Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2021-0242

Vol. **36**, No. 2, pp. 521-550
August 2024

An Inverse Averaging Finite Element Method for Solving the Size-Modified Poisson-Nernst-Planck Equations in Ion Channel Simulations

Ruigang Shen[1,2], Qianru Zhang[2,3] and Benzhuo Lu[2,*]

[1] *School of Mathematics and Computational Science, Guangxi Applied Mathematics Center (GUET), Guangxi Colleges and Universities Key Laboratory of Data Analysis and Computation, Guilin University of Electronic Technology, Guilin, Guangxi, 541004, P.R. China.*
[2] *LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, 100190, P.R. China.*
[3] *School of Mathematical Sciences, University of Chinese Academy of Sciences, Beijing, 100049, P.R. China.*

Received 1 December 2021; Accepted (in revised version) 29 August 2022

Abstract. In this work, an inverse averaging finite element method (IAFEM) is developed for solving the size-modified Poisson-Nernst-Planck (SMPNP) equations. Comparing with the classical Poisson-Nernst-Planck (PNP) equations, the SMPNP equations add a nonlinear term to each of the Nernst-Planck (NP) fluxes to describe the steric repulsion which can treat multiple nonuniform particle sizes in simulations. Since the new terms include sums and gradients of ion concentrations, the nonlinear coupling of SMPNP equations is much stronger than that of PNP equations. By introducing a generalized Slotboom transform, each of the size-modified NP equation is transformed into a self-adjoint equation with exponentially behaved coefficient, which has similar simple form to the standard NP equation with the Slotboom transformation. This treatment enables employing our recently developed inverse averaging technique to deal with the exponential coefficients of the reformulated formulations, featured with advantages of numerical stability and flux conservation especially in strong nonlinear and convection-dominated cases. Comparing with previous stabilization methods, the IAFEM developed in this paper can still possess the numerical stability when dealing with convection-dominated problems. And it is more concise and easier to be numerically implemented. Numerical experiments about a model problem with analytic solutions are presented to verify the accuracy and order of IAFEM for SMPNP equations. Studies about the size-effects of a sphere model and an ion channel

*Corresponding author. *Email addresses:* rgshen@guet.edu.cn (R. Shen), qrzhang@lsec.cc.ac.cn (Q. Zhang), bzlu@lsec.cc.ac.cn (B. Lu)

system are presented to show that our IAFEM is more effective and robust than the traditional finite element method (FEM) when solving SMPNP equations in simulations of biological systems.

AMS subject classifications: 35J61, 65N30, 92C40

Key words: Size-modified Poisson-Nernst-Planck equations, generalized Slotboom transform, inverse averaging finite element method, sphere model, ion channel.

---

1 Introduction

"The effects of finite particle size on electrostatics, density profiles, and diffusion have been a long-existing topic in the study of ionic solution." [30] As a continuous electrodiffusion model, the classical Poisson-Nernst-Planck (PNP) equations play an important role in the electrodiffusion reaction process and have been widely used to describe the electrodiffusion of ions and charge transport in applications including the solvated biomolecular system [29, 31], semiconductors [21, 33, 37], electrochemical systems [4, 10, 32] and ion channels [7, 11, 39]. Although the PNP equations have achieved a lot of success in various applications, it still has some limitations due to the neglected steric effects of ions in its mean-field derivation, for example, the PNP model leads to unphysical crowding of ions near charged surfaces and incorrect dynamics of ion transport, and the difference between two cations with the same charge cannot be distinguished when simulating the concentration distribution of ions. To incorporate the effects of finite particle sizes in the study of ionic solutions, many improvements are made through introducing exclusion terms from the liquid-state theory or the density functional theory (DFT), e.g. see [15, 16, 34, 36] and references therein. In addition, based on the framework of the PNP model, several versions of the modified PNP theory have been developed in the literature to account for steric effects [20, 22, 23, 25, 35, 38]. Among these theories, the Borukhov model [5] attracts people's attention because it captures basic size effects only with a simplified model. The Borukhov model modifies the free energy functional of the ionic system (mean-field approximation) by adding an ideal-gas-like solvent entropy term, which represents the unfavorable energy used to model the over-packing or crowding of the ions and solvent molecules. Thus the steric effects are taken into account in the model. Lu and Zhou by generalizing the Borukhov model get a class of size-modified Poisson-Nernst-Planck (SMPNP) equations via the inclusion of the entropy of solvent molecules in the electrostatic free-energy functional [30]. Different from many other works, the SMPNP model is able to treat multiple nonuniform particle sizes in simulations.

Comparing with the classical PNP equations [29], the SMPNP model adds a nonlinear term to each of Nernst-Planck (NP) equations aiming at describing the steric repulsion (see Eq. (2.2)). Since the new term includes sums and gradients of ion concentrations,