

Abstract for an Invited Paper
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Numerical modeling of fast gate-coupled ion permeation in ClC channels¹

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We have developed a three dimensional Brownian dynamics (BD) and discrete-state model to couple ion permeation to the motion of a putative fast gate in the ClC channels. The model channel is designed so as to represent certain essential features of ClC chloride channel, in which a glutamate side chain moves from an open state to a closed state (blocking the channel pore at a position which also acts as a binding site for Cl^- ions moving through the channel). Both BD and the discrete-state model generate results in qualitative agreement with experimental observations and consistent with the foot-in-the-door mechanism. Furthermore, we have formulated a numerical approach to calculate the discrete rate constants in our model channel using BD. The discrete-state model with the rate constants solved via BD produces results consistent with the (continuous space) multi-ion BD simulations.

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