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Examination of electroneutrality in charged, nanofluidic channels

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Abstract

Charged, nanofluidic channels containing electrolyte solution are of research interest because of their presence in many phenomena such as the transport of fluids inside the human body. Due to technological advancements, it has become possible to use long and narrow nanochannels in applications like DNA sequencing and nanofluidic diodes, which mandates the detailed study of such systems. At the nanoscale, unique physical properties are observed compared to the macroscale due to the effect of ion size and surface-dominated phenomena in such confined regimes. These unique properties have challenged the use of continuum models such as the Poisson-Nernst-Planck and Navier Stokes equations. Assumptions like complete screening of surface charge by counter-ions (i.e. electroneutrality) may not provide correct results at all levels.

In the past theoretical studies of charged, nanofluidic channels, electroneutrality is usually assumed to hold both globally (i.e. for the channel and reservoirs) and locally (i.e. for channel cross sections). However, a recent work by Levy et al., (J. Colloid Interface Sci., 579, 162-176, 2020) assuming zero-size ions, indicates that the channel may not be electroneutral, even when entrance effects are neglected. Our study goes beyond this initial investigation and employs a modified Nernst-Planck equation to examine the violation of global (GEN) and local electroneutrality (LEN). The effects of channel and reservoir dimensions, charge density on the channel surface, dielectric constants of the electrolyte and the channel, ion concentration in the reservoir, and size of ions are investigated. Violation of GEN and LEN may lie at the heart of the functionality of certain nanochannels in nature and in technological applications, and our research results provide a more rigorous examination of this phenomenon.

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