Capacitive Deionization for Desalinating Complex Streams

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Abstract

Capacitive deionization (CDI) is a desalination technology which is based on the storage of ions in the electrical double layer of a pair of oppositely polarized porous carbon electrodes, which are usually assembled using activated carbon particles (Figure 1). It is efficiently deployed for desalinating water with moderate salt content (eg in domestic water softening)[1]. To broaden its application range, CDI of 'mixed' streams - ranging from multi-ion solutions of inorganic salts to more complex mixtures of both inorganic and organic compounds such as biomass hydrolysates [2] - is investigated.

To date, however, there are no models available which can reliably predict preferential removal of ions from multi-ion streams by means of CDI, or which can be used as a design tool for improving e.g. cell design geometries. Several aspects make CDI a challenging process to model: it is a discontinuous (sequences of charging and discharging steps) and multiscale (macroscale, interparticle and intraparticle scale, Figure 2) problem that involves mass transport through charged porous media and which - due to operation at voltages much above the thermal voltage - exhibits highly non-linear behavior of the electrical double layer [4]. The use of ion exchange membranes in CDI cells strongly improves their performance, but adds a further layer of complexity to the modelling effort.

VITO is in the process of developing a COMSOL Multiphysics® model which incorporates these different aspects. Starting from a base model using empirically corrected mass transport coefficients and a (weakly non-linear) Gouy-Chapman based description of the electrical double layer (Figure 3), we are sequentially incorporating a more sophisticated effective medium approximation for the porous transport, more highly non-linear EDL descriptions, solvent effects, laminar mixing in the feed channel by the presence of spacers (Figure 4), the occurrence of electron-transfer reactions, etc. Coupling a microscale model component to the macroscale model component that represents the CDI cell will allow to more accurately model the non-equilibrium behavior of the electrical double layer in micropores whose diameter is smaller than the Debye length scale.

Reference

[1] Huyskens C et al. Capacitive deionization for water treatment: Screening of key performance parameters and comparison of performance for different ions. Desalination 2013;328:8–16.
[2] Huyskens C et al. Membrane capacitive deionization for biomass hydrolysate desalination. Sep Purif Technol 2013;118:33–9.
[3] Porada S et al. Review on the science and technology of water desalination by capacitive deionization. Prog Mater Sci 2013;58:1388–442.
[4] Kilic M et al., Steric effects in the dynamics of electrolytes at large applied voltages. I. Double-layer charging. Phys Rev E 2007;75.

Figures used in the abstract

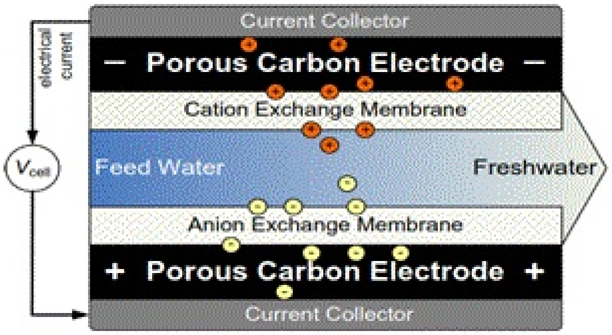

Figure 1: Principle of CDI [3].

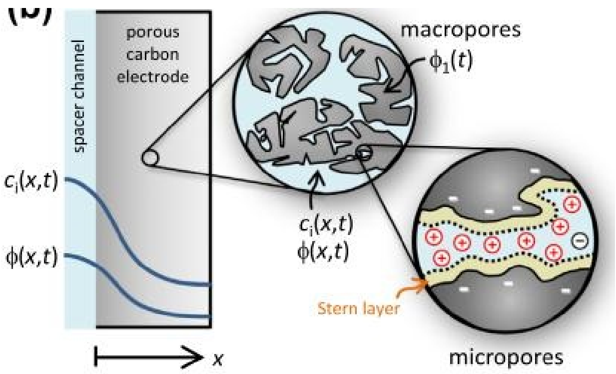

Figure 2: Relevant scales for a bimodal hierarchical porous electrode [3].

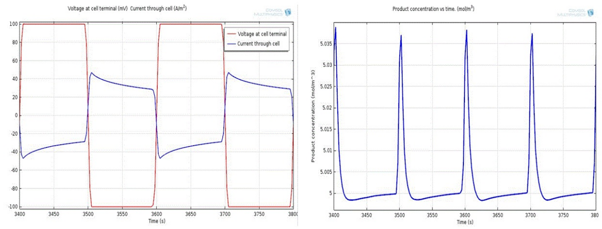

Figure 3: Applied voltage, current response and product concentration for a basic CDI model (constant voltage CDI with reverse voltage desorption)

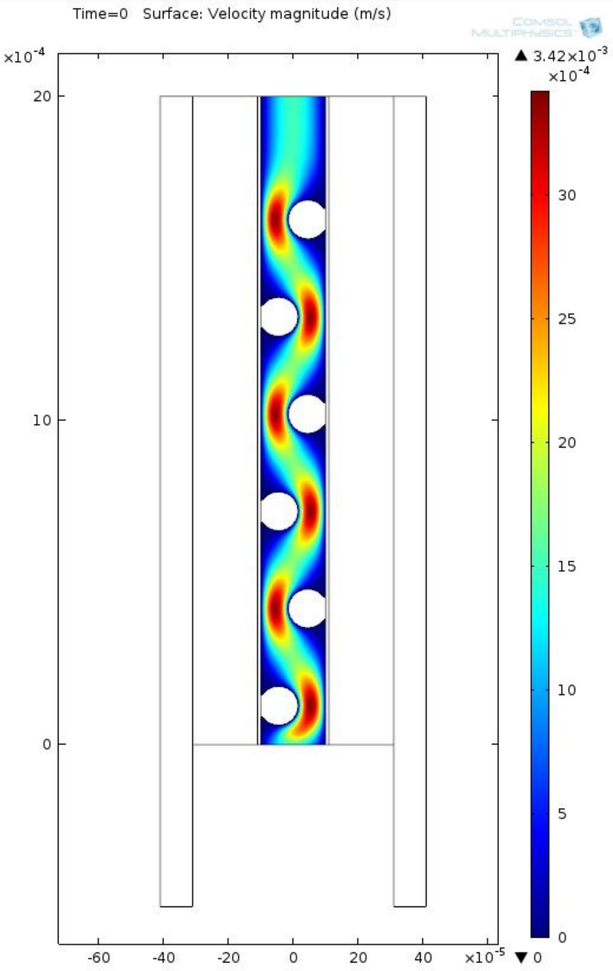

Figure 4: Cell geometry and fluid flow velocity through spacer channel.