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Flow mixing and electric potential effect of binary fluids in micro/nano channels

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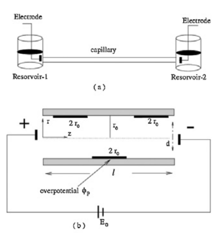
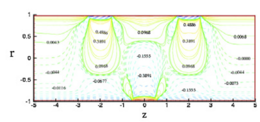
HIGHLIGHTS

- The present work deals with the electroosmotic mixing of chemical species in a circular nano-channel using Nernst Plank model.
- The present model has the flexibility to handle multivalent ions and no symmetric conditions will be assumed at the centerline.
- The pressure and vertical flow variation has been found in the transverse flow direction.
- A strong pressure gradient is developed above the overpotential region which increases the mixing performance.
- The streamlines and mole fraction distribution follows a tortuous path above the non-uniform potential for both weak and strong solution.

GRAPHICAL ABSTRACT



1. Flow domain with the overpotential region.



2. Voritcity contours formed along the channel with diameter 60 nm and overpotential value 0.2.

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ABSTRACT

In the present study, mixing enhancement is analyzed due to the multi component species transport with the variation of surface potential. The formation of vortices along the flow region due to wall heterogeneity and the solution molarity of a circular channel is discussed. The numerical solutions are obtained using the coupled Nernst–Planck equation, the Poisson equation, and the Navier–Stokes equations. A finite volume based approach is adopted to compute the mass, potential and flow profiles using Nernst–Plank model which can be valid for higher surface potential. A flow recirculation is induced due to the strong pressure gradient at the overpotential region which increases the mixing performance. The streamlines and mole fraction distribution follows a tortuous path above the non-uniform potential and the flow properties of strong solution deviates more compared to weaker solution due to induced pressure gradient which is created by the flow phase difference.

1. Introduction

Electroosmotic flow is used as a main transport technique in lab-on-a-chip technology (LOC), which allows the integration of various components in a microdevice [30]. Fluid flow in micro scale

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Nomenclature

l	cylinder length [m]
d	cylinder diameter [m]
$\vec{n}_i$	molar flux of species i [mol m^{-2} s^{-1}]
D_i	diffusion coefficient [m^2 s^{-1}]
X_i	species mole fraction (anion or cation)
$\vec{E}*$	electric field [Volt m^{-1}]
$\vec{u}*$	mass average velocity [m s^{-1}]
R	general gas constant [J mol^{-1} K^{-1}]
T	Fluid temperature [K]
F	Faraday's constant [C mol^{-1}]
N_A	Avagadro number [mol^{-1}]
U_i	mobility of species i, D_i/RT [m N^{-1} s^{-1}]
z_i	valence of species i (−1 for −ve ion and 1 for +ve ion)
M_i	molecular weight [kg mol^{-1}]
U_0	electroosmotic velocity (Smoluchosky velocity) [m s^{-1}]
Re	Reynolds number, $U_0 d/\nu$
ϵ_e	permittivity [C m^{-1} v^{-1}]
ρ_e	charge density [C m^{-3}]
ϕ_0	potential scale [v]
f	dimensionless cation
g	dimensionless anion
p	dimensionless pressure, $p^*/(\mu U_0/d)$
Sc	Schmidt number, $\frac{\nu}{D_i}$
Pe	Peclet number, $Re.\ Sc$
u	non-dimensional θ-component of velocity, u^*/U_0
w	non-dimensional z-component of velocity, $w*/U_0$
v	non-dimensional r-component of velocity, $v*/U_0$
z	non-dimensional horizontal distance, $z^*/2r_0$
r	non-dimensional radial distance, r^*/d

Greek

λ	Debye layer thickness [nm]
ρ	density of the fluid [kg m^{-3}]
ν	kinematic coefficient of viscosity [m^2 s^{-1}]

Superscript

*, $\rightarrow$	dimensional quantity

devices is a key concept for LOC technology for specific analysis of high throughput in chemistry, biology and medicine. The micro mechanisms for flow and mass transfer (microfluidics) are widely used in many fields such as chemical synthesis, drug delivery and biochemistry while tiny amounts of samples, reactants and space are consumed [31]. Since, the characteristic length in micro fluidics are in micro or nano meter range, the fluid transport are controlled by viscous forces rather than inertial effects [32].

The electroosmotic circulation growth closed to a capillary resulting a fluid motion when an externally supplied electric field is interacting actively with the charged fluid and the resulting motion is known as electroosmotic flow (EOF) [29]. In EOF, an electric double layer (EDL) is formed near the interface where the concentration of the ions are higher and the applied external electric field causes the movement of ions inside this layer. Mixing is an important component in microfluidic systems since it has large scale of applications in chemical synthesis and drug mixing in drug delivery devices [15]. During the mixing process, EDL plays an important role due to the interaction of driving bulk flow [33]. Extensive studies have been performed to explore the nature and characteristics of electroosmotic flows in micro and nanoscale devices (Ajdari [6], Liu et al. [2], Erickson and Li [7], Conlsk et al. [24], Luo [9] Tian et al. [1], Bhattacharyya and Nayak [4], Bhattacharyya and Nayak [5]). Based on the above studies it is predicted that EOF mixing is strongly influenced by the characteristic attributes of the capillary surfaces. Hence, the mass and flow variation for mixing are dependent on the ζ-potential, which is influenced by pH, ionic strength, the dielectric constant of the solution.

An experimental study for EOF is performed by Lim et al. [32] to enhance the mixing in micromixtures using various channel geometries. They have experimented using both direct current (DC) and alternating current (AC) using various lengths of constrictions. The results suggest that mixing efficiency is mostly influenced by the constriction length, AC amplitude and frequency of the applied electric field. A detailed study is made by Xu et al. [31] to study mathematically the effect of the constriction length with the periodic electric field. The flow effect due to both electroosmosis with pressure driving force in micro and nano-channels for mixing is studied by Bhttacharyya and Bera [34]. The species mixing is dependent on the intensity of the vortices induced due to the potential patches in heterogeneous channel. They found that vortical flow developed along the channel surface due to overpotential electric field and blocks causes a stronger mixing. The strength of concentration is an important factor for mixing since the vortex size is growing above the heterogeneous surface.

The potential distribution and flow profiles close to a surface heterogeneity has been studied by Yariv [35], where a step jump in potential along the channel surface is used for heterogeneity. The numerical results are obtained using a Poisson–Bolzmann (PB) distribution with the Debye–Huckel approximation for the flow governing equations. The EOF in micro channel with a step change in surface ζ-potential has been studied by Park et al. [18]. The validation of PB-model for EOF in micro and nano channel made by Wang et al. [19]. The flow properties and species transportation in a nanochannel is studied by Yaroshchuk [20]. He used a virtual computation technique to visualize the overlapping of double layers in the diffuse part of EDL.

Ramirez and Conlisk [15] performed a study on EOF by suddenly changing the channel cross section area which is a simple model for fabrication flaw. The study concludes that for asymmetrical boundary conditions of charge and concentrations flow vortices and recirculation regions are formed. The nonlinear distribution of potential and mole fraction on EOF is studied by Chen and Conlisk [36] due to the convective effects by Nernst Planck model. They found that the potential and species variation are different in Boltzmann model for strong electric field. Mostly, researchers are using PB-model for EOF in homogeneous and heterogeneous channels and it is questionable when EDL thickness is in the order of channel height. In this case the core neutrality is not preserved [24]. The distribution of ions does not consider the external electric field and the convection effect due to the Bolzmann equation. The convection effects cannot be neglected in EOF closed to a surface heterogeneity due to step jump of potential or roughness [29].

The motivation of the present work is to study the flow and species transport in a circular nano-channel with the variation of electrolyte strength due to NP-model with wall heterogeneity. In the present analysis, the externally applied conditions such as, electric field strength, species concentration and over-potential strength, which accelerates the mixing are discussed. Validation of NP- and PB-model (i.e. center line symmetry) with steady EOF is made, since NP-model does not require any symmetry condition along the centerline and there is no restriction for the low surface potential [37]. The usual top hat flow profile and neutral core, depicts a planar EOF for thin EDL and are absent for thick EDLs. The non-zero pressure gradient induces a strong convection effect for solute transport. With the increase of nanochannel height the electroosmotic flow enhancement is also observed (Bera and Bhattachryya [21]). In this regard the diameter of the channels are varied between 20 nm and 60 nm and obtained the flow and