## An Isothermal Model for Predicting Performance Loss in PEMFCs from BOP Leachates

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In the development of proton exchange membrane fuel cells (PEMFCs), the cost of balance of plant (BOP) materials and their effect on PEMFC durability can retard commercialization.<sup>1</sup> One opportunity to decrease these costs would be to use off-the-shelf materials rather than custommade materials if leachates from the less expensive materials do not affect performance and lifetime. To understand contamination mechanisms and their impacts on PEMFCs, experimental studies conducted and found the sensitivity of performance to the low levels of contamination.<sup>2-9</sup>

A model for contamination of a PEMFC which includes adsorption on the Pt catalyst, absorption into the membrane, and ion-exchange with ionomeric components is presented. The model predictions for three sources of voltage (i.e., performance) loss account for two-dimensional timedependent contamination along the channel and into the membrane as shown in Figure 1. The model is developed by considering the well-known chemical engineering concepts of Langmuir adsorption, partition coefficients, plug flow reactors (PFRs), and dimensionless analysis. The phenomena are shown to be controlled by three important dimensionless groups: a Damhköler number for the contamination reaction rate, a capacity ratio, and a coverage ratio for each contamination mechanism. Also, techniques are presented for translating the liquid phase thin film rotating disk electrode measurements of isotherms to the required in-situ parameters of the gas-phase model.<sup>9</sup>

For typical parameters, the predicted voltage loss in the electrode by an ion-exchange mechanism shows slower reaction rates but greater performance losses than other mechanisms. More broadly, the model also provides a tolerance limits for contamination.



Figure 1. Schematic of a channel and a control volume for a model (a) electrode (b) membrane contamination

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## References

[1] K. O'Leary and B. Lakshmanan Paper #1036 presented at the 220th ECS Meeting & Electrochemical Energy Summit in Boston, MA, Oct. 13, 2011.

[2] H. N. Dinh, H. Wang, C. S. Macomber, K. O'Neil, and KC Neyerlin, Paper #34 presented at the 243<sup>rd</sup> ACS National Meeting, San Diego, CA 2012.

[3] C. S. Macomber, J. Christ, H. Wang, B, S. Pivovar and H.

N. Dinh, ECS Trans., 50(2), 603-618, (2013).

[4] Md. Opu, M. Ohashi, H. Cho, C. S. Macomber, H. N. Dinh, J. W. Van Zee, ECS Trans., 50(2), 619-634 (2013).

[5] M. Das, M. Ohashi, K. O'Leary, B. Lakshmanan, R.Reid, C.S. Macomber, H.Wang, H. Dinh, and J. W. Van Zee,

Abstract #1039, 220<sup>th</sup> ECS Meeting, Boston, MA (2011).

[6] H. Cho, M. Ohashi, and J. W. Van Zee, ECS Trans. 41(1), 1487-1499 (2011).

[7] H. Cho, Md. Opu, M. Ohashi, and J. W. Van Zee, Paper #1295, presented at the 222<sup>nd</sup> ECS Meeting & Honolulu PRiME 2012, HI, Oct. 09, 2012.

[8] H. Cho, O. Masato, and J. W. Van Zee, Electrochim. Acta. (2013) Submitted

[9] H. Cho, Ph.D. dissertation, Department of Chemical Engineering, University of South Carolina 2013.