Experimental and theoretical Brownian dynamics analysis of ion transport during cellular electroporation of E. coli bacteria

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Abstract

Escherichia coli bacterium is a rod-shaped organism composed of a complex double membrane structure. Knowledge of electric field driven ion transport through both membranes and the evolution of their induced permeabilization has important applications in biomedical engineering, delivery of genes and antibacterial agents. However, few studies have been conducted on Gram-negative bacteria in this regard considering the contribution of all ion types. To address this gap in knowledge, we have developed a deterministic and stochastic Brownian dynamics model to simulate in 3D space the motion of ions through pores formed in the plasma membranes of E. coli cells during electroporation. The diffusion coefficient, mobility, and translation time of Ca2+, Mg2+, Na+, K+, and Cl− ions within the pore region are estimated from the numerical model. Calculations of pore's conductance have been validated with experiments conducted at Gustave Roussy. From the simulations, it was found that the main driving force of ionic uptake during the pulse is the one due to the externally applied electric field. The results from this work provide a better understanding of ion transport during electroporation, aiding in the design of electrical pulses for maximizing ion throughput, primarily for application in cancer treatment.