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Molecular dynamics study of an electro-kinetic fluid transport in a charged nanochannel based on the role of the stern layer

M. Rezaei [a,*], A.R. Azimian [b], D. Toghraie [b]

[a] Mechanical Engineering Department, Isfahan University of Technology, Isfahan, Iran

[b] Mechanical Engineering Department, Khomeinshahr Branch, Islamic Azad University, Khomeinishahr/Isfahan, Iran

HIGHLIGHTS

- Effects of electric field and temperature are studied on the electro-osmotic flow.
- The electro-osmotic velocity is a fourth order function of the electric field.
- The electro-osmotic velocity changes linearly with temperature.
- An increase in the studied parameters leads to a reduction in stern layer capacity.
- The stern layer capacity reduction delays the charge inversion phenomenon.

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ABSTRACT

Electro-osmotic flow of an aqueous solution of NaCl has been studied using the molecular dynamics simulation. The main objective of this work is to investigate the effects of the electric field and temperature on the flow properties considering the role of the stern layer. By increasing any of the mentioned parameters, the electro-osmotic velocity grows. It is found that the electro-osmotic velocity is a fourth order function of the electric field, while it changes linearly with temperature. Similar trends of change are found for the EDL thickness. By an increase in the studied parameters, a reduction in the stern layer capacity is observed. In this situation, more moving ions are located in the diffuse layer, which are dragging other particles. This is one of the causes that increase the electro-osmotic velocity, a matter which was not predicted by previous researches. A consequence of the stern layer capacity reduction is that in the systems under the influence of higher temperatures or stronger electric fields, charge inversion phenomenon occurs at higher wall charges.

1. Introduction

Electro-osmotic flow is one of the best known methods of fluid transport based on the electro-kinetic phenomenon. When an ionized solution makes a contact with a stationary charged surface, it attracts the counter-ions of the solution and repels the co-ions; therefore, an electric double layer (EDL) with a net positive or negative charge develops near the surface. By applying an external electric field in a direction tangential to the surface, the fluid will be dragged by the moving ions in the EDL and a nearly uniform flow called electro-osmotic transport will be generated in the channel.

* Corresponding author. Tel.: +98 9132083062; fax: +98 3113660011.
E-mail addresses: Majid-Rezaei@me.iut.ac.ir (M. Rezaei), Azimian@iaukhsh.ac.ir (A.R. Azimian), Toghraee@iaukhsh.ac.ir (D. Toghraie).

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Nomenclature

V_{LJ}	Lennard-Jones potential
σ	Respective Lennard-Jones size
$V_{Coulomb}$	Coulomb potential
q	Electrical charge
r	Separation distance between two particles
v	Velocity
δ	EDL thickness
F	Driving force
σ_s	Surface charge density
ε	Depth of the potential well
r_{cutoff}	Cut off radius
T	Temperature
ϵ_0	Vacuum permittivity
ρ_ϵ	Electric charge density
z	Valance number
n	Ion concentration
E	Electric field strength
M	Molarity

The electro-osmotic flow was first reported by F.F. Reuss [1]. He showed that water could be forced to flow through a clay plug by applying an electric field. To reach to more accurate investigations, the EDL properties must be considered and analyzed as the base of the electro-osmotic flow. Helmholtz [2]developed the electric double layer theory, which relates the electrical parameters to flow parameters for electro-osmotic transport.

Since late twentieth century researchers have begun to use numerical simulation to study the electro-osmotic flow [3–5]. Patankar and Hu [6] developed a finite volume scheme to simulate the electro-osmotic flows in complicated geometries and studied the electro-osmotic injection at the intersection of two channels. Arnold et al. [7] modeled the electro-osmotic flow using finite element method (FEM) combined with the characteristic-based split (CBS) algorithm to solve the coupled Navier–Stokes equations.

Investigations done by Qiao and Aluru [8] showed that classical numerical methods which are based on the continuum theories are not able to predict all aspects of the electro-osmotic behaviors. Therefore, researchers began to use particle based methods which are more accurate. Hence, various studies done on the electro-osmotic flow using these methods, such as Dissipative Particle Dynamics method (DPD) [9,10], Molecular Dynamics simulation (MD) [11,12], etc. In the present study, the molecular dynamics simulation which is one of the most accurate particle based methods is used. It is applied to simulate the electro-osmotic flow and investigate the effects of some important parameters on the properties of this flow. One of the most important advantages of the MD simulation is its ability to predict the behavior of the ions within the stern layer. This helps us to do better analysis considering both parts of the EDL namely the stern layer and the diffuse layer.

Some primary studies were done on the effective parameters by previous researchers such as Tian et al. [13]. In the present work it is attempted to offer a close look at the effects of two important parameters namely temperature and the electric field on the flow behavior. This is done by considering the changes in the structural properties of the EDL especially the role of the stern layer.

The first parameter is the electric field strength, which is one of the most important flow controlling parameters. In the electro-osmotic flow, the driving force could be from different sources. It could be from a single direction electric field or a periodically varying direction field [14,15]. It is also possible to have an extra source such as a pressure field [16,17]. In the present work, the first case is investigated by changing the electric field strength.

The second parameter studied in this work is temperature. This parameter has significant effects on the properties of the molecular systems. Jelinek et al. [18] reported that at larger values of temperature, a stronger electro-osmotic flow forms in the system. The aim of the present study is to investigate the trend of the changes made by the temperature in the electro-osmotic velocity and to find the cause of these changes considering the behavior of the stern layer.

In this study, we have a special consideration on the properties of the stern layer. One of the important phenomena based on the action of the stern layer is charge inversion phenomenon. In fact, in the systems with highly charged walls, the net charge of the counter-ions attracted in the stern layer exceeds the wall charge and consequently a reversed flow starts to develop in the domain [19,20]. It is of interest to study the effects of temperature and applied electric field on the mentioned phenomenon.

The present work could make a good contribution to cover shortcomings of other works. The extension of this article and the previous published works [21–24] provide the engineers a good option for future studies regarding simulation of flows in nanochannels.