## Modeling CO poisoning and O<sub>2</sub> bleeding in PEM Fuel Cells

Qiangu Yan, Qinyun Liu, Junxiao Wu<sup>\*</sup> Center for Advanced Vehicular Systems, Box 5405, Mississippi State University, MS 39762-5405

CO is one of the trace components in hydrogen fuel which is produced from hydrocarbon reforming process. CO can adsorb at Pt surface due to its special molecular structure and thus blocks the access of new reactant molecules to the surface active centers. Therefore, CO is a severe poison to Pt catalyst in PEM fuel cells; it reduces fuel cell performance significantly even at levels of 1-10 ppm. A fuel cell which would be useful for commercial applications would preferably be tolerant of CO levels at 100 ppm or greater. There are several ways to mitigate the CO-poisoning. Researchers have been able to formulate more tolerant catalysts by adding metals like ruthenium to the platinum [1]. A second option is to operate fuel cell at higher temperature such as 120 °C [2]. Bleeding a trace of O2 into anode fuel flow is the another method to reduce CO poisoning [3].

A multi-resolution [4,5] mathematical transient model of a PEM fuel cell anode catalyst layer has been developed in this study. Adsorption, desorption and electro-oxidation of carbon monoxide and hydrogen, as well as the heterogeneous oxidation of carbon monoxide and hydrogen with oxygen are modeled to simulate CO poisoning and oxygen bleeding.



Figure 1. Influence of CO concentrations on PEMFC performance.



Figure 2. CO poisoning and recovery process over a PEM fuel cell



Figure 3. Effects of O<sub>2</sub> bleeding on PEMFC performance

Reference

- Schmidt VM, Brokerho! P, Hohlein B, Menzer R, Stimming U. 1994, *Journal of Power Sources* 49(1):299-314
- Zawodzinski TA, Karuppaiah C, Uribe F, Gottesfeld S. 1997. In *Electrode Materials and Processes for Energy Conversion and Storage I*, Srinivasan S, McBreen J, Khandkar AC, Tilak VC (eds); Proceedings of the Electrochemical Society, vol. 97-13. The Electrochemical Society, Inc.: Pennington, 139-146.
- 3. Wilson M, Derouin C, Valerio J, Gottesfeld S. 1993. Proceedings of the Intersociety Energy Conversion Engineering Conference 1:1203-1208.
- Wu, J. and Liu, Q., 2003 "Integrated Multiresolution Fuel Cell Simulation," in the 204<sup>th</sup> ECS Proceedings of Power Sources for Transportation Applications, Landgrebe, A.R., ed., in press.
- Wu, J. and Liu, Q., 2004 "Simulation Aided PEM Fuel Cell Design and Performance Evaluation," First International Conference on Fuel Cell Development and Deployment, Storrs, CT.

<sup>\*</sup> Corresponding author, e-mail: jwu@cavs.msstate.edu