Investigation of Transport Phenomena in PEMFC through 1-D Macro-homogeneous Model

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INTRODUCTION

Proton exchange membrane fuel cells (PEMFCs) show great promise thanks to high efficiency, good energy density, and lack of emissions. However, high cost and limited durability remain significant barriers to widespread adoption. The most effective way to reduce PEMFC cost is by improving power density, thereby reducing the required stack size and the cost associated with every component. Optimizing power density requires a very detailed understanding of transport losses, water management, and PEMFC degradation.

To study transport losses, water management, and the effects of PEMFC degradation, a 1-D macro-homogeneous model of the PEMFC has been developed, incorporating a flooded agglomerate model of oxygen transport through the ionomer in the cathode catalyst layer. The model is used to simulate electrochemical impedance spectroscopy (EIS), and several processes are identified that have important effects on impedance.

MODEL DESCRIPTION

The overall model consists of seven component models describing the various layers of the PEMFC: flow fields, gas diffusion layers, catalyst layers, and the membrane. A 0-D mass balance is used for the flow fields to incorporate the effects of gas stoichiometry. The anode is simulated as a 0-D fully reversible hydrogen electrode. The remaining components are simulated as 1-D macro-homogenous domains. Transport in the membrane and the ionomer phase of the cathode catalyst layer is simulated using the concentrated solution theory model of Fuller and Newman(1). Gas transport is treated with the Stefan-Maxwell multicomponent diffusion equations. Oxygen transport through the ionomer film in the cathode catalyst layer is modeled with a spherical agglomerate model, incorporating an active core and an inactive ionomer film. The model is transient, allowing the calculation of impedance through direct application of a waveform and analysis of the response.

RESULTS

A typical Nyquist plot of impedance as simulated by the model is shown in Figure 1. The double layer capacitance has been excluded to improve the resolution of individual processes. When double layer capacitance is included, a direct comparison to experimental results can be made. Several membrane thicknesses are investigated to reveal the impact of water transport in the membrane. A high frequency loop is observed due to oxygen diffusion into the agglomerate. At low frequencies, two loops overlap, with the relative size and position influenced by the membrane thickness. These overlapping loops are caused by oxygen diffusion in the gas diffusion layer and water transport in the membrane. As the membrane thickness is increased, the water transport loop grows and shifts to lower frequencies. This can be observed in the Bode phase plot in Figure 2, where the 50 µm membrane shows a noticeable low frequency peak.

Experimental EIS spectra are typically analyzed through equivalent circuits. The oxygen diffusion process is usually included through a Warburg impedance component. However, the membrane hydration process identified at low frequencies is often neglected. By simulating impedance with a PEMFC model instead of an equivalent circuit model, a more complete picture of the impedance response is obtained.

ACKNOWLEDGMENTS

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REFERENCES

1. T. F. Fuller and J. Newman, J. Electrochem. Soc., **140**, 1218 (1993).

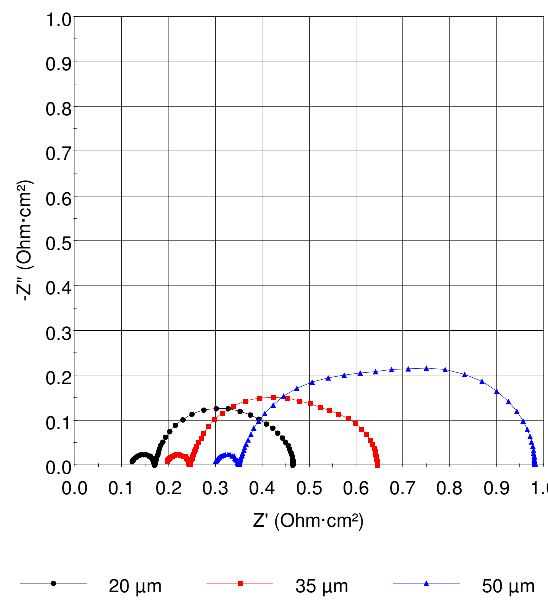

Figure 1. Nyquist plot of imaginary vs. real impedance for varying membrane thickness. Cell temperature was 60 °C, with anode and cathode (air) gas stoichiometries of 1.2 and 1.5, respectively. Inlet gases were at 50% relative humidity.

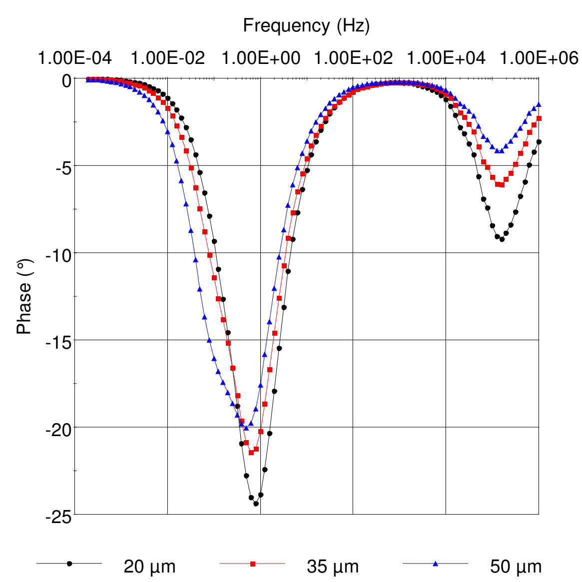

Figure 2. Bode phase plot of phase vs. frequency for verying membrane thickness.