Electrochemical Evaluation of a Planar SOFC under Phosphine Induced Degradation

Hayri Sezer[1,2] , Tao Yang[1,2] and Ismail B. Celik[1,2]
[1]National Energy Technology Laboratory, U.S. Department of Energy; [2]Mechanical and Aerospace Engineering Department

Office of Research and Development

Introduction

- Anode performance degradation due to fuel contaminants is the main drawback to utilization coal syngas in SOFC.
- Accelerated testing using high contaminant concentrations in fuel is often employed to quickly characterize the degradation behavior.
- A degradation model once calibrated/validated against accelerated tests could be used to predict degradation rates and/or cell-life time.
- The degradation behavior inside a planar cell is studied under 0.1 A/cm^2 current load and 10 ppm phosphine
- To assess the overall cell performance at any given degradation stage, the electrochemical behavior (polarization and impedance) of the cell, is analyzed.

Model Description

- DREAM-SOFC, a transient 3D model for SOFCs developed at WVU, is used

3D transport equation for the coverage (of species *i*) and degradation model (Cayan et al. 2011)

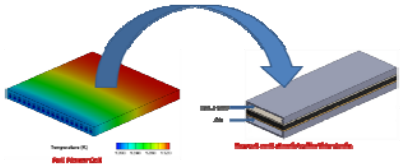
$$\frac{\partial \theta_i}{\partial t} = D_\theta \nabla^2 \theta_i + \omega_{\theta_i}$$

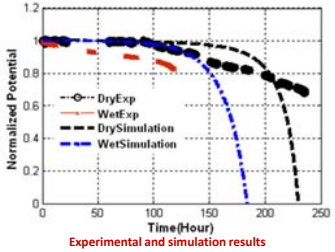
Source term for contaminants $\omega_{\theta_X} = k_{f,X} y_X \theta_{Ni} - k_{b,X} \theta_{Ni-X}$

- **Porosity as a function of Coverage** $\varepsilon = \varepsilon_0 (1 - \theta_{Ni-X})^p$
- **Exchange current density as a function of coverage**
- **Activation over potential is calculated via Butler-Volmer equation**
- **Model parameters are calibrated with one-dimensional degradation model using results from accelerated button cell testing.**

$$H_2 + 2Ni \underset{k_{b,H_2}}{\overset{k_{f,H_2}}{\rightleftharpoons}} 2(Ni-H)$$

$$PH_3 + Ni \underset{k_{b,PH_3}}{\overset{k_{f,PH_3}}{\rightleftharpoons}} Ni-PH_3$$





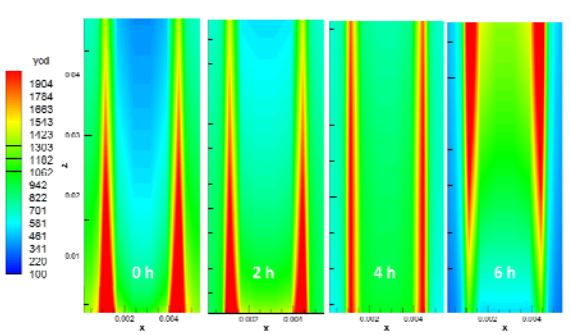
Experimental and simulation results of Button cell degradation

Geometry Parameters of the planar SOFC	
Anode thickness	50 μm
Electrolyte thickness	170 μm
Cathode thickness	50 μm
Fuel channel height	2.5 mm
Air Channel height	2.5 mm
Cell length	5 cm
Current collector width	1.28 mm
Channel width	3 mm
Conditions and parameters for simulation	
Fuel inlet composition (Mole fractions)	99.99% H2 + 10ppm PH3
Fuel inlet temperature (K)	1073
Air inlet Composition (Mole fractions)	21% O2
Air inlet temperature (K)	1073
Pressure (atm)	1.01325
External Boundaries	Adiabatic
Current density (A/cm2)	0.1
Fuel Utilization (%)	12.5
Air Utilization (%)	1.25
Anode porosity	0.480
Cathode porosity	0.45

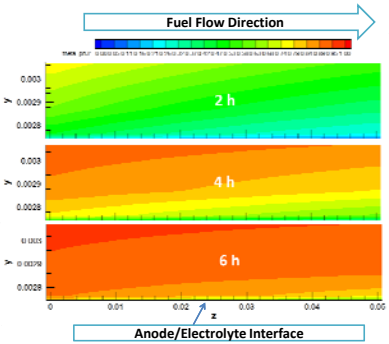
Contact

Dr. Ismail Celik
MAE Department, West Virginia University, Morgantown, WV26506
Ph: 304 293 3209 Fax: 304 293 6689
E-mail: ismail.celik@mail.wvu.edu
URL: http://cfd.mae.wvu.edu/

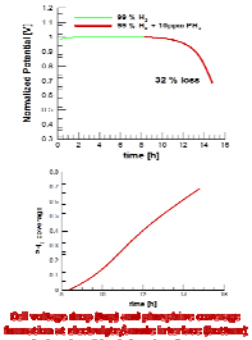
Results



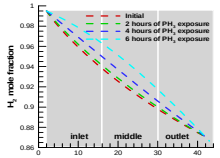
Current density (A/m^2) distribution in active layer at different times

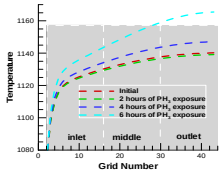


Variation of PH_3 coverage inside anode

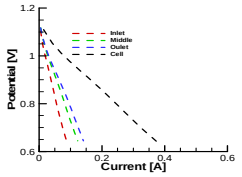


Cell voltage drop [top] and phosphine coverage fraction at electrolyte/anode interface [bottom] during phosphine induced performance degradation

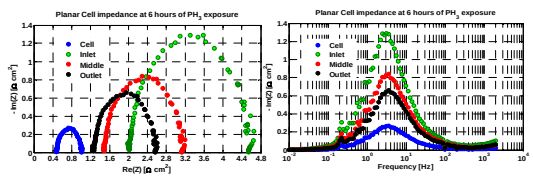




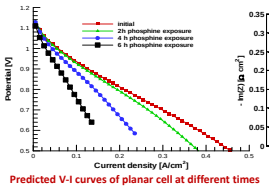
Hydrogen mole fraction (top) and Temperature (bottom) variation along the fuel channel at different times of phosphine exposure



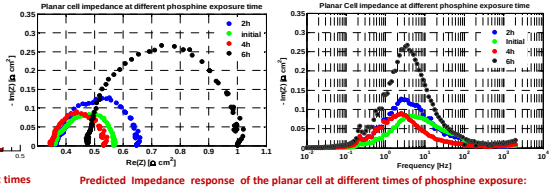
Predicted V-I curves of planar cell at 6 hours of phosphine exposure in different sections of the cell



Predicted impedance response of planar cell at 6 hours of phosphine exposure in different sections of the cell : Nyquist(left), bode (right) representations



Predicted V-I curves of planar cell at different times of phosphine exposure



Predicted Impedance response of the planar cell at different times of phosphine exposure: Nyquist(left), Bode (right)

Conclusion

- The deactivation of anode in planar cells exposed to contaminants is spatially non-uniform; this alters the current distribution inside the cell. Such behavior is not observed in button cells.
- Current redistribution leads to variable the polarization resistance in different regions of the cell.
- Ohmic resistance changes with the time due to temperature variation.
- Predicted V-I curves at different stages of degradation show that the cell failure is accelerated by a decrease in the limiting current.
- Predicted polarization behavior and the impedance response yield consistent results.

Acknowledgement

This work is conducted under US DOE (Department of Energy) EPSCoR Program. It is jointly sponsored by US DOE Office of Basic Energy Sciences, NETL (National Energy Technology Laboratory), WV State EPSCoR Office and the West Virginia University under grant number DE-FG02-06ER46299. Dr. Tim Fitzsimmons is the DOE Technical Monitor. Dr. R. Bajura is the Administrative Manager and Dr. I. Celik is the Technical Manager and the Principal Investigator of this project.

U.S. DEPARTMENT OF ENERGY | the ENERGY lab National Energy Technology Laboratory

Carnegie Mellon PENNSTATE West Virginia University URS