Modeling the Adsorption of Ions on Electrodes in a Flow Cell

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Abstract

A variety of applications, like membrane separation processes, batteries, electrochemical cells and fuel cells need a good understanding of the ion transport in electrolytes under concentration and electrochemical potential gradients. It is also possible to bring about charge based separation in response to an applied electric field, like in the case of electrochemical cells and electrosorption based separation processes.

In the present work, we have modeled a flow in a channel (Figure 1) to study electrosorption of ions on electrodes placed on the opposite walls using COMSOL Multiphysics®. The system is modeled with Poisson-Nernst-Planck (PNP) equation, which is a basic continuum model for simulating ionic flow in an open ion channel along with incorporating Langmuir model for adsorption of ions on the electrodes. The extent of variation in ion electrosorption from the feed solution (Figure 2) has been studied at various applied potential and solution velocity. The preferential adsorption of different ions is also modeled using aqueous solutions containing $NaCl$, $NaHCO_3$, $Ca(HCO_3)_2$ and $CaCl_2$.

It is seen that increasing the applied potential as well as decreasing the flow enhances the electrosorption. Simulations were also conducted with different cations (Na^+, Ca^{2+}) and anions (Cl^-, HCO_3^-). A similar trend was observed with applied potential and flow rate. The model will be extended further to include the effect of porosity and the effect of double layer capacitance.

Reference

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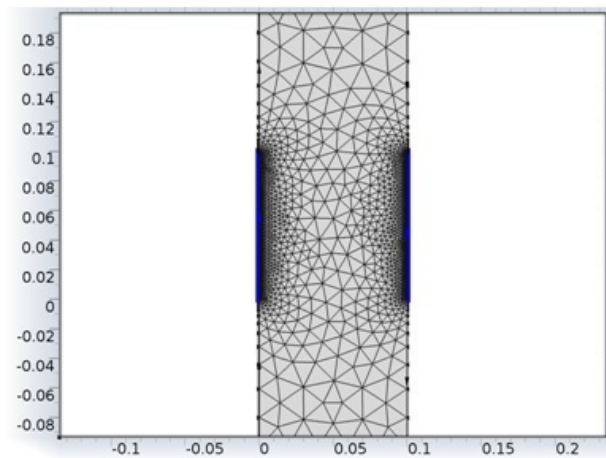
Figures used in the abstract

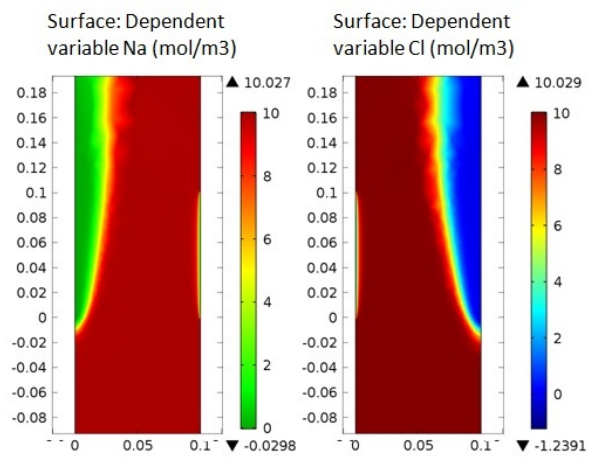**Figure 1**: Flow cell with distributed mesh.

Figure 2: Concentration profiles (Na+ and Cl-) showing ion adsorption on electrodes.