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Amer Alizadeh, Moran Wang

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Reverse Electrodialysis through Nanochannels with Inhomogeneously Charged Surfaces and Overlapped Electric Double Layers

Amer Alizadeh and Moran Wang*

Department of Engineering Mechanics and CNMM, Tsinghua University, Beijing, China

ABSTRACT: Modeling of electro-chemo-mechanical transport phenomena in simple (nanochannel) or complex (nanoporous media) geometries with inhomogeneous surface charge and overlapped electric double layers remains challenging. This bottleneck originates from lack of a comprehensive model to predict the local surface charge density based on the variable local solution properties. This work aims to propose a model, so-called representative bulk layer (RBL), which makes the chemically non-isolated solid-liquid interfaces (due to the electric double layers interaction) as isolated interfaces by introducing a local effective bulk ion concentration. Using RBL together with the electrical triple layer model to provide boundary conditions for the multi-physio-chemical transport equations (PNP+NS), we investigate the reverse electrodialysis (RED) in nanochannels. Our modeling results indicate that the length of an ion-selective membrane not only influences the ionic current but also the logarithm of the slope of current-voltage curve increases linearly with the ratio of nanochannel length to height. This interesting finding inspires us to propose a dimensionless relation for the current-voltage curve that is independent of the nanochannel dimensions. The present contribution numerical framework could shed light on the electro-chemo-mechanical transport mechanism through nanofluidic devices and membranes.

Keywords: chemically non-isolated interface, electrokinetic transport, overlapped electric double layer, reverse electrodialysis, representative bulk layer model, local surface charge

^{*} Corresponding author: mrwang@tsinghua.edu.cn

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