Poisson-Nernst-Planck Simulations for Enzyme and Nanopore System

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Abstract

The Poisson-Nernst-Planck equations are widely used in simulating the electro-diffusion processes for nanoscale biological system. Here, we apply the Poisson-Nernst-Planck equations to acetylcholinesterase system as well as nanopore and solve the equations with finite element method. We compare the numerical results of substrate-enzyme system with Debye-Hückel limiting law, based on a linearized Poisson-Boltzmann model and known for its accurate predictions in dilute solutions. It is observed that both charged substrate and product together contribute like a non-reactive species in numerical simulation, and our Poisson-Nernst-Planck model recovers the Debye-Hückel limiting law well. For nanopore, we observe the ion current rectification phenomenon in steady state, which is influenced by nanopore geometry, electrolyte concentration and surface charge density. Moreover, nanopore scanning is simulated by time-dependent Poisson-Nernst-Planck equations, and the profile of current-voltage behavior is presented.

Keywords: PNP equation, FEM, electro-diffusion process, AChE, DHL law, nanopore, scan