Stochastic Diffusion of Calcium Ions Through a Nanopore in the Cell Membrane Created By Electroporation

O. Henao[1], V. Gómez[1], I. De La Pava[1], J. Sánchez [1]

[1]Grupo Fisiología celular y aplicada, Universidad Tecnológica de Pereira, Pereira, Risaralda, Colombia

Abstract

In this work we simulated the diffusion of calcium ions through a nanopore created in the cell membrane by electroporation, in presence and absence of the external electric field responsible of the membrane permeabilization. First we solved the set of coupled differential equations that describe the process of ionic diffusion in a 2D nanopore model using COMSOL Multiphysics® software (Figure 1) [1][2], and then we carried out a simulation of the stochastic molecular dynamics of the calcium ions in the nanopore using MATLAB® [3][4][5]. The electric field in the stochastic diffusion model was obtained through the Electrostatics interface of the AC/DC Module. Our first approach was to export the computed values of the electric field to a text file and then loaded them into MATLAB, afterwards we used the COMSOL LiveLink™ for MATLAB® instead, with no alteration in the final behavior of the probabilistic distribution of the Calcium ions in the nanopore (Figure 2-4). Finally we compared the results obtained in both simulations. We found a difference of about one order of magnitude in the values of the ionic flux in the nanopore, while the qualitative description of the diffusion process evolution was similar in both cases.

Reference

[1] Dongqing Li, Saeid Movahed,"Electrokinetic Transport through the Nanopores in Cell Membrane during Electroporation", Journal of Colloid and Interface science, Volume 369, 442-452 (2011).

[2] Stephen J. Beebe, "Bioelectrics in Basic Science and Medicine: Impact of Electric Fields on Cellular Structures and Functions", Journal of Nanomedicine and Nanotechnology, Volume 4, 1-8 (2013).

[3] Daniel T. Gillespie, "The Mathematics of Brownian Motion and Johnson Noise", American Association of Physics Teachers, Volume 64, 225-240 (1996).

[4] Steven S. Andrews, Tuan Dinh et al., "Stochastic Models of Biological Processes", Encyclopedia of Complexity and Systems Science, 8730-8749 (2009).

[5] Steven S. Andrews, Tuan Dinh et al., "Stochastic Simulation of Chemical Reactions with Spatial Resolution and Single Molecule Detail", Physical Biology, Volume 1, 137–151 (2004).

Figures used in the abstract

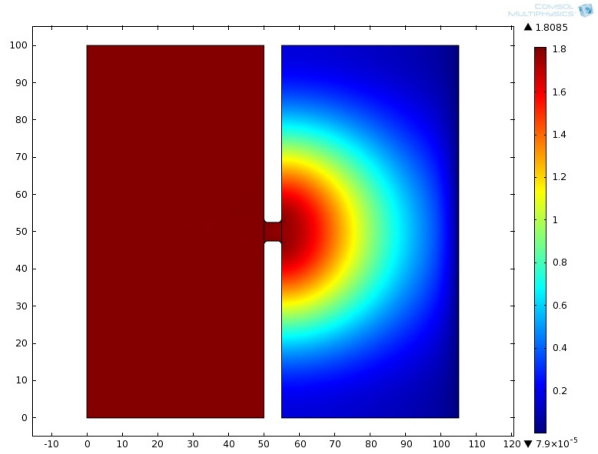

Figure 1: Calcium concentration profile in the nanopore after the application of the external electric field.

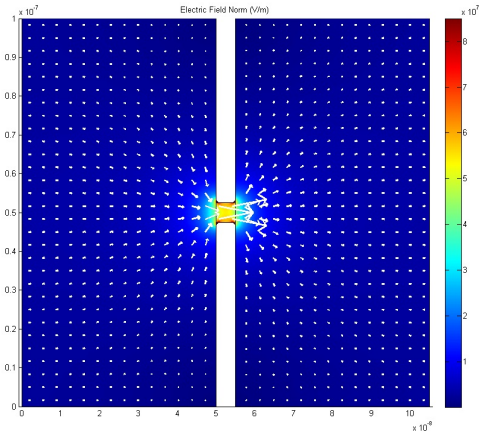

Figure 2: Electric field obtained with the COMSOL LiveLink™ for MATLAB®.

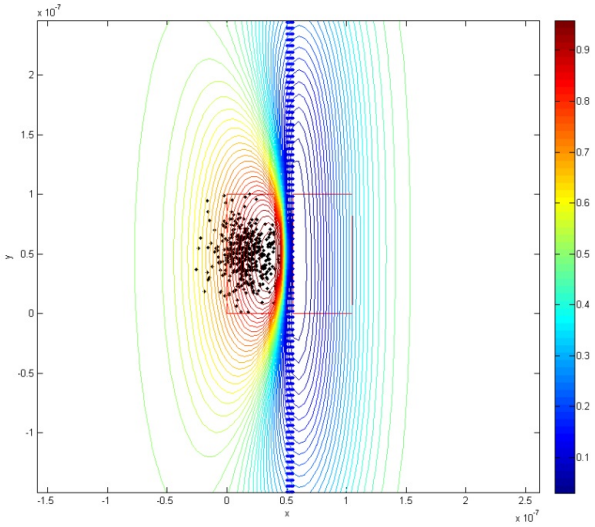

Figure 3: Probabilistic distribution of the Calcium ions in the nanopore before the application of the external electric field.

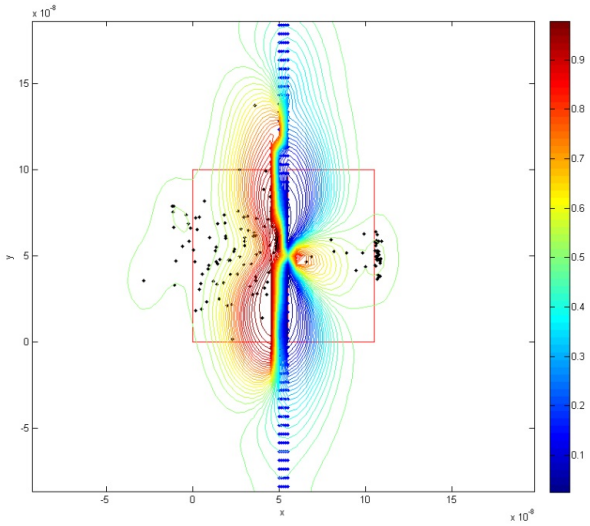

Figure 4: Probabilistic distribution of the Calcium ions in the nanopore after the application of the external electric field.