A Computational Study on the Effect of Steam on SOFC Anode Degradation due to Phosphine

Hayri Sezer, S. Raju Pakalapati, Huang Guo, Bruce Kang, Ismail B. Celik
National Institute for Fuel Cell Technology, West Virginia University, Morgantown, WV

Introduction

- Experimental results show that electrochemical degradation of anode supported SOFCs due to PH$_3$ is dependent on steam concentration of fuel
- A possible mechanism for this dependence is formation of different secondary phases of Phosphor under wet and dry conditions
- An existing degradation model is modified to take into account these new phenomena.
- Voltage-Current (V-I) curves and impedance behavior was obtained based on porosity and conductivity changes during the gradual degradation process

Model Description

- 1D Degradation model computes the gas phase diffusion, contaminant coverage, and the cell potential along the anode thickness during the gradual degradation process.
- Experimental results are used to calibrate model parameters
- The parameters are different for wet and dry conditions

Model Equations

Monolayer adsorption mechanism

\[
X + Ni \stackrel{k_{f,x}}{\rightleftharpoons} Ni - X
\]

H$_2$ + 2Ni $\rightleftharpoons k_{a,o} / k_{a,x} \times 2(Ni - H)$

1D transport equation for the coverage (of species $i$)

\[
\begin{align*}
\frac{\partial \theta}{\partial t} &= D_\theta \left( \frac{\partial^2 \theta}{\partial z^2} + \omega_{\theta} \right) \\
\omega_{\theta} &= k_{f,x,y} \theta_{\alpha} - k_{a,x} \theta_{\alpha,x} \\
\omega_{\theta_{\alpha,x}} &= k_{f,x,y} \theta_{\alpha} - k_{a,x} \theta_{\alpha,x} \\
\theta_{\alpha,x} + \theta_{\alpha} + \theta_{\alpha,H} &= 1
\end{align*}
\]

Gas phase Species Distribution Equation in Porous media

Activation loss from BV

Eq. with modified exchange current density

\[
J_{o,H_2} = c_i \left( \frac{y_{H_2,act}}{y_{H_2,ref}} \right) \exp \left( - \frac{E_{act,H_2}}{R_T} \right) \left( 1 - \theta_{\alpha,H_2} \right)
\]

Charge conservation equation

\[
\frac{1}{c} \frac{\partial \phi}{\partial t} = \frac{\partial}{\partial z} \left( \frac{\partial \phi}{\partial z} \right)
\]

Results

- Conductivity $\sigma = \sigma_0 \left( 1 - \theta_{\alpha,X} \right)^{\phi}$
- Porosity $\varepsilon = \varepsilon_0 \left( 1 - \theta_{\alpha,X} \right)^{\phi}$

Conclusions

- Sensitivity of anode degradation to steam concentration is attributed to different Ni-P secondary phases formed under wet and dry conditions
- Different parameters are used in the model for wet and dry cases to account for secondary phase differences.
- The predicted V-I curves show that during the degradation, the limiting current for the cell decreases gradually and the activation losses also increase.
- The impedance curves also show that series resistance increased gradually whereas the activation losses increase abruptly after remaining more or less constant for 100 hours.