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Application of Helmholtz EDL Theory in a Pore Network Model for Studying Capacitive Deionization

Thursday, 3 June 2021 15:10 (15 minutes)

Research interest in Capacitive Deionization (CDI) as a novel approach for water desalination has increased significantly over the past decade or more. CDI shows significant promise for desalinating brackish or low salinity waters due to a decrease in the energy consumption per ion removed compared to conventional desalination methods such as reverse osmosis [1], [2]. Capacitive Deionization works by storing ions in Electrical Double Layers (EDL) on a pair of oppositely charged porous electrodes. One of the objectives of research surrounding CDI is to increase the salt adsorption capacity of the electrodes used. Past research has shown that pore microstructure has a significant effect on CDI performance including salt adsorption capacity [3]. Pore network modelling is a tool used by researchers in other research areas to study the effect of pore structure on transport in porous media. Pore network modelling uses a resistor in series like network of pores and throats to determine transport properties. Pore network modelling has yet to be utilized in capacitive deionization modelling work. Available capacitive deionization modelling work couples transport equations with appropriate EDL model. The uptake rate of ions into the electrical double layer is determined from EDL theory [4]. It is to the best of our knowledge that no one else has applied EDL theory to a pore network model. Therefore, before a pore network model of a full CDI cell can be developed, appropriate EDL theory must be applied to a pore network model. One such EDL model is the famous Helmholtz model. This was, to the best of our knowledge, the first EDL model to be used in CDI modelling work [5]. Helmholtz assumed a capacitor like EDL structure where charges near the electrode-electrolyte interface are separated and equally compensated. In this work, the application of Helmholtz EDL theory to a pore network model is demonstrated. Electroneutrality in the macropores, equal cation and anion diffusivities, and no flow was assumed simplifying our capacitive deionization model to a transient fickian diffusion algorithm with Helmholtz reaction term coupled with a transient ionic transport algorithm [6]. A pore network simulation was conducted on a small two-dimensional network of 36 pores subdivided into anode, cathode, and spacer pores. OpenPNM was used to do the pore network simulation while COMSOL Multiphysics was used as reference solution to validate the implementation of Helmholtz. The conclusions of this work was that the pore network model correctly applied Helmholtz EDL theory. This is the start of using pore network modelling to study capacitive deionization.

Time Block Preference

Time Block C (18:00-21:00 CET)

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