Using CFD to Understand the Effects of CO Poisoning in a PEMFC

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Introduction

Murthy et al.[1] have shown the effect of temperature and pressure on the tolerance of MEAs to relatively high concentrations of CO and they reported rates of poisoning for these conditions. In another paper[2] Murthy et al. showed that effect of gas diffusion layer (GDL) depends on the concentration of CO in a H_2 mixture. Bender[3] has experimentally studied CO distributions with a segmented electrode. Recently Nwoga and Van Zee[4, 5] used the steady state data from Refs. 1 and 2 and a modified model similar to that of Springer et al.[6] to estimate parameters for adsorption isotherms and of CO and H_2. They used these parameters to predict the measured rates of poisoning and recovery as a function of temperature, pressure, and CO concentration.

The objective of this work is to use a three-dimensional (3-D) model to predict the effect of CO on PEMFC performance by combining the CO model of Nwoga and Van Zee[4, 5] and the 3-D PEMFC model of Lee et al.[7]. This combined model includes flow behavior, species transport, heat transfer, water phase change, and CO adsorption isotherms. This model allows for the prediction of the distributions of CO coverage and H_2 coverage on the available platinum and ruthenium catalysts. This model is based on equilibrium and rate constants and their changes with temperature and pressure.

Figure 1 shows typical experimental performance curves for a PRIMEA® MEA for various CO concentrations.[2] The model predictions will be compared with these data for an experimental 25-cm^2 PEMFC geometry (triple serpentine flow-field). Figure 2 shows the predicted current density and CO distributions for a straight channel 10-cm long PEMFC. In that figure the anode catalyst is exposed to 1000 ppm CO concentration at an average current density of 0.45 A/cm^2 for a cell voltage of 0.4 V. The average CO surface coverage in Figure 2b is 0.67.

Numerical Procedure

A control volume technique based on a commercial computational fluid dynamics was used to solve the coupled governing equations. The software requires specification of species source terms, electrochemical, water phase change, and new subroutines were written to model the adsorption isotherms and isobars for the CO poisoning effect.

Acknowledgment

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References

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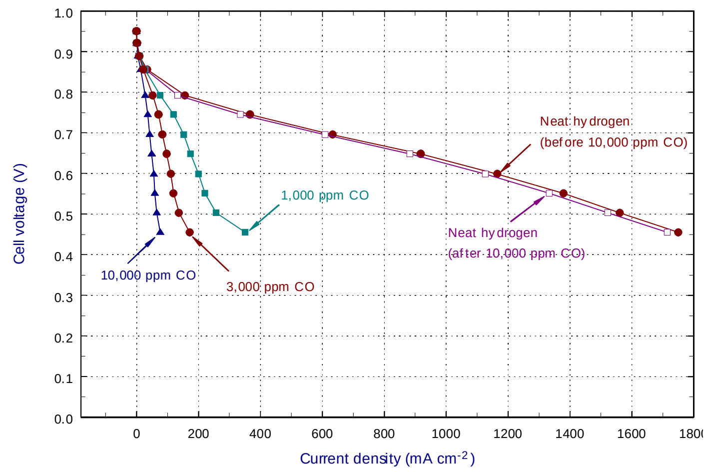

Figure 1. Effects of CO on the performance of a PEM fuel cell (Tcell = 70 °C, T_H(A/C) = 85/75 °C, P(A/C) = 101/101 kPa)

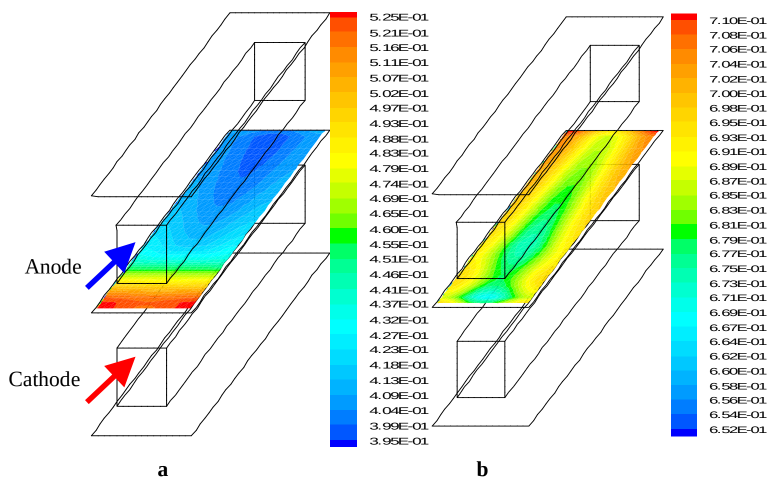

Figure 2. The distributions of local current density (Fig. 2a) and local CO coverage (Fig. 2b) on anode catalyst surface of 10-cm straight channel long PEMFC at Vcell of 0.4 V correspond to Iavg of 0.45 A/cm^2 for 1000 ppm concentration of CO.

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