

## **427n Signal Transduction Reactions at Cell Membranes: Comparison of Continuum Theory and Brownian Dynamics Simulations**

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Biochemical transduction of signals received by living cells typically involves molecular interactions and enzyme-mediated reactions at the cell membrane, a problem that is analogous to reacting species on a catalyst surface or interface. We have developed an efficient Brownian dynamics algorithm that is especially suited for such systems and have compared the simulation results with various continuum theories through prediction of effective enzymatic rate constant values. We specifically consider reaction versus diffusion limitation, the effect of increasing enzyme density, and the spontaneous membrane association/dissociation of enzyme molecules. In all cases, we find the theory and simulations to be in quantitative agreement. This algorithm may be readily adapted for the stochastic simulation of more complex cell signaling systems.