Prediction of SOFC Performance via Multi-Physics Simulation Tool with Realistic Microstructure Properties

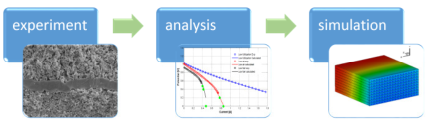
Tao Yang[1,2], Ismail Celik[1,2], Hayri Sezer[1,2], Harry Finklea[1,3], Kirk Gerdes[1]
[1]National Energy Technology Laboratory, Morgantown, WV,
[2]Mechanical and Aerospace Engineering Department, West Virginia University, Morgantown, WV
[3]Bennett Department of Chemistry, West Virginia University, Morgantown, WV

Introduction

- Simultaneous calibration of polarization curves and impedance behavior is necessary for SOFCs model developments, but was largely neglected in the literature.
- Tens of parameters are nonlinearly coupled in the multi-physics model of SOFCs, so that large number of datasets are needed for model calibration.
- The accurate prediction of cell performance at different air/fuel utilization conditions, as well as different working loads, should also be considered for model developments.
- The present study aims to find the way of determining the essential properties of fuel cells via efficient combination of experiments and numerical simulations.

Model Description

Physics-based SOFC Analysis Procedure



Governing Equations

- **Charge conservation**

Electrode phase

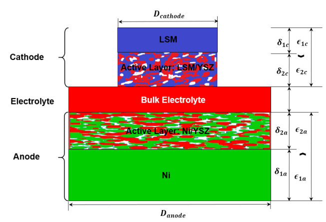
$$a_{\text{int}} C_{DL} \frac{\partial \varphi_e - \partial \varphi_i}{\partial t} + \nabla \cdot (-\sigma_e \varphi_e) = i_F$$

Electrolyte phase

$$a_{\text{int}} C_{DL} \frac{\partial \varphi_e - \partial \varphi_i}{\partial t} + \nabla \cdot (-\sigma_i \varphi_i) = -i_F$$

Dense electrolyte

$$\nabla \cdot (-\sigma_i \varphi_i) = 0$$



- **Species transportation**

$$\varepsilon \frac{\partial \phi}{\partial t} = \nabla (D_\phi^{eff} \phi) - S_\phi$$

- **Butler-Volmer type equations**

$$i_{Fa} = i_{0a} l_{TPB,a} \left(P_{H_2}\right)^a \left(P_{H_2O}\right)^b \{\exp(\frac{\alpha F \eta_a}{RT}) - \exp[-\frac{(1-\alpha) F \eta_a}{RT}]\}$$

$$i_{Fc} = i_{0c} l_{TPB,c} \left(P_{O_2}\right)^m \{\exp(\frac{\alpha F \eta_c}{RT}) - \exp[-\frac{(1-\alpha) F \eta_c}{RT}]\}$$

- **Diffusion coefficients**

$$D_\phi^{eff} = \frac{\varepsilon}{\tau^n} \left(\frac{1 - \alpha_{im} y_i}{D_{i,m}} + \frac{1}{D_{Ki}} \right)^{2/3}$$

- **Effective conductivity**

$$\sigma_i^{eff} = \frac{V_i}{\tau_i^2} \sigma_{i0}$$

Microstructure Properties

- **Length of triple phase boundary** (L.C.R. Scheneider et al. 2006)

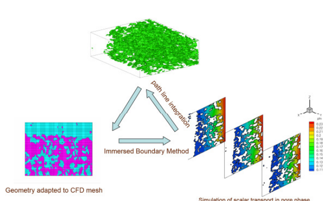
$$l_{TPB} = \frac{3D}{r^2} \sqrt{1 - \left(\frac{D_0}{D}\right)^{1/3}} \Phi_{io} (1 - \Phi_{io}) Z$$

- **Interface area between ion-conducting and electron-conducting phase** (A.M. Gokhale et al. 2009)

$$a_{\text{int}} = \frac{r}{2} l_{TPB}$$

- **Tortuosity** (M. Matyka et al. 2008)

$$\tau_i = V_i^{-p}$$



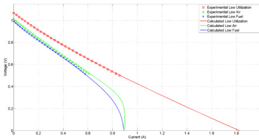
(S. Pakalapati et al.)

Contact

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

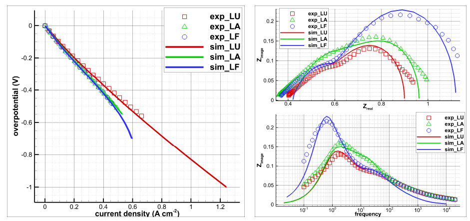
Results

Calibration Procedures for Button Cell



Polarization analysis of measured V-I curves

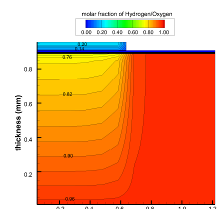
variables	values from EPA	refined values in simulations
$i_{0a}\ (A \cdot m^{-3})$	1.29×10^8	7.0×10^8
$i_{0c}\ (A \cdot m^{-3})$	1.02×10^8	2.66×10^8
a	1.66	0.425
b	0.34	0.75
m	0.46	0.25



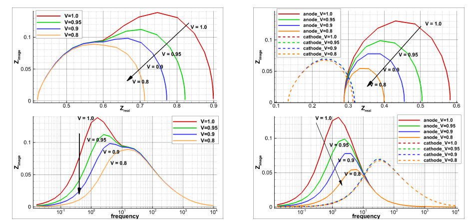
Simultaneous calibration of polarization curves and impedance behavior

Parameters	Values
Thickness of anode (μm)	900
Thickness of anode (μm)	50
Thickness of anode (μm)	10
Anode conductivity ($\Omega^{-1} \cdot m^{-1}$)	4.63×10^3
Electrolyte conductivity ($\Omega^{-1} \cdot m^{-1}$)	0.4
Cathode conductivity ($\Omega^{-1} \cdot m^{-1}$)	6.34×10^3
Reference specific capacitance at Ni/YSZ interface ($F \cdot m^{-3}$)	1.43×10^8
volumetric exchange current density in anode $i_{0a}\ (A \cdot m^{-3})$	7.0×10^8
exponent 'a' in the anode exchange current relation	0.425
exponent 'b' in the anode exchange current relation	0.75
Reference specific capacitance at LSM/YSZ interface ($F \cdot m^{-3}$)	3.075×10^7
volumetric exchange current density in cathode $i_{0c}\ (A \cdot m^{-3})$	2.66×10^8
exponent 'm' in the anode exchange current	0.25
Porosity in support layer	0.48
Porosity in active layer	0.23

Detailed Analysis of Processes Inside Electrodes

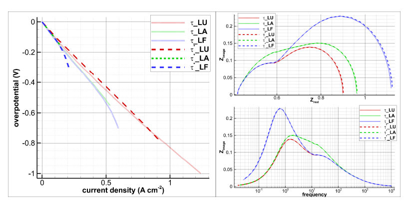


Air/fuel fraction distribution within electrode

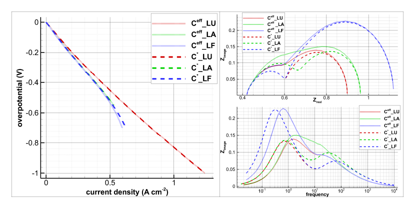


Performances with different working loads and impedance of electrodes

Effects of Using Partial Data Sets

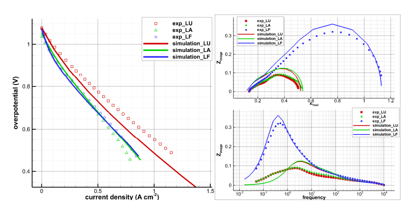


Results with calibration of impedance behavior only

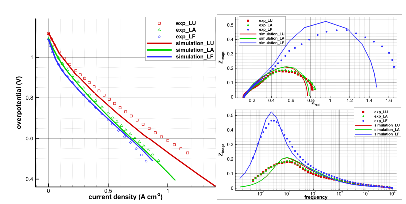


Results with calibration of polarization curves only

Further Application (Effects of Infiltration)



Calibrated results of baseline cell



Calibrated results of Co-infiltrated cell

Conclusions

- A physics-based tool, combining experiments, empirical polarization analysis, and multi-physics numerical simulations, is developed for prediction and analysis of SOFC performance.
- Experimental datasets are analyzed in conjunction with empirical polarization analysis to extract essential information of the fuel cell, and finally refined by multi-physics numerical simulations.
- Microstructure properties are incorporated for in-depth understanding of processes within electrodes.
- The present study demonstrates that at least three different air/fuel flow conditions are needed to produce a set of complete data for better understanding of the processes occurring within SOFCs.
- This procedure can also predict the SOFC performances for different utilization cases and working loads, as well as cell performance due to microstructural changes, such as infiltration and degradation.

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