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

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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

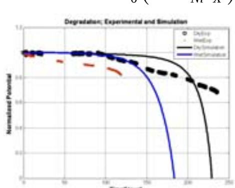
Model Description

- 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

Parameter	Dry (%0 H_2O)	Wet (%3 H_2O)
Temperature, °C	800	800
Current density, A/cm²	0.6	0.6
D_X^{eff}, m²/s	1×10^{-6}	1×10^{-6}
$k_{f,X}$, s⁻¹	0.5	0.5
m	0.4	0.4
n	7.0	7.0
p	0.5	2.0
q	2.0	2.0

Conductivity $\sigma = \sigma_0 \left(1-\theta_{Ni-X}\right)^q$

Porosity $\varepsilon = \varepsilon_0 \left(1-\theta_{Ni-X}\right)^p$



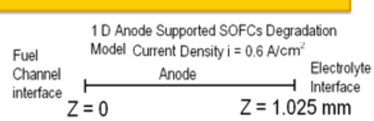
Degradation Model comparison with experimental data

Model Equations

Monolayer adsorption mechanism

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

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



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

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

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

$$\omega_{\theta_{Ni-H}} = k_{f,H}\, y_{H_2}\, \theta_{Ni}^2 - k_{b,H}\, \theta_{Ni-H}^2$$

$$\theta_{Ni-X} + \theta_{Ni-H} + \theta_{Ni} = 1$$

Gas phase Species Distribution Equation in Porous media

$$\varepsilon \frac{P}{RT}\frac{\partial y_i}{\partial t} = \frac{\partial}{\partial z}\left(\frac{P}{RT} D_i^{eff} \frac{\partial y_i}{\partial z}\right) + R_i + S_i$$

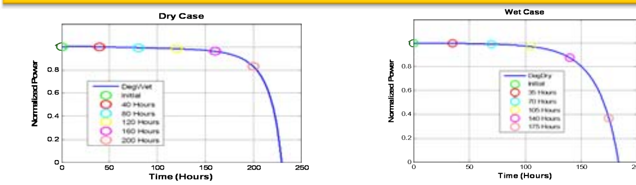
Activation loss from BV Eq. with modified exchange current density

$$i_{o,H_2} = c_1 \left(\frac{y_{H_2,\mathrm{int}}}{y_{H_2,ref}}\right) \exp\left(-\frac{E_{act,H_2}}{R_u T}\right)\left(1-\theta^m_{Ni-X,\mathrm{int}}\right)^n$$

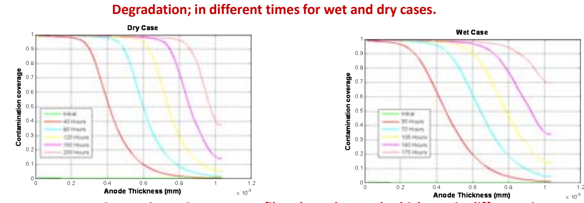
Charge conservation equation

$$\frac{1}{c}\frac{\partial \phi}{\partial t} = 0 = \frac{\partial}{\partial z}\left(\sigma \frac{\partial \phi}{\partial z}\right)$$

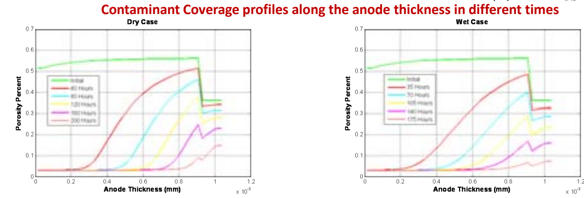
Results



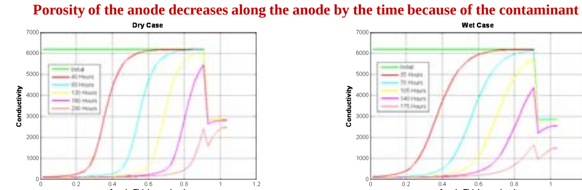
Degradation; in different times for wet and dry cases.



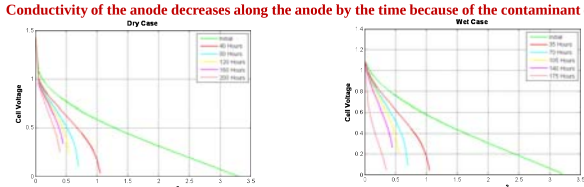
Contaminant Coverage profiles along the anode thickness in different times



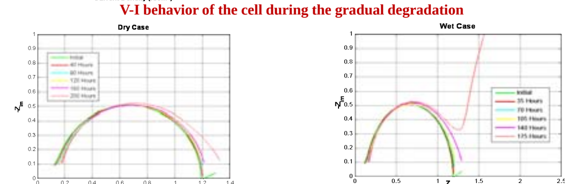
Porosity of the anode decreases along the anode by the time because of the contaminant coverage.



Conductivity of the anode decreases along the anode by the time because of the contaminant coverage.



V-I behavior of the cell during the gradual degradation



Impedance response of the cell during the gradual degradation

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.

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