Modeling, Simulation and Characterization of Ionic Transport and Impedance in PEM Fuel Cells

Investigators: Peter M. Pinsky, Mechanical Engineering; David M. Barnett, Materials Science and Engineering and Mechanical Engineering, Stanford University

Sponsor: Global Climate and Energy Project

Objective: Solid polymer fuel cells promise to be an efficient power source for mobile and stationary applications with the potential for a greatly reduced environmental impact. The investigators will examine the properties of solid polymer membranes through modeling of ion transport, impedance, diffusion and atomic force microscopy imaging. Increased understanding of the ion behavior at the Nernst diffusion layer of the membrane surface could enable new classes of solid polymer fuel cell membranes with increased mass transport.

Background: Ion-selective membranes have found a wide range of applications in electrochemical technologies, including proton exchange membrane fuel cells (PEMFCs). However, the ionic diffusion behavior under current load conditions is not completely understood. It is known that concentrations of individual ions exhibit great variation across the Nernst diffusion layer at the membrane surface and it is thought that these local ion changes significantly influence mass transport across the membrane.

Impedance measurements, quantifying the response of a material to an applied varying voltage, have become a standard procedure to determine membrane properties. Factors contributing to the experimental results are poorly understood, and hence modeling the physical processes involved in the impedance measurement could greatly enhance the usefulness of this technique.

Atomic force microscopes are used for imaging small-scale surfaces, but the dynamics of the related measurements are not well defined. The charged tip of an atomic force microscope interacts with surface charges and the space charge layer on surfaces such as membranes. Since membrane charge characteristics may be inhomogeneous, imaging these variations could prove crucial to understanding the functionality of membranes. Research is needed to obtain a better understanding of the relationship between the image obtained and the charge distributions present on the membrane.

Approach: Combining the Nernst-Plank expression for ion transport with the Nernst-Einstein relation for ion mobility would allow extensions of existing ion transport models to two and three dimensions. Diffusion of ions and solvent through the membrane can also be considered. Ion and solvent transport in a typical solid polymer membrane is illustrated in Figure 1. The model will include electrochemical kinetics, current distribution, hydrodynamics, and multi-component transport, allowing for general geometry and boundary conditions as well as an accurate treatment of nonlinearities.

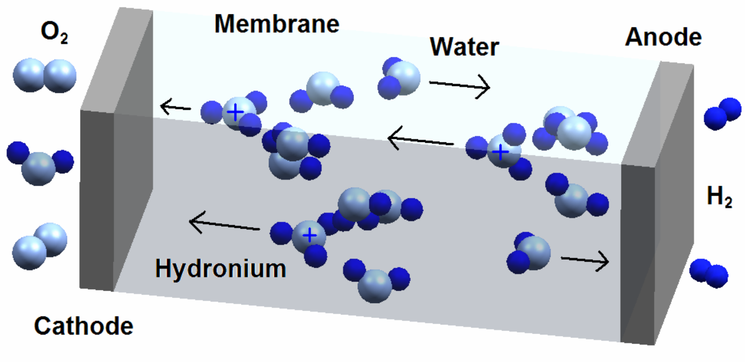

Figure 1: Hydronium ion transport and solvent diffusion in a solid polymer membrane fuel cell

Simulations of impedance measurements in two and three dimensions including nonlinear regions of high electric field will be performed. The models will serve to improve interpretation of measurement results and assist in the development of scaling laws for fuel cell performance based on impedance measurements.

In order to more effectively use an atomic force microscope for the investigation of fuel cell membranes for quantitative imaging, a model of the mechanical and electrical dynamics of the probe tip will be developed. Images obtained through measurement will contain much spatial and temporal information about the sample being measured. This model will assist in the deconvolution of membrane property information from the resulting images. A hypothetical example comparing atomic force microscopy measurements and the actual geometry of a circular array of charges is presented in Figure 2. The model can be verified by, for example, assuming various charge distributions, constructing an image catalogue for comparison with observation, and looking to obtain matches.

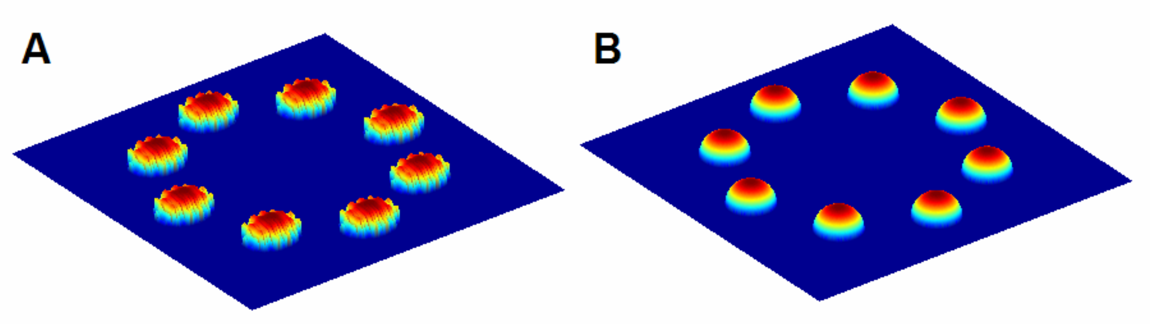

Figure 2: Hypothetical example of atomic force microscopy data (A) obtained from scanning a charge array (B).

Contact: Peter Pinsky, pinsky@stanford.edu