Multicomponent conduction and selectivity of biological channels

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We consider multispecies conduction and selectivity of narrow biological filters such as KcsA [1] and NaChBac [2]. We use equilibrium statistical theory to find filter occupation and conductivities when coupled to the bath solutions with mixed types of conducting ions. The analysis of the filter conduction and selectivity conduction and selectivity is thus reduced to the analysis of the effective grand canonical distribution of ions within the filter [3], energy spectra, and density of the states within the filter [4]. The effects of energy quantization due to discrete number of ions and due to dehydration are taken into account. To account for the interaction between fluxes of different species within the channel we introduce Maxwell-Stefan theory [5] of the ion channel conduction. The fluxes of various species through the filter are obtained analytically in the limit of weak coupling. The theory is applied to derive Eisenman relations of the filter selectivity from the condition of nearly diffusion limited conduction in KscA channel.

The model predictions are compared with experimental results using self-consistent kinetic equations. The transition rates in kinetic model are derived using effective grand canonical ensemble. A good agreement with the experiment is demonstrated. An application of the theory to analysis of the channel mutation experiments are discussed.

- [1] Morais-Cabral, J. H. H., Zhou, Y. & MacKinnon, R., Nature, 414, 37-42 (2001).
- [2] Payandeh, J., Scheuer, T., Zheng, N., & Catterall, W. A., Nature, 475(7356), 353–358 (2011).
- [3] Roux, B. B., Allen, T. W., Berneche, S., & Im, W., Quarterly Reviews of Biophysics, 37(1), 182–189 (2004).
- [4] D.G. Luchinsky, W.A.T. Gibby, I.K. Kaufman, D.A. Timucin, & P.V.E. McClintock, Preprint arXiv:1604.05758v3 (2016).
- [5] Wesselingh, J. A., Vonk, P., & Kraaijeveld, G., The Chemical Engineering Journal and the Biochemical Engineering Journal, 57(2), 75–89 (1995).