

Impact of Marangoni Stress and Mobile Surface Charge on Electrokinetics of Ionic Liquids Over Hydrophobic Surfaces

Authors : Somnath Bhattacharyya

Abstract : The mobile adsorbed surface charge on hydrophobic surfaces can modify the velocity slip condition as well as create a Marangoni stress at the interface. The functionalized hydrophobic walls of micro/nanopores, e.g., graphene nanochannels, may possess physisorbed ions. The lateral mobility of the physisorbed ions creates a friction force as well as an electric force, leading to a modification in the velocity slip condition at the hydrophobic surface. In addition, the non-uniform distribution of these surface ions creates a surface tension gradient, leading to a Marangoni stress. The impact of the mobile surface charge on streaming potential and electrochemical energy conversion efficiency in a pressure-driven flow of ionized liquid through the nanopore is addressed. Also, enhanced electro-osmotic flow through the hydrophobic nanochannel is also analyzed. The mean-field electrokinetic model is modified to take into account the short-range non-electrostatic steric interactions and the long-range Coulomb correlations. The steric interaction is modeled by considering the ions as charged hard spheres of finite radius suspended in the electrolyte medium. The electrochemical potential is modified by including the volume exclusion effect, which is modeled based on the BMCSL equation of state. The electrostatic correlation is accounted for in the ionic self-energy. The extremal of the self-energy leads to a fourth-order Poisson equation for the electric field. The ion transport is governed by the modified Nernst-Planck equation, which includes the ion steric interactions; born force arises due to the spatial variation of the dielectric permittivity and the dielectrophoretic force on the hydrated ions. This ion transport equation is coupled with the Navier-Stokes equation describing the flow of the ionized fluid and the 3fourth-order Poisson equation for the electric field. We numerically solve the coupled set of nonlinear governing equations along with the prescribed boundary conditions by adopting a control volume approach over a staggered grid arrangement. In the staggered grid arrangements, velocity components are stored on the midpoint of the cell faces to which they are normal, whereas the remaining scalar variables are stored at the center of each cell. The convection and electromigration terms are discretized at each interface of the control volumes using the total variation diminishing (TVD) approach to capture the strong convection resulting from the highly enhanced fluid flow due to the modified model. In order to link pressure to the continuity equation, we adopt a pressure correction-based iterative SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm, in which the discretized continuity equation is converted to a Poisson equation involving pressure correction terms. Our results show that the physisorbed ions on a hydrophobic surface create an enhanced slip velocity when streaming potential, which enhances the convection current. However, the electroosmotic flow attenuates due to the mobile surface ions.

Keywords : microfluidics, electroosmosis, streaming potential, electrostatic correlation, finite sized ions

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