte solution are assumed to be constant.

The mass conservation equation for the ion species is written as

$$\frac{\partial C_m}{\partial t} + \frac{\partial J_{mj}}{\partial x_j} = 0, \quad (3)$$

$$J_{mi} = -\frac{ez_m D_m}{k_B T} C_m \frac{\partial \phi}{\partial x_i} - D_m \frac{\partial C_m}{\partial x_i} + C_m u_i, \quad (4)$$

where C_m and \mathbf{J}_m denote the concentration and the flux of an ion, respectively, with $m = a$ for the anion and $m = c$ for the cation. Here, e is the unit charge, k_B is Boltzmann's constant, and T is the temperature. The constants z_m and D_m are the valence and the diffusion coefficient of species m , respectively. Equation (4) is referred to as the Nernst–Planck model [28], where the first, second, and third terms on the right-hand side of the flux equation are the contributions of electrochemical migration, diffusion, and convection of the electrolyte solution, respectively.

Finally, the electrical potential ϕ is governed by the following Poisson equation:

$$\varepsilon \frac{\partial^2 \phi}{\partial x_j^2} = -\rho_e, \quad (5)$$

where ε is the dielectric constant of the electrolyte solution. The local charge density ρ_e is defined in terms of the ion concentration as

$$\rho_e = \sum_m F z_m C_m, \quad (6)$$

where F is Faraday's constant. With this local charge density, the body force \mathbf{F} in Eq. (2) is defined as the interaction with the electric field:

$$F_i = -\rho_e \frac{\partial \phi}{\partial x_i}. \quad (7)$$

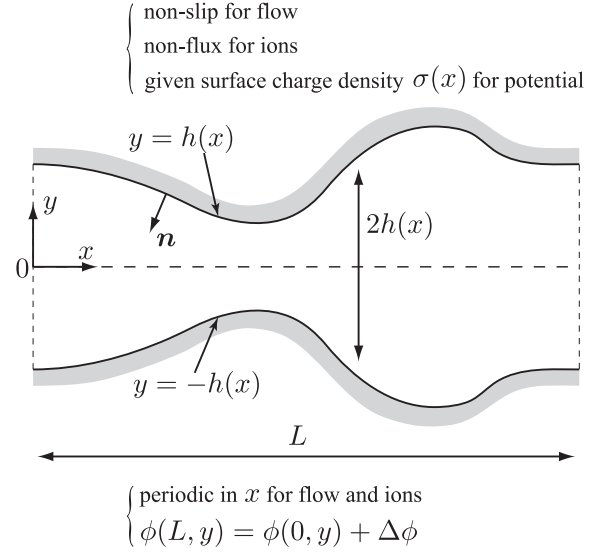


Fig. 1. Geometry of the problem.

If the convection term in Eq. (4) is negligible compared with the other two terms and a unique value of potential is defined at $C_m = C_0$, integration of Eq. (4) yields the Boltzmann distribution $C_m = C_0 \exp(-ez_m \phi / k_B T)$. With this formula, Eq. (5) reduces to the Poisson–Boltzmann equation. In the electrokinetic flows considered in the present paper, however, although the convection term is sufficiently small, specifying a unique potential value at $C_m = C_0$ is difficult because of the external potential gradient. We therefore apply the original set of equations described here in the numerical simulations in Section 5. Then the ion distribution affected by the external potential is obtained as shown in Section 5.2, which the Poisson–Boltzmann equation decoupled from the external potential field fails to capture.

2.3. Boundary conditions on solid–liquid interface

For the flow velocity, the ordinary non-slip condition is assumed at the solid–liquid interface:

$$u_i = 0, \quad \text{at } y = \pm h(x). \quad (8)$$

Note that in nano-scale flows, the simple non-slip condition is not sufficient and so a model describing the slip taking place at the interface is necessary. However, since the scale of the problems considered in the present paper is relatively large (at a scale of micrometers), we assume the non-slip condition to be valid. For the ion concentration, no flux goes across the boundary, which is formulated simply as

$$n_j J_j = 0, \quad \text{at } y = \pm h(x), \quad (9)$$

where \mathbf{n} is the unit normal vector pointing inward to the fluid region. If we substitute Eq. (4) into Eq. (9), then we have

$$-\frac{ez_m D_m}{k_B T} C_m n_j \frac{\partial \phi}{\partial x_j} - D_m n_j \frac{\partial C_m}{\partial x_j} + C_m n_j u_j = 0. \quad (10)$$

This form of the Neumann-type boundary condition seems rather complex to implement in the lattice Boltzmann method. However, with the scheme for the Nernst–Planck model described in the next section we can impose this condition in a simple manner. Finally, the boundary conditions for the electrical potential are given as the following Neumann-type condition:

$$-\varepsilon n_j \frac{\partial \phi}{\partial x_j} = \sigma, \quad \text{at } y = \pm h(x). \quad (11)$$

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