Distributed Electrochemistry Modeling Tool for Simulating SOFC Performance and Degradation

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OVERVIEW

Improving the durability of the SOFC, especially when consuming coal gas or alternative fuels such as land-fill gas, is essential to making SOFCs practical for stationary and distributed power generation. In general, SOFC performance and durability is adversely affected by reactions that cause unwanted changes to the electrode microstructures such as grain coarsening, cracking, clogging of pores, and the formation of secondary phases. The distributed electrochemistry (DEC) modeling tool is being developed to investigate the electrochemistry within the membrane-electrode assembly (MEA) of the SOFC and to help quantify the effects of these unwanted reactions. The DEC model calculates the current-voltage (I-V) performance of the cell based on the local multi-physics and properties of the electrode microstructure, which can varying through the MEA. The model has been validated with experimental button cell data and has been used to investigate changes in performance with changes in local conditions and properties within the MEA.

OBJECTIVES

- Develop a multi-dimensional cell-level distributed electrochemistry model that can simulate SOFC performance by solving the coupled and spatially varying multi-physics that occur within the MEA.
- Validate the model for an SOFC operating on various fuel gas compositions.
- Investigate the effect of local conditions, microstructure, and electrode degradation on the electrochemical performance.

DEC MODEL FEATURES

- Resolves local conditions in SOFC based on the reactive transport, electrochemistry, and operating conditions
- Calculates global electrical performance based on local electrochemistry
- Investigates effects of local conditions & microstructure on cell performance
- Effects of electrode degradation on cell performance (under development)

MULTI-PHYSICS GOVERNING EQUATIONS

Conservation Equations

$$\frac{\partial}{\partial x_j}(\rho u_j) = S_m$$

$$\frac{\partial}{\partial x_j}(\rho u_j Y_k + F_{k,j}) = S_k$$

$$\frac{\partial}{\partial x_j}(\rho u_j u_i - \tau_{ij}) = -\frac{\partial p}{\partial x_i} + S_p$$

Diffusion Flux: Fick's Law

$$F_{m,j} = -D_m \frac{\partial Y_{m,j}}{\partial x_j}$$

Bulk Advection: Darcy's Law

$$\frac{\partial p}{\partial x_j} = -\frac{\mu}{\kappa} u_j$$

Charge Transfer: Modified Butler-Volmer

$$i_F^V = i_{0,e} \lambda_{TPB}^V \left[\exp\left(\frac{\alpha_a F \eta_{act,e}}{RT}\right) - \exp\left(-\frac{\alpha_c F \eta_{act,e}}{RT}\right) \right]$$

Electric Potential: Poisson's Equation

$$\sigma_{elyt}^{eff} \left(\frac{\partial^2 E_e}{\partial x_j^2}\right) = -i_F^V$$

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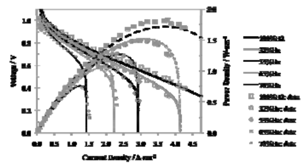
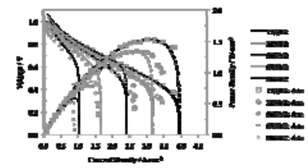
DEC MODEL VALIDATION

- **DEC model validation with experimental data: Global voltage and power density for various fuel mixtures at different operating currents.**

	Thickness, micron	Volume fraction			Particle radius, micron		Pore radius, micron	Tortuosity factor
		YSZ	Pores	Ni/LSM	YSZ	Ni/LSM		
Anode	1100	0.274	0.35	0.376	0.5	0.5	0.5/0.8	2.5
Electrolyte	10	1.0	0.0	0.0	–	–	–	–
Cathode	30	0.315	0.35	0.335	0.5	0.5	0.5	2.5





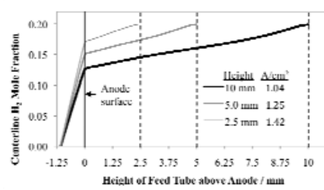
ANODE OPTIMIZATION EXERCISE

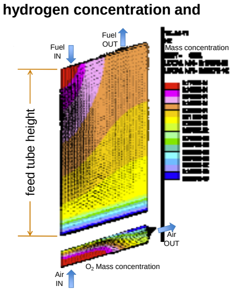
- **Optimization of SOFC performance by systematically adjusting anode microstructural properties**

Step	Structural parameters changed	Physics effected compared to baseline	Current density, A/cm² at 0.8 V
1	Baseline (1100 mm anode)	Baseline physics	0.862
2	+Model anode thickness decreased to 550 mm	Increased gas transport	0.914
3	+Increase porosity and pore size in anode support layer (from 0.35 to 0.45, and 0.8 mm to 2.0 mm)	Increased gas transport	0.935
4	+Increase YSZ fraction in anode base layer (from 0.274 to 0.35, porosity decreased from 0.35 to 0.30)	90% increase in ionic conductivity, 23% increase in TPB, and decreased gas transport in base layer	1.162
5	+Decrease particle radius of YSZ and Ni from 0.5 to 0.3 mm, increase porosity back to 0.35 (slight decrease in YSZ and Ni compared to Step 4)	70% increase in ionic conductivity, 300% increase in TPB, and return to gas transport in base layer as in case 3	1.401

EXPERIMENTAL DESIGN & SETUP

- **Height of fuel feed tube above anode affects hydrogen concentration and cell performance**





CONCLUSIONS

- Developed the DEC modeling tool which can accurately reproduce experimental data at various operating voltages and gas compositions.
- The validated modeling tool can predict trends in SOFC performance due to changing electrode microstructure.
- Experimental designs and setups can be evaluated for their effectiveness before construction.
- The DEC model can now be expanded to look at degradation and performance problems of interest to the SECA industrial team members. Such as:
  - Ni oxidation due to fuel supply interruption
  - sulfur poisoning of the anode in an auxiliary power supply unit

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For more information about the science seen here, please contact:

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