PNP Equations with Steric Effects: A Model of Ion Flow through Channels

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The flow of current through an ionic channel is studied using the energetic variational ap- proach of Liu applied to the primitive (implicit solvent) model of ionic solutions. This approach allows the derivation of self-consistent (Euler-Lagrange) equations to describe the flow of spheres through channels. The partial differential equations derived involve the global interac- tions of the spheres and are replaced here with a local approximation that we call steric PNP (Poisson-Nernst-Planck). Kong combining rules are used and a range of values of steric inter- action parameters are studied. These parameters change the energetics of steric interaction but have no effect on diffusion coefficients in models and simulations.

Calculations are made for the calcium (EEEE, EEEA) and sodium channels (DEKA) previously studied in Monte Carlo simulations with comparable results. The biological function is quite sensitive to the steric in- teraction parameters, and we speculate that a wide range of the function of channels and transporters, even enzymes, might depend on such terms. We point out that classical theories of channels, transporters, and enzymes depend on ideal representations of ionic solutions in which nothing interacts with nothing, even in the enormous concentrations found near and in these proteins or near electrodes in electrochemical cells for that matter. We suggest that a theory designed to handle interactions might be more appropriate. We show that one such theory is feasible and computable: steric PNP allows a direct comparison with experiments measuring flows as well as equilibrium properties. Steric PNP combines atomic and macro- scales in a computable formulation that allows the calculation of the macroscopic effects of changes in atomic scale structures (size about 0.1 nm) studied very extensively in channology and molecular biology.