A Generalized Poisson-Nernst-Planck Equations with Inhomogeneous Dielectric Permittivity for Ion Selectivity in Ion Channels

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Abstract

The electric diffusion process around the biomolecule in the solution can be described by electric potential and ion concentration distributions. The Poisson-Nernst-Planck (PNP) equations have been widely used to study the ion transport problems in many systems of physics and chemistry. In this work, we present a generalized PNP equations with variable dielectric permittivity. To derive the generalized PNP equations, we propose a complete mean field free energy of a charged system within a finite inhomogeneous dielectric domain with Neumann/Dirichlet boundary conditions. For inhomogeneous electrolyte with ionic concentration-dependent dielectric permittivity, if we consider the non-equilibrium state, there exist ion transport process in the system. Then we derive the generalized PNP equations under different boundary conditions. Some numerical simulations are made in a simplified cylindrical nanopore and in a realistic model of a potassium channel. The new generalized PNP equations can model selectivity of ion channel and distinguish different ionic species in the solvent.

Keywords: Generalized Poisson-Nernst-Planck equations; Variable dielectric; Ion selectivity; Ion channels.