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

Authors : Jiahui Song

Abstract : The application of an electric field can cause poration at cell membranes. This includes the outer plasma membrane, as well as the membranes of intracellular organelles. In order to analyze and predict such electroporation effects, it becomes necessary to first evaluate the electric fields and the transmembrane voltages. This information can then be used to assess changes in the pore formation energy that finally yields the pore distributions and their radii based on the Smolchowski equation. The dynamic pore model can be achieved by including a dynamic aspect and a dependence on the pore population density into the pore formation energy equation. These changes make the pore formation energy E(r) self-adjusting in response to pore formation without causing uncontrolled growth and expansion. By using dynamic membrane tension, membrane electroporation in response to a 180kV/cm trapezoidal pulse with a 10 ns on time and 1.5 ns rise- and fall-times is discussed. Poration is predicted to occur at times beyond the peak at around 9.2 ns. Modeling also yields time-dependent distributions of the membrane pore population after multiple pulses. It shows that the pore distribution shifts to larger values of the radius with multiple pulsing. Molecular dynamics (MD) simulations are also carried out for a fixed field of 0.5 V/nm to demonstrate nanopore formation from a microscopic point of view. The result shows that the pore is predicted to be about 0.9 nm in diameter and somewhat narrower at the central point.

Keywords : high-intensity, nanosecond, dynamics, electroporation
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