Biophysical Journal (1993) 64:A22

M-PM-WS4-2

POISSON-NERNST-PLANCK *(PNP)* THEORY OF AN OPEN IONIC CHANNEL.

((Robert Eisenberg and Duanpin Chen)) Dept. of Physiology, Rush Medical College, 1750 W. Harrison, Chicago IL

The structure of an ionic channel is the location of its atoms and their permanent electric charge. The electric field within a channel's pore is determined by all types of charge, namely the permanent charge of the channel protein, the mobile charge of ions within the pore, and the induced charge in pore and protein. Permanent charge is significantly shielded by permeating ions whose concentration and flux in turn depend on the electric field. A channel and its contents form a thoroughly coupled system, requiring simultaneous analysis of electric field and electro-diffusion, as do semiconductors like transistors. Asymptotic analysis of a *PNP* theory gives surprising results. Even though its pore is always open, in just one conformation, and its ions are points, able to flow through each other, its net and unidirectional fluxes are *not* independent if the pore contains an access resistance or selectivity filter. Rather, the fluxes vary together, as bath concentrations are varied. The electric field changes shape because the shielding of the permanent charge varies: potential barriers can change into potential wells (i.e., binding sites) as concentrations change. In this way, fluxes are coupled to concentrations in the bath, and to one another, as they are in traditional single file channels or mediated transport systems.

M-PM-WS4-3

POISSON-NERNST-PLANCK *(PNP)* THEORY OF IONIC CHANNELS.

((Duanpin Chen and Robert Eisenberg)) Dept. of Physiology, Rush Medical College, 1750 W. Harrison, Chicago IL

PNP theory predicts many characteristics of biological channels, although it describes a channel of just one conformation in which ionic points can flow through each other. Rectification, saturation of conductance with concentration, and flux interactions arise naturally in the theory, if the pore contains an access resistance or selectivity filter, because the shape of the electric field changes with experimental conditions. The spatial variation (1) of ionic charge (2) of potential (3) and of the energy of the charge at that potential reveals how each characteristic of real channels can arise even in such an oversimplified model. When the permanent charge distribution has four maxima, as in thyristors or "Numa rings", three *IV* relations satisfy the steady-state equations. Two are stable. One contains few ions to shield the permanent charge or carry current, perhaps corresponding to a closed channel. The other contains enough ions to shield the permanent charge and carry a large current, perhaps corresponding to an open channel. The unstable state may describe a transient or inactivating channel. We have constructed and are integrating a time dependent version of the *PNP* theory to see if the evolution or switching of these states can account for the time dependent properties of channels.