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הפקולטה להנדסה כימית
ע״ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar

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Room 6

Modeling of ion equilibrium and transport in membranes

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MSc Seminar

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Ion-selective membranes play a crucial role in various technological fields, e.g., water, energy, and recovery of resources. For instance, water purification and desalination technologies use membranes to selectively remove ions from water, while in energy applications such as fuel cells or electrolyzers they are used as selective ion conductors. The importance of membranes lies in their ability to separate ions, molecules, water, by blocking the transport of certain species while allowing the passage of desired ions.

However, standard theoretical frameworks, such as the Poisson-Boltzmann equation, Donnan model, or Manning model, which rely on mean-field approaches, are employed to compute averaged potentials and concentrations, from which ion permeabilities are derived. These models fail to fully explain the transport trends observed experimentally. Consequently, important effects such as ion association arise, which cannot be adequately treated within mean-field approaches.

Unlike previous models, the ‘pore model’ framework offers a non-mean-field treatment and, in addition, considers membrane heterogeneity. This model was inspired by Bjerrum's treatment of ionic solutions but accounts for the fact that ions present within water-rich pores are still strongly affected by the dielectric exclusion due to surrounding low-dielectric matrix. As a result, ion association effects are still highly significant due to the confined, low-dielectric environment, but the description of ion transport in membrane systems is much impoved, compared with the approximation of that membrane as a homogeneous medium .

The model was examined on non-charged cross-linked poly(ethylene glycol) diacrylate (XLPEGDA) hydrogels. Published experimental result of partition coefficients and conductivity were analyzed using the pore model for various salts species and concentration, including LiCl, NaCl, and KCl., and, with appropriate adjustments, a good agreement was found This research establishes a physically framework for modeling non-ideal thermodynamic interactions using membrane physical properties. That can be expanded into charged systems, improving the prediction of ion uptake, selectivity, and conductivity in commercial ion-exchange membrane.