

MECHANICAL ENGINEERING STUDENT SEMINAR

Thursday, February 02, 2023, at 13:00, Online: technion.zoom.us/BestSeminarEver

Theory of monovalent ion selectivity using capacitive deionization electrodes

Zohar Sahray

Adviser: Assoc. Prof. Matthew Suss

Capacitive deionization (CDI) is a fast-emerging membraneless water treatment technology, commonly applied to brackish water desalination and water treatments. A typical CDI cell consists of two microporous carbon electrodes separated by a dielectric separator. Predicting the storage dynamics of each species for a feedwater with multiple ions is challenging, as it depends on time, cell parameters, operational parameters, and electrolyte properties. Ion selective removal, specifically, is gaining increased attention for emerging complex water treatments. For instance, treating brackish or waste waters for direct use in agriculture requires retaining minerals such as Ca^{2+} , Mg^{2+} , and SO_4^{2-} , while selectively removing monovalent species such as Na^+ and Cl^- . Several parameters can be tuned to enhance monovalent selectivity at short charging times, including micropore chemical charge, and anode placement (upstream or downstream). To explain different selectivity mechanisms, we used a dynamic model for a flow-through electrode CDI cell which describes ion transport, ion size effects, and chemically treated electrodes. We unravel several effects which lead to monovalent selectivity and suggest a mechanistic explanation. Leveraging our mechanistic understanding, we discover and explain a novel operational regime for perfect monovalent selectivity and chemical-free ion exchange functionality using CDI.

