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ACCEPTED MANUSCRIPT

A three-ions model of electrodiffusion kinetics in a nanochannel

Táňa Sebechlebská, Pavel Neogrády, Ivan Valent*

Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University, Mlynská dolina, 842 15 Bratislava, Slovak Republic

Abstract

Nanoscale electrodiffusion transport is involved in many electrochemical, technological and biological processes. Developments in computer power and numerical algorithms allow for solving full time-dependent Nernst-Planck and Poisson equations without simplifying approximations. We simulate spatio-temporal profiles of concentration and electric potential changes after a potential jump in a 10 nm channel with two cations (with opposite concentration gradients and different mobilities) and one anion (of uniform concentration). The temporal dynamics shows three exponential phases and damped oscillations of the electric potential. Despite the absence of surface charges in the studied model, an asymmetric current-voltage characteristic was observed.

Keywords: Ion transport, Electrodiffusion, Ion channel, PNP theory, Time-dependent Nernst-Planck-Poisson equations, Ion current rectification ICR

1. Introduction

Conforming to a general principle all systems out of equilibrium try to reach a minimum of the free energy. Phenomena occurring in electrolyte solutions during the equilibration include chemical reactions, solvation, or transport of ions. Ion transport due to a gradient of the electrochemical potential, known as electrodiffusion, is described at molecular level by the

*Corresponding author
Email address: valent@fns.uniba.sk (Ivan Valent)

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