Pressure driven transport of neutral macro-solute in microchannel with porous wall at high surface potential

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ABSTRACT

Mass transport of macro-solutes under streaming potential in a microchannel with porous wall is presented in this study. The streaming field under high wall potential and overlapping electric double layer with coupled velocity and concentration of neutral solutes is computed numerically in this work. Streaming potential increases by 7 folds as κH decreases from 0.7 to 0.1 at $\zeta = -50$ mV, where, κ^{-1} is Debye length, H is channel half height and ζ is wall zeta potential. Mass transport in terms of Sherwood number is calculated including osmotic effect of the solution and selective retention of macrosolutes. Electroviscous effects resulting from streaming potential and overlapping electric double layer at higher wall zeta potential have significant effect on velocity field and the mass transport of macrosolutes. Apparent viscosity due to this effect increases upto 3.2 times the solution viscosity at $\kappa H = 0.2$ for $\zeta = -50$ mV. This effect is intensified upto 4 times at higher wall potential, $\zeta = -200$ mV at $\kappa H = 0.5$. At these points, the velocity profile suffers the most adversely affecting the mass transfer reducing Sherwood number to 4 (about 5 times reduction compared to higher κH) at $\zeta = -200$ mV and $\kappa H = 0.5$. Sherwood number reduces by three to four folds at the critical κH values, representing the minimum. The induced electrical field due to the streaming potential is higher compared to axial pressure drop for $|\zeta| > 50$ mV at $\kappa H < 0.3$. The electric double layer overlaps for the values of κH upto 0.7 corresponding to $\zeta = -50$ mV. In case of high ζ (-200 mV), the centerline potential can be as high as 75% of the wall potential for $\kappa H = 1.5$. The minimum wall Peclet number ($\overline{Pe_w}$) occurs at $\kappa H = 0.5$ for $\zeta = -200$ mV, which is five times less than the situation without electrokinetic effects.

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1. Introduction

Flow through microchannels under the influence of electrokinetic effects is a promising area of research [1,2]. The transport phenomena associated with electrokinetic flow in microchannels is useful to quantify microscale heat and mass transfer. Fluid flow combined with heat transfer has been studied by various researchers in microscale heat exchanger [3], micro-chip cooling [4], microelectronic-mechanical-systems (MEMS) [5], microreactors [6], etc. The corresponding mass transport problem has applications in transdermal drug delivery [7,8], electrolyte transport in fuel cells [9], transport in hydrogel [10], etc.

Typically, the electrokinetic flow in microchannel can be categorized in four different regimes: electroosmosis, electrophoresis, flow due to streaming field and sedimentation potential. Electroosmosis and electrophoresis occur only in presence of electric field and can occur in conjugation with the pressure gradient. Mass transport in electro kinetically actuated pressure driven flow has already been theoretically analyzed for rectangular channels [11]. The semi-analytical solution approach quantifies the solute transport and dispersion for small zeta potential varying in x and y dimensions. Solute transport in microchannels can also be affected by surface reaction or adsorption which can occur during DNA hybridization or catalytic reaction in micro-reactors [12,13]. The dynamics of chemical reaction as well as adsorption affecting the solute transport was studied. The different regimes of diffusion controlled or reaction kinetics controlled or adsorption dominant are also identified based on the system configuration and operating conditions. In the absence of external field, the streaming field and sedimentation potential are both generated due to the advection of the mobile counterions by non-electrical forces. The mass transport associated with such electrokinetic flows can be augmented by changing the electrolyte concentration, dimensions of the channel, and tuning the surface potential of the channel walls. In case of

Nomenclature

c	concentration of the macrosolute, kg/m^3
c_0	inlet concentration of the macrosolute, kg/m^3
c_p	concentration of the permeate, kg/m^3
c_p^*	non-dimensional permeate concentration of the macrosolute, c_p/c_0
$\overline{c_p*}$	length averaged non-dimensional permeate concentration of the macrosolute
c_w	concentration of macrosolute over the porous wall, kg/m^3
c_w*	non-dimensional wall concentration of the macrosolute, c_w/c_0
$\overline{c_w*}$	length averaged non-dimensional wall concentration of the macrosolute
D	diffusivity of the macrosolute, m^2/s
d_e	hydraulic diameter of the channel, m
e	charge of an electron, C
E_{st}	streaming field, V/m
H	half height of the channel, m
I_{cond}	conduction current, A
I_{ionic}	total ionic current, A
I_{str}	streaming current, A
k	mass transfer coefficient, m/s
k_b	Boltzmann constant, m^2.kg.s^{-2}.K^{-1}
K_W	dissociation constant of water, 10^{-14}
L	length of the microchannel, m
L_p	permeability of the porous wall, Pa.s
m	relative error in shooting technique, refer to Eq. (37)
n^+	number concentration of the cation, numbers/mol
n_+^0	cation number concentration at the center of the channel, number/mol
n_-	number concentration of the anion, numbers/mol
n_-^0	anion number concentration at the center of the channel, number/mol
n_{Cl^-}	number concentration of the chloride ion in solution, numbers/mol
N_d	number of water molecules dissociated into H$_3$O$^+$ and OH$^-$
$n_{H_3O^+}$	number concentration of the hydronium ion in solution, numbers/mol
$n_{H_3O^+}^0$	number concentration of hydronium ion at the channel center, numbers/mol
$\overline{n_{H_3O^+}}$	average number concentration of the hydronium ion in solution, numbers/mol
n_{K^+}	number concentration of the potassium ion in solution, numbers/mol
n_{OH^-}	number concentration of the hydroxide ion in solution, numbers/mol
$n_{OH^-}^0$	number concentration of hydroxide ion at the channel center, numbers/mol

$\overline{n_{OH^-}}$	average number concentration of the hydroxide ion in solution, numbers/mol
N_S	density of the charged surface, sites/m^3
Pe_w	wall Peclet number
$\overline{Pe_w}$	length averaged wall Peclet number
pH	negative logarithm (base 10) of H$_3$O$^+$ molar concentration in the solution
pH_{ZPC}	pH of the solution at which the charged surface is neutral
p_x	axial pressure gradient, Pa/m
$r^\pm$	radius of the cation or anion, m
R_r	real retention of the porous wall
Sh	Sherwood number
$\overline{Sh_L}$	length averaged Sherwood number
T	temperature, K
u	overall velocity profile, m/s
$u_{cond}^\pm$	conduction velocities of cation and anion, m/s
u_p	average cross sectional velocity ($=p_x H^2/3\mu$), m/s
v_w	transverse velocity (quantified as permeation rate), m/s
x	axial co-ordinate, m
y	vertical co-ordinate, m
z	valence of the cation or anion in case of symmetric electrolyte

Greek symbols

α	non-dimensional term defined in Eq. (4), $\alpha = \frac{ze\psi}{k_B T}$
α_1, α_2	co-efficient for computing osmotic pressure using power law, (unit of α_1 is Pa.m$^{3\alpha_2}$.kg$^{-3\alpha_2}$)
δ	parameter defined in Eq. (6)
ε_0	permittivity of vacuum, 8.854×10^{-12} CV^{-1}.m^{-1}
ε_r	relative permittivity of the electrolyte medium
$\varepsilon_{1,2,3}$	relative tolerance for convergence of ψ_C, n_-^0 and n_+^0
$\Delta\pi$	osmotic pressure difference between wall and permeate side, Pa
ΔP_w	gauge pressure inside the channel, Pa
ΔpK	difference of the dissociation constants
κ	inverse of Debye layer thickness, m^{-1}
μ	solution viscosity, Pa.s
μ_{app}	apparent solution viscosity due to electroviscous phenomena, Pa.s
π	osmotic pressure of solution, Pa
σ_0	surface charge density, C/m^3
ψ	EDL potential distribution, V
ψ_C	EDL potential at the center of the channel, V
ψ_N^*	non-dimensional Nernst potential, ψ_N/ζ
ζ	wall zeta potential, V

flow due to the streaming field, the overall flow is hindered by the conduction current, which is manifested in apparent increase in viscosity of the fluid, recognized as the electroviscous effects [14–17]. Impact of the electroviscous effects results in reduced efficiency of the system, as reported by Wang et al. [18] in the case of nanofluidic channels. However, the above mentioned studies deal with microchannels with impervious walls.

Electrokinetic flow in microchannels with porous walls has potential application in electrokinetic transport and separation of biomolecules [19], microfluidic separation systems [20], basic clinical diagnostics [21], etc. However, studies on mass transport in microchannel are mostly limited to quantification of dispersion of micro-solutes (electrolytes) [22–24], in an impermeable conduit.

Few reports are available for studies on mass transport of neutral macrosolute across the porous wall in a microchannel. De and coworkers recently reported mass transport of neutral solutes in a microchannel with porous wall under the combined action of Poiseuille flow and external electric field [25–28]. There has been a recent analytical study on the shear dispersion of the neutral solutes by electroosmotic flow in a microchannel and microtube with porous walls by Dejam et al. [29,30]. They have used Reynolds decomposition technique to solve for the coupled flow-species system. A 1D diffusion dominated species transport equation in the porous medium has been prescribed instead of the interface mixed boundary condition. The shear dispersion coefficient depends on the Debye–Hückel parameter, Poiseuille contribution fraction and