Analysis of SOFC Impedance Using Simulations and Experiments Together

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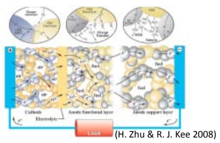
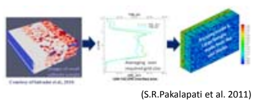
Office of Research and Development

Objectives

➢ **Multiphysics model**



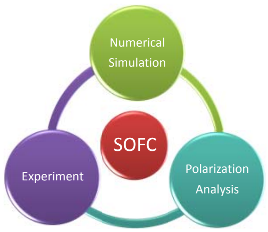
(H. Zhu & R. J. Kee 2008)



(S.R.Pakalapati et al. 2011)

➢ **Objective**

- Develop a physics based SOFC simulation tool for design analysis, diagnostics, and degradation/life-time predictions.



Methodology

➢ Multi-scale, multidisciplinary approach

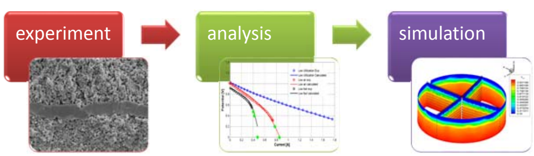
➢ Molecular dynamics modeling for estimation of reaction rates and the macroscopic material properties

➢ Continuum level modeling for cell level performance analysis

➢ Effective exchange of data and predictions among various levels of modeling and among modeling and experiments

➢ Multiphysics model validated against experiments

➢ Impedance calculation in time domain



Sketch of procedures in our physics based SOFC simulation tool

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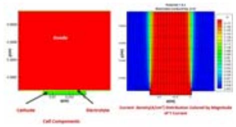
Polarization Analysis

➢ **Ohmic Resistance**

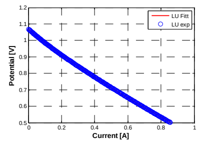


2D simulation of electric field for ohmic resistance.

Electrolyte Cond: 0.13

	Potential	anode	cathode	electrolyte	Cell
Variable cond	0.1	0.0091	0.0138	0.1475	0.1705
Uniform cond	0.1	0.0035	0.0056	0.1462	0.1552
Variable cond	0.5	0.0091	0.0138	0.1435	0.1664
Uniform cond	0.5	0.0035	0.0056	0.1462	0.1552

➢ **Exchange Current Density Using Butler-Volmer Equation**



i_{0a}	0.3152
i_{0c}	0.2165
$\lambda = i_{0c}/i_{0a}$	0.6869
R_Ω	0.41

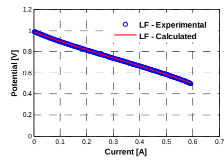
Polarization analysis for low air/fuel utilization (LU) case

Anode: $$i_{F,a} = i_{0,H_2}\left(\frac{P_{H_2}}{P_{H_2}^{\infty}}\right)^a\left(\frac{P_{H_2O}}{P_{H_2O}^{\infty}}\right)^b\times\left\{exp\left(\frac{F\eta_a}{RT}\right) - exp\left(-\frac{F\eta_a}{RT}\right)\right\}$$

Cathode: $$i_{F,c} = i_{0,O_2}\left(\frac{P_{O_2}}{P_{O_2}^{\infty}}\right)^m\times\left\{exp\left(\frac{F\eta_c}{RT}\right) - exp\left(-\frac{F\eta_c}{RT}\right)\right\}$$

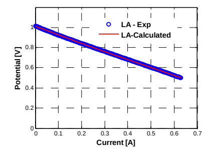
General type Butler-Volmer equation which is also used in the impedance simulation

➢ **Concentration Effects**



i_{0a}	0.4000
i_{0c}	0.2165
a	1.377956
b	0.9121
i_L	0.9000
R_Ω	0.41

Polarization analysis for low fuel (LF) supply case



i_{0a}	0.3152
i_{0c}	0.196057
m	0.606697
i_L	0.9000
R_Ω	0.41

Polarization analysis for low air (LA) supply case

Impedance Simulation

➢ **Charge conservation**

- electrode phase

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

- electrolyte phase

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

- bulk electrolyte

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

➢ **Species transport**

$$\frac{\partial(\epsilon\phi)}{\partial t} = \nabla(D^{eff}\nabla\phi) - \dot{S}$$

➢ **Effective diffusion coefficients** (F. N. Cayan et al. 2009)

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

$$D_{i,m} = \frac{1-y_i}{\sum_{k\neq i}\frac{y_k}{D_{ik}}} \quad with \quad D_{ik} = 0.001858\frac{[T^3(M_i+M_k)/M_iM_k]^{1/2}}{p\sigma_{ik}^2\Omega_D}$$

$$D_{Ki} = \frac{2}{3}\left(\frac{8RT}{\pi M_i}\right)^{1/2}\bar{r} \quad Knudsen\ Diffusion$$

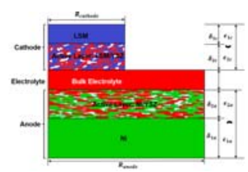
$$\alpha_{im} = 1 - \left(\frac{M_i}{M_m}\right)^{1/2}$$

➢ **Structural properties** (empirical relations)

$$a_{int} = a_0(\epsilon_0/\epsilon)^{2/3} \quad or\ from\ experiment$$

$$\tau = \tau_0(\epsilon/\epsilon_0)^{-0.5} \quad or\ from\ theoretical\ calculations$$

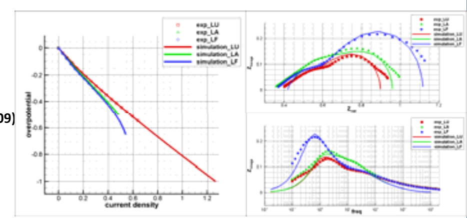
$$l_{TPB} = \frac{3d}{r^2}\sqrt{1-\left(\frac{d_0}{d}\right)^{\frac{1}{3}}}\phi_{i0}(1-\phi_{i0})Z \quad \phi_{i0} = \frac{\epsilon_Y}{\epsilon_Y+\epsilon_L} \quad Z \cong 6.3$$



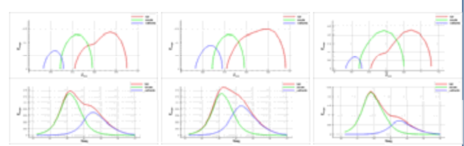
Sketch of button cell geometries in impedance simulation

	Analysis	Simulation
i_{0a}	8.55E8	7.0E8
i_{0c}	0.93E8	2.66E8

Comparison of exchange current densities from polarization analysis and those in simulation



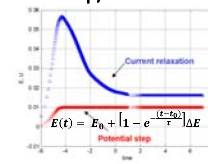
Simulation results for different utilization cases and the validation against experiments: *(left)* polarization curve, *(right)* impedance behavior.



Impedance contributions from anode/cathode for different utilization cases: *(left)* low utilization case, *(middle)* low air supply case, *(right)* low fuel supply case.

Relaxation Impedance Simulation

➢ **Potential step/Current relaxation & FFT analysis** (Bessler 2008)



An example of potential step and current relaxation

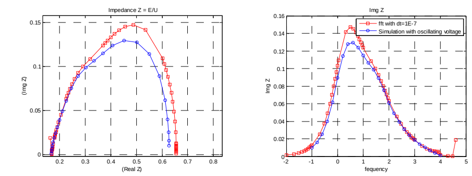
$$E^*(\omega) = \int_{-\infty}^{\infty} E(t)exp(-j2\pi\omega t)dt$$

$$I^*(\omega) = \int_{-\infty}^{\infty} I(t)exp(-j2\pi\omega t)dt$$

$$Z^*(\omega) = \frac{E^*(\omega)}{I^*(\omega)}$$

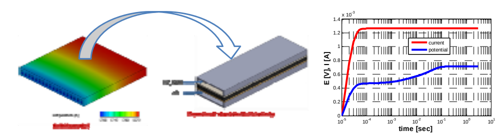
Formula for Fourier analysis

➢ **Button Cell**

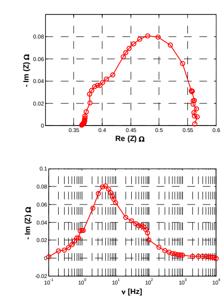


Results of Relaxation impedance simulation for button cell: *(left)* Nyquist plot, *(right)* Bode plot

➢ **Planar Cell**



Cell Geometry	
Anode thickness	50 µ
Electrolyte thickness	170 µ
Cathode thickness	50 µ
Channel length	5.1 cm
Channel width	3.048 cm
Current Collectors width	1.524 cm
Fuel Composition	
H2 %	99.00
H2O %	1.00
Fuel utilization %	12.50
Air Composition	
O2 %	21.00
N2 %	79.00
Air utilization	12.50
Electrical Properties	
Anode conductivity	
Current density	0.1 A/cm2
Total current	0.311 A



Results of Relaxation impedance simulation for planar cell

Acknowledgement

Acknowledgement

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