

Abstract Submitted
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Surface functional groups in capacitive deionization with porous carbon electrodes ALI HEMMATIFAR, DIEGO I. OYARZUN, Stanford University, JAMES W. PALKO, University of California, Merced, STEVEN A. HAWKS, MICHAEL STADERMANN, Lawrence Livermore National Lab, JUAN G. SANTIAGO, Stanford University, STANFORD MICROFLUIDICS LAB TEAM, LAWRENCE LIVERMORE NATIONAL LAB TEAM — Capacitive deionization (CDI) is a promising technology for removal of toxic ions and salt from water. In CDI, an applied potential of about 1 V to pairs of porous electrodes (e.g. activated carbon) induces ion electromigration and electrostatic adsorption at electrode surfaces. Immobile surface functional groups play a critical role in the type and capacity of ion adsorption, and this can dramatically change desalination performance. We here use models and experiments to study weak electrolyte surface groups which protonate and/or deprotonate based on their acid/base dissociation constants and local pore pH. Net chemical surface charge and differential capacitance can thus vary during CDI operation. In this work, we present a CDI model based on weak electrolyte acid/base equilibria theory. Our model incorporates preferential cation (anion) adsorption for activated carbon with acidic (basic) surface groups. We validated our model with experiments on custom built CDI cells with a variety of functionalizations. To this end, we varied electrolyte pH and measured adsorption of individual anionic and cationic ions using inductively coupled plasma mass spectrometry (ICP-MS) and ion chromatography (IC) techniques. Our model shows good agreement with experiments and provides a framework useful in the design of CDI control schemes.

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