Model Evaluation of Thermal Effects Created by Cell Membrane Electroporation

Authors : Jiahui Song

Abstract : The use of very high electric fields (~ 100kV/cm or higher) with pulse durations in the nanosecond range has been a recent development. The electric pulses have been used as tools to generate electroporation which has many biomedical applications. Most of the studies of electroporation have ignored possible thermal effects because of the small duration of the applied voltage pulses. However, it has been predicted membrane temperature gradients ranging from 0.2×109 to 109 K/m. This research focuses on thermal gradients that drives for electroporative enhancements, even though the actual temperature values might not have changed appreciably from their equilibrium levels. The dynamics of pore formation with the application of an externally applied electric field is studied on the basis of molecular dynamics (MD) simulations using the GROMACS package. Different temperatures are assigned to various regions to simulate the appropriate temperature gradients. The GROMACS provides the force fields for the lipid membranes, which is taken to comprise of dipalmitoyl-phosphatidyl-choline (DPPC) molecules. The water model mimicks the aqueous environment surrounding the membrane. Velocities of water and membrane molecules are generated randomly at each simulation run according to a Maxwellian distribution. For statistical significance, a total of eight MD simulations are carried out with different starting molecular velocities for each simulation. MD simulation shows no pore is formed in a 10-ns snapshot for a DPPC membrane set at a uniform temperature of 295 K after a 0.4 V/nm electric field is applied. A nano-sized pore is clearly seen in a 10-ns snapshot on the same geometry but with the top and bottom membrane surfaces kept at temperatures of 300 and 295 K, respectively. For the same applied electric field, the formation of nanopores is clearly demonstrated, but only in the presence of a temperature gradient. MD simulation results show enhanced electroporative effects arising from thermal gradients. The study suggests the temperature gradient is a secondary driver, with the electric field being the primary cause for electroporation.

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