An application of Shockley's recombination and generation theory to biological ion channels

Sai Hu, Karl Hess
Computational Electronics Group, Beckman Institute, University of Illinois,
Urbana, IL, 61801, USA
email: saihu@uiuc.edu

We have applied the Shockley-Read-Hall (SRH) model for the generation and recombination of charge carriers to biological ion channels. We show how to include this important effect in the traditional PNP model and how to provide a bridge between the microscopic particle methods (such as MD, Monte Carlo) and the macroscopic continuum models such as PNP that always need to be part of a multi-scale approach. We refer to our method by the acronym TR-PNP where "TR" indicates the inclusion of the trapping and releasing processes of ions at certain trapping or binding sites.

The idea is to use the software of computational electronics developed to solve Shockley's equations. In particular we have used PROPHET, with help of the Stanford TCAD group, to simulate biological ion channels beyond the level that was achieved up to now in PNP simulations of the bio-physics community. We have included into the continuum type PNP simulations particle like properties and dynamics such as capture and release of ions. The considerable reduction of effective diffusion coefficients can be well simulated and understood that way. The saturation effect observed in current-concentration curves, which is not predicted by the conventional PNP model, has been successfully reproduced in our TR-PNP simulation. We also demonstrate that PROPHET can easily be used to perform both steady state and time dependent simulations for ion channels. Furthermore, our numerical results show that capture and even gating phenomena in ion channels are very likely to be accurately simulated by our method. The timescale can be microseconds, far beyond the range of molecular dynamics simulations. Our results also demonstrate the useful role of PROPHET simulations in a multi-scale simulation approach.

A full journal publication of this work will be published in the Journal of Computational Electronics.

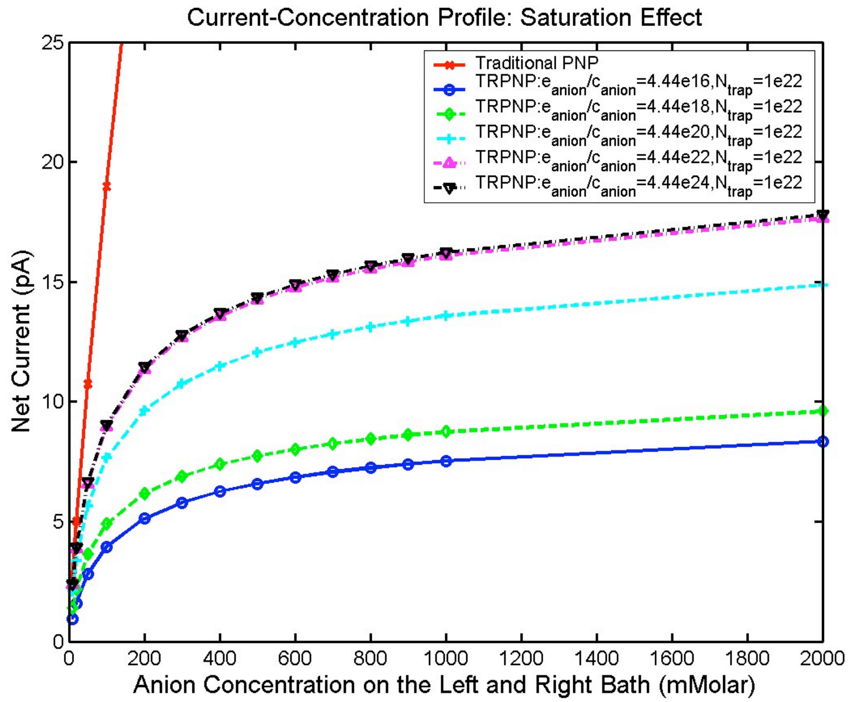

Figure 1: The saturation effect of current-concentration curves predicted by our TR-PNP model, compared with the almost linear relationship from the traditional PNP model

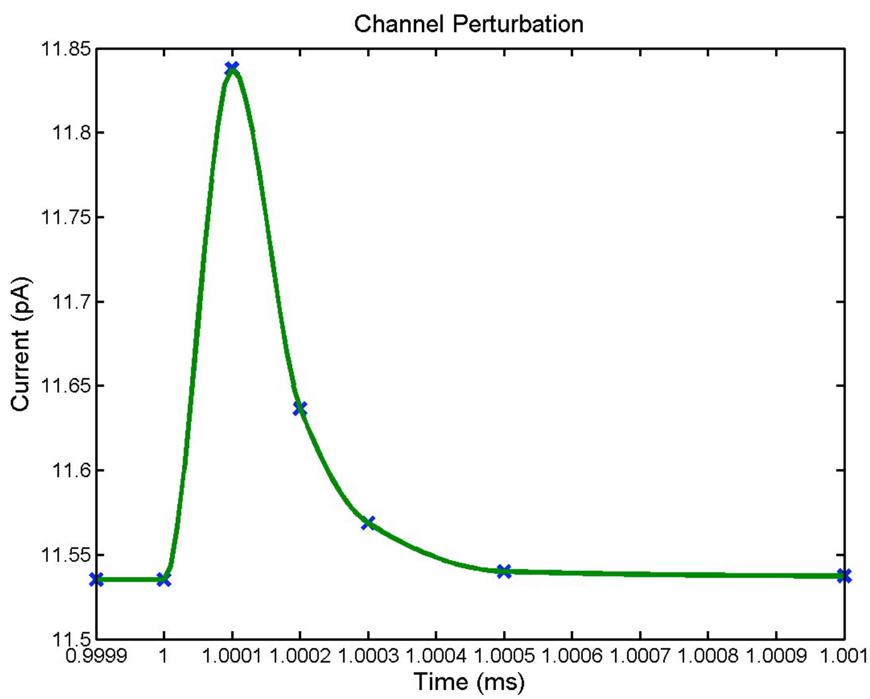

Figure 2: The evolution of the current initiated by the perturbation related to anions release at time t=1.0ms

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