

# Parallel Computation of Electroosmotic Flow in Micro- and Nanochannel

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**Key Words:** Electroosmotic Flow, Micro/nano Flow

## ABSTRACT

Electrokinetics induced by external electric field has emerged as a promising means for manipulating fluid motion and associated species transports in micro- and/or nanochannels adopted in microfluidic devices [1]. A premise for electroosmosis is the presence of a net fluid charge. For a neutral electrolyte solution, such a situation occurs only in the limited region, called the Debye layer or EDL (electric double layer), adjacent to the liquid-solid interface [2]. The thickness of EDL  $\lambda$  depending on concentration of the solution is usually less than several ten nanometers. In the conventional microchannels, the height,  $h$  encompasses the range from several to hundred micrometers, i.e.,  $\lambda/h \ll 1$ . The evolution of net charge in EDL leads to insignificant influences on the electric and chemical balance of the bulk fluid. The consequences are that the flow in the bulk of the channel has a plug-like uniform profile and the velocity is proportional to the applied electric field. The effects of EDL could be modeled by the slip boundary conditions.

Remarkable advance in microfabrication technology enables to manipulate nanofluidic devices in which  $h \sim O(100\text{nm})$ . Separation of a selected material from a picoliter of sample becomes practical. As the length scale of the channel is reduced, the resolution to EDL becomes crucial. An extreme case is that two Debye layers forming on the top and bottom boundaries are overlapped. The simplification based on the very thin EDL assumption is not valid any longer. EDL gives a direct impact on the structures of electroosmotic flow in the bulk of the fluid [3]. A few atomistic computations examined the EDL in nanochannels (e.g., [4]). The dimension considered was  $O(10\text{nm})$  and the channel of height  $O(100\text{nm})$  is still challenging. There have been the continuum-based numerical efforts to describe the detailed structure of EDL [5-7]. Most of these studies assumed the Boltzman equilibrium with a constant reference value for electric potential. The interaction between EDL and the bulk of the fluid were not taken into account. Various numerical attempts have been devoted to the full scale simulation of non-equilibrium electroosmotic flow, but, a successful numerical model without defects are still under question.

In this study, a numerical model is developed for simulating non-equilibrium electroosmotic flow in micro- and nanochannels. The Guoy-Chapman model is adopted to compute the flow and electric potential. The governing equations are

$$\rho \frac{\partial \bar{u}}{\partial t} + \rho \bar{u} \cdot \nabla \bar{u} = -\nabla p - \rho_e \bar{E} + \nabla \cdot (\eta \nabla \bar{u}) \quad (1)$$

$$\nabla \cdot \bar{u} = 0 \quad (2)$$

$$\vec{E} = \nabla\Phi \quad (3)$$

$$\Phi = \phi + \psi \quad (4)$$

$$\nabla \cdot (\epsilon \nabla \phi) = 0 \quad (5)$$

$$\nabla \cdot (\epsilon \nabla \psi) = -\rho_e \quad (6)$$

$$\rho_e = e \sum n_i z_i, \quad (7)$$

$$\frac{\partial n_i}{\partial t} + \vec{u} \cdot \nabla n_i = \nabla \cdot (D_i \nabla n_i) + \nabla \cdot (\mu_i n_i \nabla \Phi) \quad (8)$$

where  $\vec{u}$  is velocity vector,  $t$  time,  $p$  pressure,  $\vec{E}$  electric field,  $\Phi$  electric potential,  $\rho$  density,  $\rho_e$  charged density,  $\eta$  viscosity,  $e$  unit charge of a proton.  $n_i$ ,  $z_i$ ,  $D_i$  and  $\mu_i$  viscosity, the concentration (number density), valence and diffusivity of  $i$ -th ionic species, respectively.

It is noteworthy that, as in equation (4), the electric potential is divided into two parts: the electric potential due to the externally imposed electric field  $\phi$  and the natural potential induced by the presence of EDL,  $\psi$ . It is noted that an inevitable hurdle is the numerical stiffness stemming from the strong nonlinearity of the electric body force term. A strategic decomposition is conducted as

$$\nabla p + \rho_e \vec{E} = (\nabla p^* + \nabla p_{ES}) + \epsilon \nabla^2 \psi (\nabla \phi + \nabla \psi) \quad (9)$$

Here, a physically-reasonable consideration is adopted; the electric field due to the induced natural potential does not affect the electroosmotic flow. Thus, it can be assumed that the electric body force due to  $\nabla \psi$  is balanced by electrostatic pressure gradient  $\nabla p_{ES}$  likely in dealing with the gravitational body force due to hydrostatic pressure distribution. The usefulness of this approach will be described in more detail.

Another typical feature of the present model is that The Nernst-Planck equation (8) is employed to trace unsteady transports of ionic species, i.e., time-dependent net charge density. A new set of boundary conditions based on the physically-meaningful quantity surface charge density  $\sigma$  are designed rather than using the conventionally employed zeta potential:

$$\epsilon \frac{\partial \psi}{\partial y} = \sigma \quad \text{and} \quad \frac{\partial n_i}{\partial y} + n_i \frac{e z_i}{kT} \frac{\sigma}{\epsilon} = 0 \quad (10)$$

For numerical solution to the governing equations with the prescribed boundary conditions, a finite volume numerical model is developed. The model is essentially based on the fractional time step method. Spatial discretization are implemented on the collocated grid network and central differencing is used. The target problem is characterized by the channel of which height is submicron and the typical thickness is still  $O(10\text{nm})$ . Full scale simulation with retaining sufficient resolution to EDL requires intensive computation. In order to accommodate huge computational requirement, the numerical model has been developed for parallel computing.

The backbone of parallelism is domain decomposition. The use of collocated grid system was to avoid complexity of the code for parallel implementation. The parallel programming model is message passing and the standard MPI is used. The major subroutines for interprocess communication are modularized for simple code structure and easy debugging. The key subroutine calling for intensive computation is the matrix solver. After testing several matrix solvers, a conjugate gradient method was selected since it provided good scalability. The parallel performance of the model has been tested on a IBM p690 system a linux-based PC cluster. The speed-up characteristics and related issues will be discussed more in detailed.

A test problem, as schematically illustrated in Figure 1, is examined. The device is a flow passage consisting of a channel of a relatively large height  $h$  (microchannel) and a contraction part of a small height  $a$  (nanopore). Considered is that  $h$  is much larger than the Debye length  $\lambda$  while  $a$  is of  $O(\lambda)$ , i.e., a nanopore is located in a microchannel. In the core of the microchannel, the fluid is electrically neutral and there is no net charge since  $h \gg \lambda$ . However, in the core of

the nanochannel, there exists net charge since the two EDLs are overlapped. These establish a difference of natural potential near the entrance and exit of the nanochannel, which may play a role to trap charged proteins. Numerical computation was conducted to explore this idea.

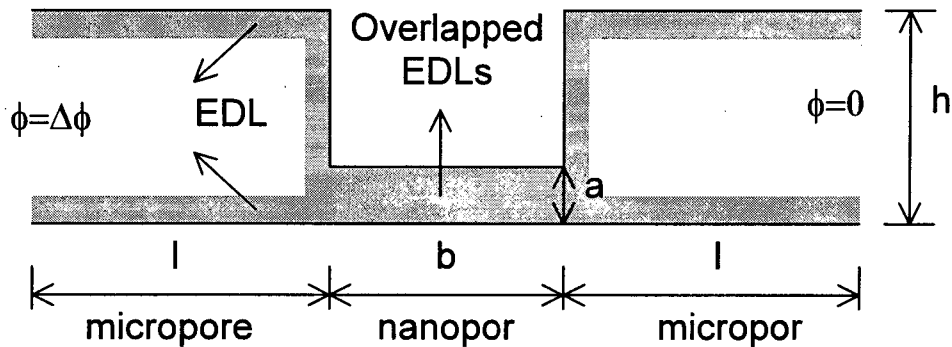


Fig. 1 Schematic illustration of electroosmotic flow in a micropore with a nanopore junction

Numerical computation was conducted for a specific set of parameters:  $a/h=1/4$ ,  $\lambda/h=1/10$ ,  $l/h=6$ ,  $b/h=4$ ,  $\zeta_0 = \sigma\lambda / \varepsilon = -2.35$ ,  $Re=\rho U h/\eta=5 \times 10^{-4}$ ,  $Sc=\eta/\rho D=10^3$ . The fluid is assumed to be an 1:1 symmetric electrolyte such as KCl. In real devices, the length of the channel is much larger than the height. For computational brevity, only a small section of flow passage is selected as computational domain. As mentioned before, the structure of EKF in microchannel is of boundary-layer type while in nanochannel the EDLs are overlapped ( $\lambda/a=2/5$ ). This condition for electrokinetic flow resembles to a real situation in which the flow velocity  $U=0.4\text{mm/s}$ , zeta potential  $\zeta=-50\text{mV}$  and  $h=100\text{nm}$ .

Fig. 2 shows the steady-state solution. The externally-imposed electric potential  $\phi$  displays a steeper variation in nanochannel than in microchannel. If  $a/h$  decreases further, the change in  $\phi$  takes places mainly in the nanopore section. The contour plot of natural potential  $\psi$  illustrates the typical EDL structures anticipated. In the micropores, there exists distinct EDLs on the charged walls and an electrically neutral interior core between two EDLs. In the nanopore, the EDLs are overlapped. The streamlines are concentrated in the nanopore having a larger magnitude of electric field

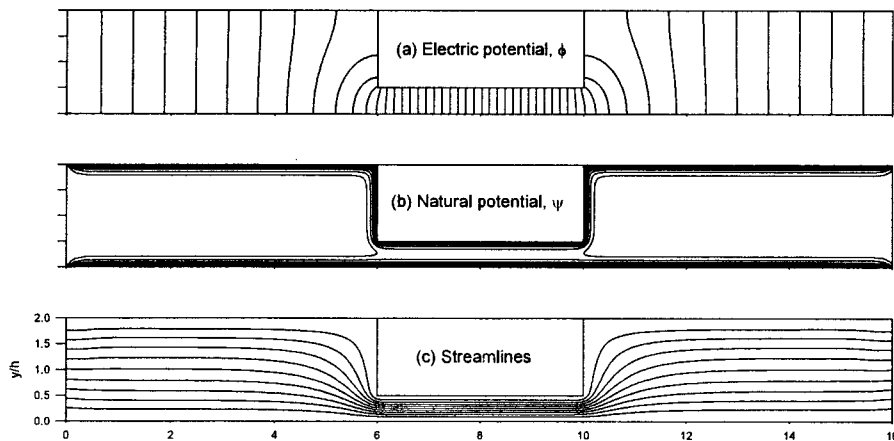


Figure 2 Structure of electroosmotic flow in a microchannel with a nanopore. Contour plots for (a) externally imposed potential  $\phi$ ; (b) natural potential  $\psi$ ; (c) streamlines.

In order to exemplify the effects of nanopore, both of  $\phi$  and  $\psi$  are plotted in Fig. 3 as well as the total electric potential  $\phi+\psi$ . A local maximum of potential is visible near the exit of the nanopore. If we consider the transport of negatively charged protein, it move toward positive charge (i.e., toward the region of higher value of  $\phi+\psi$ . There may be a strong possibility that proteins could be captured at the exit of the nanopore.

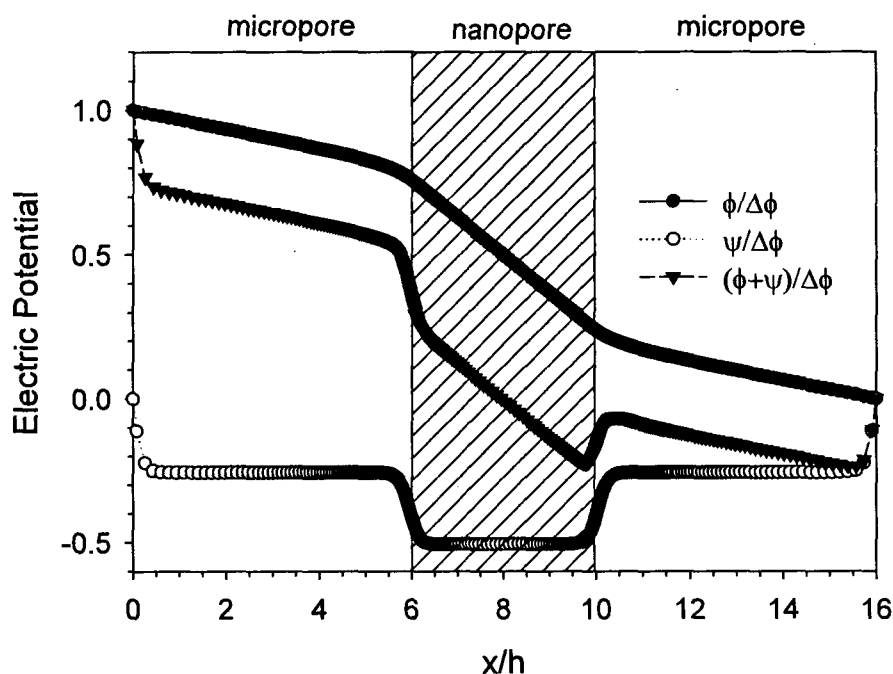


Fig. 3. Distribution of electric potential along the channel at the mid-height of nanopore ( $y/h=1/8$ ).

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