Molecular Dynamics Simulation Studies of Thermal Effects Created by High-Intensity, Ultra-Short Pulses Induced Cell Membrane Electroporation

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Abstract : The use of electric fields with high intensity (~ 100kV/cm or higher) and ultra short pulse durations (nanosecond range) has been a recent development. 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 effects that drive 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. MD simulations of a lipid layer with constant electric field strength of 0.5 V/nm at 25 °C and 47 °C are implemented to simulate the appropriate thermal effects. 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. The high background electric field is typically used in MD simulations to probe electroporation. It serves as an accelerated test of the pore formation process since low electric fields would take inordinately long simulation time. MD simulation shows no pore is formed in a 1-ns snapshot for a DPPC membrane set at a temperature of 25°C after a 0.5 V/nm electric field is applied. A nano-sized pore is clearly seen in a 0.75-ns snapshot on the same geometry, but with the membrane surfaces kept at temperatures of 47°C. And the pore increases at 1 ns. The MD simulation results suggest the possibility that the increase in temperature can result in different degrees of electrically stimulated bio-effects. The results points to the role of thermal effects in facilitating and accelerating the electroporation process.

Keywords : high-intensity, ultra-short, electroporation, thermal effects, molecular dynamics
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