

Modeling a Non-Flooding Hybrid Polymer Electrolyte Fuel Cell and Related Diffusion-Migration-Reaction Systems

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Abstract

Introduction: Understanding the mass and charge transport behavior of heterogeneous systems that include diffusion, migration, and reaction of ions is important in fuel cells, batteries, and other electrochemical applications. Here, a numerical model for charged species transport and reaction has been developed to simulate the electrochemical behavior of a novel type of "non-flooding" hybrid polymer electrolyte fuel cell, and further extended to a more generalized system. The non-flooding cell consists of proton exchange membrane and anion exchange membrane half-cells which have been pressed together on either side of a porous intermediate layer. Such a design is intended to improve the water management inside the fuel cell by shifting water production from the electrodes to the porous layer, allowing excess water to be wicked to the exterior of the cell. [1] While the design has been experimentally validated, initial performance was poor compared to conventional fuel cells. This was hypothesized to be due to a large ionic resistance contributed by the porous layer. [2] Use of COMSOL Multiphysics: A one-dimensional, time-dependent Poisson-Nernst-Planck model was developed using the Transport of Diluted Species physics with migration and reaction terms, as well as the Electrostatics physics. The model was used to determine the ionic resistance of the porous layer under varying current loads. The effects of varying the thickness, porosity, and temperature of the porous layer were also investigated. Results: Resistance values from the model agreed closely with experimental results for the effective resistance of the entire fuel cell, confirming the hypothesis that nearly all of the cell's resistance is due to the porous layer (Figure 1). Resistance was found to increase with temperature and with porous layer thickness. It was observed that the porous layer behaves as a non-Ohmic electrolyte since the number of charge carriers is current-dependent. It was further determined that electron conduction in the solid scaffold of the porous layer is crucial to maintaining electroneutrality, resulting in extremely high ionic resistance when the layer is electronically insulating. To illustrate its potential wider applicability, the model was generalized by allowing for the generation of insoluble reaction products. In the system modeled, aqueous solutions of silver nitrate and sodium chloride are introduced to opposite sides of a porous membrane and the precipitation of solid AgCl is allowed via the reaction $\text{Ag}^+(\text{aq}) + \text{Cl}^-(\text{aq}) \rightarrow \text{AgCl}(\text{s})$. The accumulation of precipitate in the pore space is presumed to reduce the local porosity. This behavior was approximated in the model by reducing the effective ionic diffusivities commensurate to the ratio of AgCl concentration to its known molar volume. As the reaction zone becomes choked with precipitate, the ionic conductivity was found to drop off sharply due to this diffusivity reduction. Conclusion: In this presentation, the utility of COMSOL Multiphysics in

determining the behavior of nonlinear systems involving diffusion, migration, and reaction of ions will be demonstrated. The ability to determine both local and global behaviors will be shown. More complex systems related to multiphase electrochemistry are being explored and will be discussed briefly.

Reference

1. W. Shen, F.-Y. Zhang, A.K. Prasad, J.L. Hertz, *Electrochem. Soc. Trans.* 33 (2010) 2011–2016.
2. W. Shen, A.K. Prasad, J.L. Hertz, *Electrochem. Solid-State Lett.* 14 (2011) B121–B123.

Figures used in the abstract

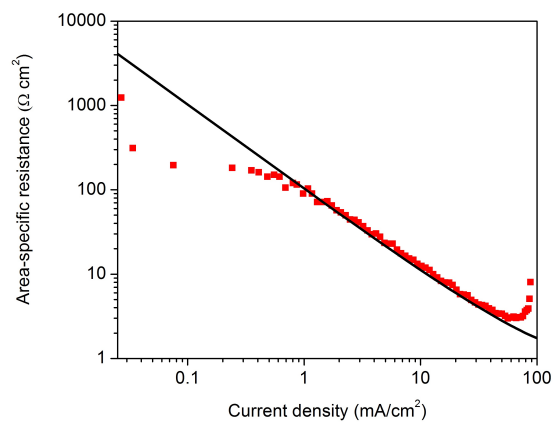


Figure 1: Modeled area-specific resistance of a 100 μm-thick hybrid fuel cell porous layer at 30°C as a function of current density, compared to experimental resistance data for the entire hybrid fuel cell under the same conditions.