**Specification of Ion Channel Problem**

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The electric potential is computed from the Poisson equation with a source term equal to the charge generated by the ions, including the permanent charge. For the continuum description of ion transport, the Nernst-Planck (NP) equations are used, which involve a diffusion term as well as a drift term caused by the electric field (ideal electrostatic potential), an external confining potential, and the excess electro-chemical potential. A computational model and domain  that describes the bath and channel is a coupled system of the form (after suitable scaling)

 (1)

 (2)

Here  denotes a relative charge of the -th species,  the mobility, and  is a scaled variable depending on the dielectric coefficient, elementary charge, and typical values of the concentrations The potentials  are computed as variations of an energy functional, i.e.,

 (3)

which is of the form

 (4)

The functional  includes electrostatic interaction via the electric field (the first two terms), diffusion (the logarithmic term), external action via potentials , and also direct electric and chemical interactions. Note that the Poisson equation (1) can be seen as an equilibrium condition for this energy, i.e.,

 (5)

Besides the specific exchange terms in energy and potentials, the PNP equations (1), (2) are a standard model for electrodiffusion of charged species (cf. [Ru90]), which has well-known applications to semiconductors (cf. [VR50, MRS90]). A major difference between electrodiffusion and semiconductors is that it is easy to control the concentrations of the different species in the bath independently of the applied potential, while it is not easy (or even usually possible) to control the concentration of holes or electrons independent of the contact potential.

Boundary conditions for the ion channel problem are of the form

 (6)

Here the boundary is split into , where  is the insulated part and  denotes the normal derivative. Since there are usually two baths,  will consist of two separated components, and the boundary values are typically constant on each component. The potential  (or rather the difference of  between the left and right bath) denotes an applied voltage, and  are the bath concentrations of the free species, which are constrained by the charge neutrality condition

 (7)

Note that the confined species is usually modeled at equilibrium, which is equivalent to the zero flux boundary condition (for the constrained ions) on the whole boundary. The total number of confined particles  needs to be specified to determine , giving

 (8)

The (measured) output of a channel is the current flowing out on one side, given by

 (9)

where  is one of the connected components of  and  denotes the flux of species  given by

 (10)

where the excess potential is defined as .

We mention that the nondimensionalization and scaling of (1), (2), (6) can be performed in an analogous way to the drift-diffusion model for semiconductors (cf. [MRS90]), and for typical values one also has to expect that  is small, i.e., the Poisson equation (1) becomes a singularly perturbed problem.

The system just described has to be coupled to some model for the excess potentials. The excess electro-chemical potentials (obtained as variations of the excess energy with respect to the particle densities) include the direct interactions between the ions, usually obtained from hard-sphere models. The external confining potential describes the external forces produced by the structure of the channel on the ionic groups of the protein that make up the permanent charge. This confined permanent charge produces the selectivity of the channel.