Abstract

This thesis presents a numerical study on the electrokinetic transport of liquid droplets and soft colloidal particles under the influence of an external electric field through a hydrogel medium. The mathematical model is based on the conservation principle, which leads to the coupled set of Navier-Stokes-Poisson-Nernst-Planck equations. The Brinkman extended Navier-Stokes model is used to formulate the flow through hydrogel medium. 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 dielectric decrement. The simplified asymptotic model for certain limiting cases under a weak applied electric field and low charge density consideration is also derived.

Chapter 1 of the thesis is introductory. In Chapter 2 the electrophoresis of a liquid droplet embedded in a polyelectrolyte hydrogel medium under the influence of an imposed electric field is considered. The surface of the droplet is considered to be charged, and the liquid filling the droplet is non-conducting. The dielectric polarization of the non-conducting droplet is also addressed in the present study. The strong electroosmotic flow (EOF) driven by the immobile charges of the gel medium creates a negatively charged drop to translate along the direction of the applied field. We have shown that a linear superposition of the droplet electrophoretic mobility in an uncharged gel medium and the background EOF due to the gel immobile charge can approximate our computed mobility for a thin Debye length in which the interaction of the immobile charge with the diffuse layer is negligible. The surface conduction enhances as the dielectric permittivity of the drop is increased. The charged gel medium is found to be efficient in size-based sorting of the liquid drops. In the subsequent chapter (Chapter 3) the electrophoresis of an uncharged non-conducting micro-sized liquid droplet in a charged hydrogel medium is studied. The dielectric polarization of the liquid drop under the action of an externally imposed electric field induces a non-homogeneous charge density at the droplet surface. The interactions of the induced surface charge of the droplet with the immobile charges of the hydrogel medium generates an electric force to the droplet, which actuates the drop through the charged hydrogel medium. A numerical study based on the first principle of electrokinetics is adopted. Dependence of the droplet velocity on its dielectric permittivity, bulk ionic concentration and immobile charge density of the gel is analyzed. The impact of the counterion saturation in the Debye layer due to the dielectric decrement of the medium is addressed. We find that the present induced charge electrokinetic mechanism in a charged gel medium creates a strong recirculation of liquid within the droplet and the translational velocity of the droplet strongly depends on its size.

In Chapter 4 the electrophoresis of a soft particle with a charged polarizable core is analyzed numerically which is supplemented by an asymptotic analysis. The hydrodynamics in both the gel medium and the soft layer encapsulating the hard core are governed by the Darcy-Brinkman model. The subtle nonlinear effects arising due to the polarization and relaxation of the double layer and the convective transport of counterions induced by the immobile charge of the soft layer are elucidated. These nonlinear effects have negligible impact when the bulk ionic concentration becomes high. The simplified model under the weak field consideration is independent of the core dielectric permittivity. However, the numerical model shows a strong dependence on core permittivity when the applied electric field is moderate. We have also addressed the ion partitioning effect when the dielectric permittivity of the soft layer is different from the gel medium. This creates a counterion saturation in the soft layer, and hence an augmentation in the electrophoresis. Subsequently, in Chapter 5 we consider the electrophoresis of a charged soft particle embedded in a charged hydrogel medium. The particle motion depends on the immobile charge of the surrounding polyelectrolyte layer (PEL) as well as the electroosmosis of the counterions. The ions are treated as charged dielectric sphere of finite radius (hydrated size of ions). The ion transport in the medium is considered to be governed by the modified Nernst-Planck equations (MNP), which takes into account the dielectric decrement, ion steric interactions, Born energy difference and dielectrophoretic interactions. The convection of the ions are governed by the Brinkman extended Navier-Stokes equations. Our computed results are in agreement for limiting cases with the existing solutions based on first-order perturbation analysis. The steric interactions and dielectric decrement creates a counterion saturation in the Debye layer of the core, which in-turn reduces the induced surface charge density. Consideration of the dielectric decrement and the Born force attenuates the counterion condensation leading to a dominance of the PEL fixed charge density. An overall conclusion of the studies reported in the thesis and an outline of the future scope are presented in Chapter 6 of the thesis.

Keywords : Navier-Stokes equations; Nernst-Planck equation; Brinkman equation; Numerical solution; Control volume method; Double layer polarization; Electrophoresis; Induced charge electrophoresis; Dielectric decrement; Ion partitioning effect; Carnahan-Starling model; Ion steric interactions.