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Diffusioosmotic flows in slit nanochannels

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Abstract

Diffusioosmotic flows of electrolyte solutions in slit nanochannels with homogeneous surface charges induced by electrolyte concentration gradients in the absence of externally applied pressure gradients and potential differences are investigated theoretically. A continuum mathematical model consisting of the strongly coupled Nernst–Planck equations for the ionic species' concentrations, the Poisson equation for the electric potential in the electrolyte solution, and the Navier–Stokes equations for the flow field is numerically solved simultaneously. The induced diffusioosmotic flow through the nanochannel is computed as functions of the externally imposed concentration gradient, the concentration of the electrolyte solution, and the surface charge density along the walls of the nanochannel. With the externally applied electrolyte concentration gradient, a strongly spatially dependent electric field and pressure gradient are induced within the nanochannel that, in turn, generate a spatially dependent diffusioosmotic flow. The diffusioosmotic flow is opposite to the applied concentration gradient for a relatively low bulk electrolyte concentration. However, the electrolyte solution flows from one end of the nanochannel with a higher electrolyte concentration to the other end with a lower electrolyte concentration when the bulk electrolyte concentration is relatively high. There is an optimal concentration gradient under which the flow rate attains the maximum. The induced flow is enhanced with the increase in the fixed surface charge along the wall of the nanochannel for a relatively low bulk electrolyte concentration.

Keywords: Diffusioosmosis; Diffusioosmotic flow; Electrokinetics; Electrokinetic flow; Nanofluidics; Electrical double layer (EDL)

1. Introduction

In recent years, there has been a growing interest in developing nanofluidic devices with features comparable in size to DNA, proteins, and other biological molecules for biological and chemical analysis [1–5]. In nanofluidic devices, it is necessary to propel fluids from one part of the device to another, control fluid motion, enhance mixing, and separate fluids. Pressure-driven flow in nanochannels is usually very difficult due to its high pressure loss with a very low volume flow rate. On the other hand, electroosmotic pumps with no moving parts are commonly used to transport liquids through nanochannels by external electric fields. Electroosmosis and electrophoresis have been widely used for fluid and particle manipulations in microfluidics and nanofluidics. Instead of externally applying an electric field, an electrolyte solution in a nanochannel can also be driven by means of diffusioosmosis through the application of gradients of solute concentration. With a concentration gradient on the order of 1 M/cm along a charged surface with a zeta potential on the order of $k_B T/e$ (k_B is the Boltzmann constant, T is the absolute temperature, and e is the elementary charge), the induced diffusioosmotic flow has a velocity on the order of μm/s [6–17]. Like the well-known electroosmosis phenomenon, diffusioosmosis originates from electrostatic interaction between the electrolyte and the charged solid's surface that is in contact with the electrolyte solution. Therefore, both electroosmosis and diffusioosmosis fall into the same category of surface-driven phenomena that take advantage of the increase of surface to volume ratio [18]. However, flow generation in nanofluidics by diffusioosmosis has received less attention than fluid motion induced by electroosmosis.

We consider a nanochannel connecting two reservoirs on either side (Fig. 1). The wall of the nanochannel is charged. The

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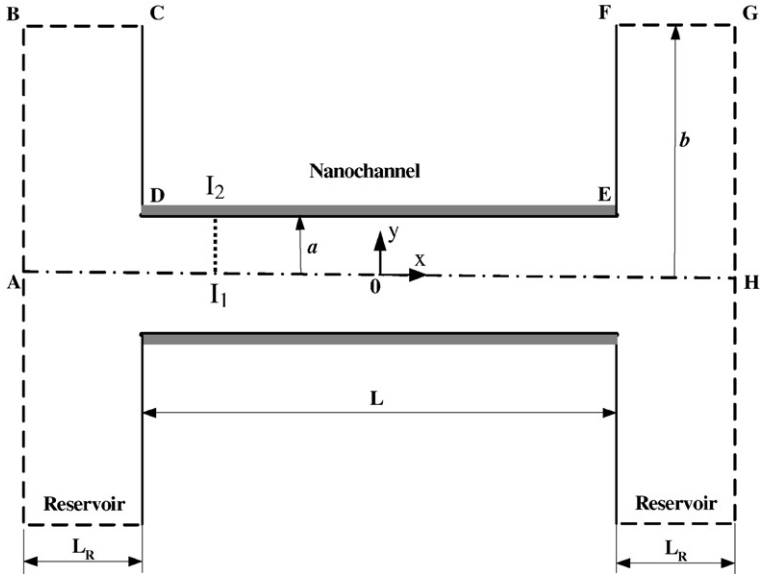

Fig. 1. Schematic of a slit nanochannel of length L and height $2a$ connecting two reservoirs on either side. The surface charge density along the wall of the nanochannel is σ_w. The length and height of the reservoir are, respectively, L_R and $2b$. When a concentration gradient of electrolyte solution is applied across the two reservoirs, a potential difference and a pressure gradient, and thus diffusioosmotic flow are induced in the absence of any external pressure gradient and potential difference.

two reservoirs contain a dilute electrolyte solution with different concentrations. Due to the electrostatic interaction between the ionic species present in the electrolyte solution and the fixed surface charge along the wall of the nanochannel, counterions accumulate in a thin liquid layer next to the solid's surface. This thin layer is known as the electrical double layer (EDL), and its thickness is typically on the order of 10 nm [19]. In the presence of an external concentration gradient of the electrolyte solution, fluid motion is generated by two mechanisms: electroosmotic and chemiosmotic effects. Due to the presence of the concentration gradient, electrolyte ions diffuse in the nanochannel, accompanied by a net diffusive flux of charge when the mobilities of the anion and cation are not equal. As a result, an electric field is induced that compensates for the net diffusive flux of charge across the nanochannel. The induced electric field, through its action on the counterions accumulated in the EDL, creates a body force that, in turn, induces fluid motion. In contrast to the electroosmotic flow driven by an externally applied electric field, the fluid motion due to the electroosmotic effect in diffusioosmosis phenomenon is driven by the induced electric field in the absence of an externally applied electric field. Although there is no externally applied pressure gradient across the channel, a pressure gradient is induced by the electrolyte gradient, which induces shear in the EDL and a flow opposite to the concentration gradient [6–18]. Therefore, the diffusioosmotic flow is driven by both the induced electric field and the induced pressure gradient in the absence of the externally applied electric field and pressure gradient. As compared to the electroosmotic flow and the pressure-driven flow, the two strategies, electroosmosis and pressure-driven, are synergetically combined in diffusioosmotic flow, yielding strongly enhanced interfacial driven flows in nanofluidic and microfluidic devices [18].

Previous investigations of diffusioosmotic flow are very limited. Most studies to date have focused on diffusioosmotic flows near plane walls and in straight conduits (i.e., capillary tubes and slits) with uniform zeta potentials or surface charges along the walls. See, for example, Keh and Ma [17] and the references cited therein. In addition, most previous analysis of diffusioosmotic flows has been subjected to several restrictions, such as a thin EDL [6,7], a sufficiently low zeta potential along the wall [8,13], and neglected effects of the ionic concentration distributions and ionic convection on the induced local electric field and pressure gradient [7,8,13,14]. Moreover, the deformation and concentration polarization of the EDL due to the convection have not been taken into account in previous work. In this paper, we study diffusioosmotic flows in slit nanochannels with uniform surface charge densities along the channel's walls. In contrast to the previous work, the current analysis accounts for the polarization of the EDL with no assumption made concerning the thickness of the EDL and the magnitude of the zeta potential or surface charge density along the wall. In addition, the effects of the reservoirs connecting the nanochannel are also taking into account in the current work.

The rest of the paper is organized as follows. Section 2 describes the full mathematical model for the fluid motion induced by both the induced pressure gradient and the induced electric field and the general multi-ion mass transport model that accounts for the polarization of the EDL. Detailed code validation is described in Section 3. The diffusioosmotic flows in slit nanochannels under various conditions are presented and discussed in Section 4. Section 5 concludes.

2. Mathematical model

Let us consider a charged slit nanochannel with length L and height $2a$ connecting two identical reservoirs on either side. Fig. 1 schematically depicts the geometry. The length and height of the reservoir are, respectively, L_R and $2b$. We assume