Abstract

This thesis presents a numerical study on the electroosmotic flow (EOF) of Newtonian and non-Newtonian fluids in a modulated micro- or nanochannel. We have also considered the EOF in a soft channel where the channel walls are coated with a polyelectrolyte layer. The objectives are to achieve enhanced fluid flow as well as current density and ion selectivity in the conduits. The impact of the interfacial slip on the EOF of a yield stress fluid is also analyzed. The mathematical models are based on the conservation principle which leads to the coupled Navier-Stokes-Nernst-Planck-Poisson equations. The Cauchy momentum equation is used for the transport of the non-Newtonian viscoplastic fluid. The Brinkman extended Navier-Stokes equations are adopted to formulate the flow through the hydrogel, modeled as a porous media. Thesis consists of five main Chapters 2-6 along with an introductory Chapter 1 and a Chapter 7 describing the overall summary and the future scope.

An enhanced EOF by a geometric modulation of the surface of a charged nanochannel is considered in Chapter 2. The nanochannel filled with single electrolyte is modulated by embedding rectangular grooves placed perpendicular to the direction of the applied electric field in a periodic manner. We have arranged the rectangular grooves in such a way that the maximum flow enhancement occurs. It is found that enhancement of flow is much higher compared to the EOF in a flat channel when the width of the grooves are much higher than its depth and the Debye length is in the order of the channel height. The EOF with larger values of the width to depth ratio of grooves approaches the EOF through a channel in which grooves are replaced by superhydrophobic patches.

An enhanced EOF through a polyelectrolyte-infused grooved channel is studied subsequently (Chapter 3). The patterned microchannel results in an enhancement in the average EOF by creating an intrinsic velocity slip at the polyelectrolyte-liquid interface. We have established an analogy between the EOF in a polyelectrolyte filled grooved-channel with the EOF in which the grooves are replaced by the charged slipping planes. We have also derived an exact analytic solution for EOF based on the linearized Poisson-Boltzmann (P-B) model under the Debye-Hückel approximation when the width of the groove is much larger than its height. The effect of current density, ion selectivity and ion partitioning on EOF of the modulated channel for different values of electrokinetic parameters are also studied.

The transport of ionic liquid through the parallel plate soft nanochannel is presented in Chapter 4. The charged rigid walls of the channel are covered by a diffuse polyelectrolyte (PE) layer which entraps immobile charges. An analytic solution of EOF for step-like PE is derived based on the linearized P-B model under Debye-Hückel approximation. This analytic solution are in excellent agreement with the numerical model for thinner Debye-length and lower values of surface charge density. The occurrence flow reversal, zero flow and perm selectivity are studied in this Chapter.

The EOF of a non-Newtonian power-law and viscoplastic fluid (Casson, Bingham and Hershel-Bulkley fluid) near a surface potential heterogeneity is studied in Chapter 5. The objective of this study is to develop vortical flow to promote mixing of neutral solutes within the microchannel. We have highlighted the limitations of the linear slip-model and the nonlinear P-B model at various flow conditions. The nonlinear effects on EOF are found to be pronounced for a shear thinning liquid whereas the EOF is dominated by the diffusion mechanisms for the shear thickening liquid. A vortex, which resembles the Lamb vortex, develops over the potential patch when the patch potential is of opposite sign to that of the homogeneous surface potential. Enhanced mixing of a neutral solute is also analyzed in the present analysis. The yield stress reduces the EOF however, it promotes solute mixing.

The EOF of a viscoplastic Herschel-Bulkley fluid through a nanochannel patterned with periodically arranged uncharged slipping surfaces and no-slip charged surfaces is analyzed in Chapter 6. The aim of this study is to achieve an EOF augmentation in a nanoconduits. The channel is modulated in such a way that the slipping plane of one wall faces the no-slip surface of the opposite wall. Such arrangement is found to produce a maximum flow enhancement as the fluid in the vicinity of the uncharged slip stripes becomes electrically non-neutral. The maximum flow enhancement occurs for lower values of flow behavior index and higher values of yield stress and slip length parameter. We have obtained an analytic solution for the power-law fluid with free-slip patches when the periodic length is much higher than the channel height. The effect of nondimensional parameters such as yield stress, periodic length, Debye length, flow behavior index and slip length parameter on current density and ion selectivity are analyzed.

Keywords: Electroosmosis; Navier-Stokes equations; Nernst-Planck equations; Poisson-Boltzmann equation; Viscoplastic fluid; Power-law fluid; Polyelectrolyte; Species mixing; Hydrophobicity; Heterogeneous ζ-potential; Ion selectivity; Ion partitioning; Numerical solution.