

Title: Effects of (small) permanent charge and channel geometry on ionic flows via classical Poisson-Nernst-Planck models

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Abstract: We examine effects of permanent charges on ionic flows through ion channels via a quasi-one-dimensional classical Poisson-Nernst-Planck (PNP) model. The geometry of the three-dimensional channel is presented in this model to a certain extent, which is crucial for the study in this paper. Two ion species, one positively charged and one negatively charged, are considered with a simple profile of permanent charges: zeros at the two end regions and a constant Q_0 over the middle region. The classical PNP model can be viewed as a boundary value problem (BVP) of a singularly perturbed system. The singular orbit of the BVP depends on Q_0 in a regular way. Assuming $|Q_0|$ is small, a regular perturbation analysis is carried out for the singular orbit. Our analysis indicates that effects of permanent charges depend on a rich interplay between boundary conditions and the channel geometry. Furthermore, interesting common features are revealed: for $Q_0 = 0$, only an average quantity of the channel geometry plays a role; however, for $Q_0 \neq 0$, details of the channel geometry matter, in particular, to optimize effects of a permanent charge, the channel should have a short and narrow neck within which the permanent charge is confined. The latter is consistent with structures of typical ion channels.