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Molecular Dynamics Simulation Studies of High-Intensity, Nanosecond Pulsed Electric Fields Induced Membrane Electroporation

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Abstract : The use of high-intensity, nanosecond electric pulses has been a recent development in biomedical. High-intensity (~100 kV/cm), nanosecond duration-pulsed electric fields have been shown to induce cellular electroporation. This will lead to an increase in transmembrane conductivity and diffusive permeability. These effects will also alter the electrical potential across the membrane. The applications include electrically triggered intracellular calcium release, shrinkage of tumors, and temporary blockage of the action potential in nerves. In this research, the dynamics of pore formation with the presence of an externally applied electric field is studied on the basis of molecular dynamics (MD) simulations using the GROMACS package. MD simulations show pore formation occurs for a pulse with the amplitude of 0.5V/nm at 1ns at temperature 316°K. Also increasing temperatures facilitate pore formation. When the temperature is increased to 323°K, pore forms at 0.75ns with the pulse amplitude of 0.5V/nm. For statistical significance, a total of eight MD simulations are carried out with different starting molecular velocities for each simulation. Also, actual experimental observations are compared against MD simulation results.

Keywords : molecular dynamics, high-intensity, nanosecond, electroporation
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