MODELING THE DIRECT METHANOL FUEL CELL ANODE

Claudia Diniz, Robert Moore, P Badrinarayanan
Fuel Cell Vehicle Modeling Program
University of California, Davis, CA 95616

Piotr Zelenay
Materials Science and Technology Division
Los Alamos National Laboratory
Los Alamos, NM 87545

This paper describes an anode model for the direct methanol fuel cell (DMFC). It is a steady state, isothermal model, in which electrochemical reaction rates are governed by the Tafel kinetics. Mass transfer and diffusion are considered in the transport equations. The main purpose of the model is to calculate the anode potential loss and methanol crossover current density using cell current density, concentration and flow rate of methanol as inputs. The model also calculates the flux of methanol at the exit of the anode, as well as methanol concentration at the anode catalyst layer and at the membrane-catalyst interface.

The transport of water, methanol and protons is theoretically described and characterized. Detailed treatments of the liquid diffusion and the catalyst layers are provided. The model findings are compared with the experimental data obtained at Los Alamos National Laboratory under the same conditions as those used in the model.

The model is capable of predicting the DMFC anode potential loss and methanol crossover. The Model is also capable of predicting the mass transport effects for a higher current range, but there was no data available for validation of this region. Further experimental validation of the model is planned as more relevant state-of-the-art anode and cell performance data become available.

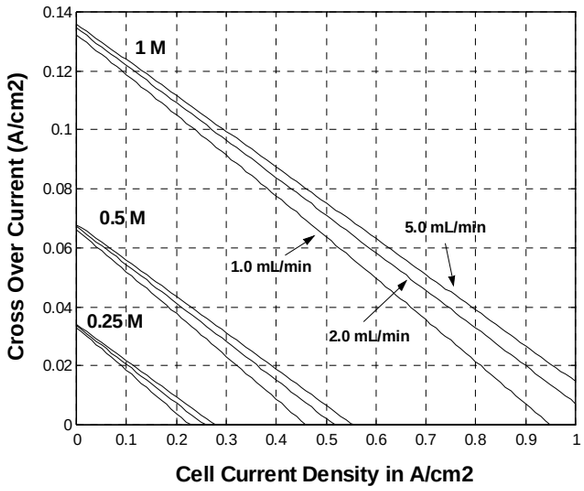

Figure 1: Influence of methanol concentration and flow rate on methanol crossover. The order in which plots for the anode feed rates of 1.0, 2.0 and 5.0 mL min^{-1} appear in the graph is the same for all three concentrations of methanol. Cell area: 5 cm^2.

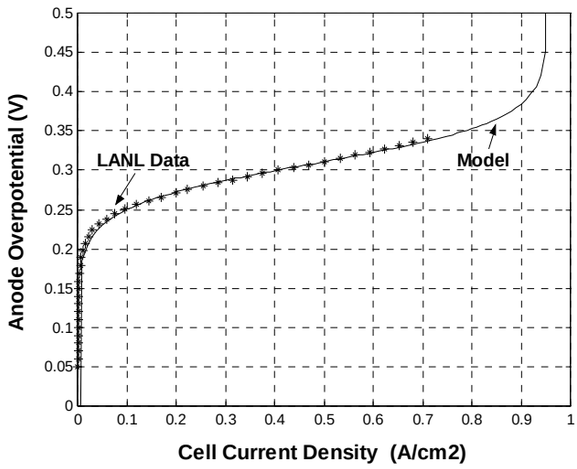

Figure 2: Model-predicted and measured dependence of the anode overpotential on cell current density; methanol concentration 1.0 M, methanol flow rate 1.0 mL min^{-1}; cell area 5 cm^2; cell temperature 100°C.

References:

S. F. Baxter, V. S. Battaglia and R. E. White, *J. Electrochem. Soc.*, **146**, 437 (1999).

X. Ren, T. E. Springer and S. Gottesfeld, *J. Electrochem. Soc.*, **147**, 92 (2000).

T. E. Springer, M. S. Wilson and S. Gottesfeld, *J. Electrochem. Soc.*, **140**, 3513 (1993).

S. C. Thomas, X. Ren and S. Gottesfeld "Direct Methanol Fuel Cells: Catalyst Ionomer Content and Anode Performance" in *Proton Conducting Membrane Fuel Cells (Second International Symposium)*, S. Gottesfeld, T. F. Fuller and G. Halpert (Eds.), Proceedings Volume 98-27, pp. 267-279, The Electrochemical Society, Pennington, New Jersey, 1999.