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Development of a High-Resolution Scheme for Solving the PNP-NS Equations in Curved Channels

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Abstract. A high-order finite difference scheme has been developed to approximate the spatial derivative terms present in the unsteady Poisson-Nernst-Planck (PNP) equations and incompressible Navier-Stokes (NS) equations. Near the wall the sharp solution profiles are resolved by using the combined compact difference (CCD) scheme developed in five-point stencil. This CCD scheme has a sixth-order accuracy for the second-order derivative terms while a seventh-order accuracy for the first-order derivative terms. PNP-NS equations have been also transformed to the curvilinear coordinate system to study the effects of channel shapes on the development of electroosmotic flow. In this study, the developed scheme has been analyzed rigorously through the modified equation analysis. In addition, the developed method has been computationally verified through four problems which are amenable to their own exact solutions. The electroosmotic flow details in planar and wavy channels have been explored with the emphasis on the formation of Coulomb force. Significance of different forces resulting from the pressure gradient, diffusion and Coulomb origins on the convective electroosmotic flow motion is also investigated in detail.

AMS subject classifications: 76D05, 76D55, 65M06, 65M22

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1 Introduction

Design of a microfluidic biochemical device to propel ionic fluids from one end to the other end has been an important research topic [1]. For an effective control of flow motion to enhance fluid mixing and to avoid flow separation, the concept of miniaturized total analysis (μTAS) proposed in the early 1990s [2] can be adopted. With the remarkable progress in μTAS, today biochemical analysis has many applications in the fields of microfludics and display [3]. One can refer to [4] for an overview of applications of magnetohydrodynamics to DC/AC electrokinetics for electroosmotic or electrophoresis/dielectrophoresis flow. The techniques exploiting the physicochemical properties of solid-electrolyte interface are referred as electroosmotics [5].

Electroosmotic flow (EOF) results from a motion of accumulated electric charges on the no-slip surfaces which are in contact with electrolyte solution. These ions are accumulated in a thin layer immediately close to the wall. This thin layer is also known as the electric double layer (EDL) or Debye layer [6]. Electrolyte away from this thin layer is neutral. Charge separation near the solid surface establishes a positive or a negative potential difference across the Debye layer. When an external electric field is applied, the counter ions in the Debye layer are attracted to the oppositely charged electrodes. Motion of these ions induces fluid flow. In other words, the electric force can be exploited as the leading factor to drive and control the movement of operating fluid and the charged species. For example, motion of beads and pigmented particles of the size ranging from a sub-millimeter to a few microns in electrode-bounded channels can be controlled using the above mechanism.

In microfluidic devices the gap between electrodes is very small and one can easily generate a highly localized and large electric field. For such devices, electric force can be used precisely for flow control. Microfluidic devices are normally featured with a much larger surface-to-volume ratio in comparison with their macroscopic counterparts. Forces relevant to surface are therefore likely to be substantially larger than the forces associated with volumes. The zeta-potential surface force established between the solid electrode and the surrounding electrolyte induces EDL formation. Within this layer, an excessive amount of free charges exists. When these charges are exposed to an electric field with non-zero component parallel to the surface, they start moving accordingly and can provide a significant pumping force to the electrolyte liquid.

In this study, the electroosmotic flowfields bounded by planar and wavy channel walls are investigated when an uniform potential difference is specified across these channels. Numerical investigation of these types of flowfield needs the solution of velocity vector to enable simulation of the transport of positive and negative ions. Non-uniform distribution of ions in a channel with charged walls results in the formation of Coulomb force which further induces fluid motion. This prompts the importance of solving the transport equations for positive and negative ions along with the Navier-Stokes equations. Thus, the study of electroosmotic flow turns out to be relevant to the analysis of incompressible Navier-Stokes equations and ion transport equations.