Numerical Study on Electrokinetic transport of charged colloids and Newtonian/non-Newtonian viscoplastic electrolytes through nanopores

Abstract

This thesis presents a numerical study on electrokinetic transport of colloidal particles through electrolyte medium and motion of Newtonian or non-Newtonian viscoplastic ionic liquids through nanopore. Dispersion of the spherical soft or rigid colloids driven by the external electric field or gravitational force is analyzed numerically. We have studied the electroosmotic flow and ion transport through a nanotube of a non-Newtonian viscoplastic fluid. Generation of the streaming field and energy conversion through pressure driven flow of ionized liquid in a polyelectrolyte coated slit channel is also addressed in the present thesis. The mathematical models are based on the conservation principle, which leads to the coupled set of Navier-Stokes-Poisson-Nernst-Planck equations. The Brinkman extended Navier-Stokes equation is used to formulate the flow through porous region. The Nernst-Planck equation for ion transport is modified to take into account the ion steric interactions due to a finite ion size and the Born energy difference arise due to the difference in dielectric permittivity of the medium. The simplified asymptotic model for certain limiting cases under a weak applied electric field and low charge density consideration is also derived. The Thesis consists of four main Chapters 2-5 along with an introductory Chapter 1 and a Chapter 6 describing the overall summary and the future scope.

In Chapter 2, we consider the electrophoresis of a diffuse soft particle under the influence of an imposed electric field with the ion partition effect. Our investigation shows that the electrophoretic velocity strongly depends on the hydrophobicity of the core, Debye layer thickness, and the difference in permittivity of the PEL with the corresponding electrolyte. The surface conduction is largely influenced by the impact of ion partition and hydrophobicity of the core. The permittivity difference can significantly increase the effective charge density, however it reduces when PEL become dense where the counterion condensation effect dominates. The dependence of the particle size on its mobility is found to be pronounced when the Debye length is lower than the particle size.

Sedimentation mechanism of a charged hydrophobic colloid under a generalized gravitational field is studied in Chapter 3. The dependence of the sedimentation velocity on the several electrokinetic properties and hydrophobic nature of the colloid is investigated. The strength of the sedimentation field and the electric body force exerted on the particle increases as the particle charge density is enhanced. Surface hydrophobicity plays an important role to influence the induced sedimentation potential which has a significant

effect on the sedimentation velocity. The sedimentation velocity decreases as the electrolyte concentration is increased and it approaches to the velocity of uncharged colloid. The generalized gravitational field manifests the size based sorting of the particles.

The EOF of a viscoplastic Herschel-Bulkley fluid through a hydrophobic cylindrical pore is analyzed in Chapter 4. The objective of this study is to achieve enhanced EOF for viscoplastic material due to the effect of the interfacial slip at the hydrophobic pore. The effect of nondimensional parameters such as yield stress, length of the membrane, Debye length, flow behavior index and slip length parameter on current density and ion selectivity are also analyzed. 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. We have developed an analytic solution for the EOF of a power-law fluid in a long hydrophobic tube. Ion concentration polarization is highly influenced by the choice of flow index parameter and Debye length. Velocity slip exhibits higher ion selectivity as well as conductance at the pore.

The generation of streaming potential and energy conversion efficiency in a charged nanochannel whose walls are grafted with diffuse polyelectrolyte layer (PEL) is extensively investigated in Chapter 5. The standard electrokinetic model is modified by incorporating the finite ion size effect and ion partitioning effect that arises due to difference in dielectric permittivity between the electrolyte and PEL. Present model incorporates the impact of the PEL-to-electrolyte dielectric permittivity difference and the ion steric repulsion through the BMCSL model which enables to consider different ion sizes. The ion steric interactions and ion partitioning effects creates a counterion saturation of the PEL when the PEL and the wall are similarly charged, which in-turn produces higher streaming field and energy conversion efficiency.

Keywords : Navier-Stokes equations; Nernst-Planck equation; Double layer polarization; Electrophoresis; Electroosmosis; Sedimentation potential; Streaming potential; Ion partitioning effect; Viscoplastic fluid; BMCSL model; Ion steric interactions; Finite Volume Method; QUICK scheme; TVD scheme.