

Analysis and Design of Fuel Cells

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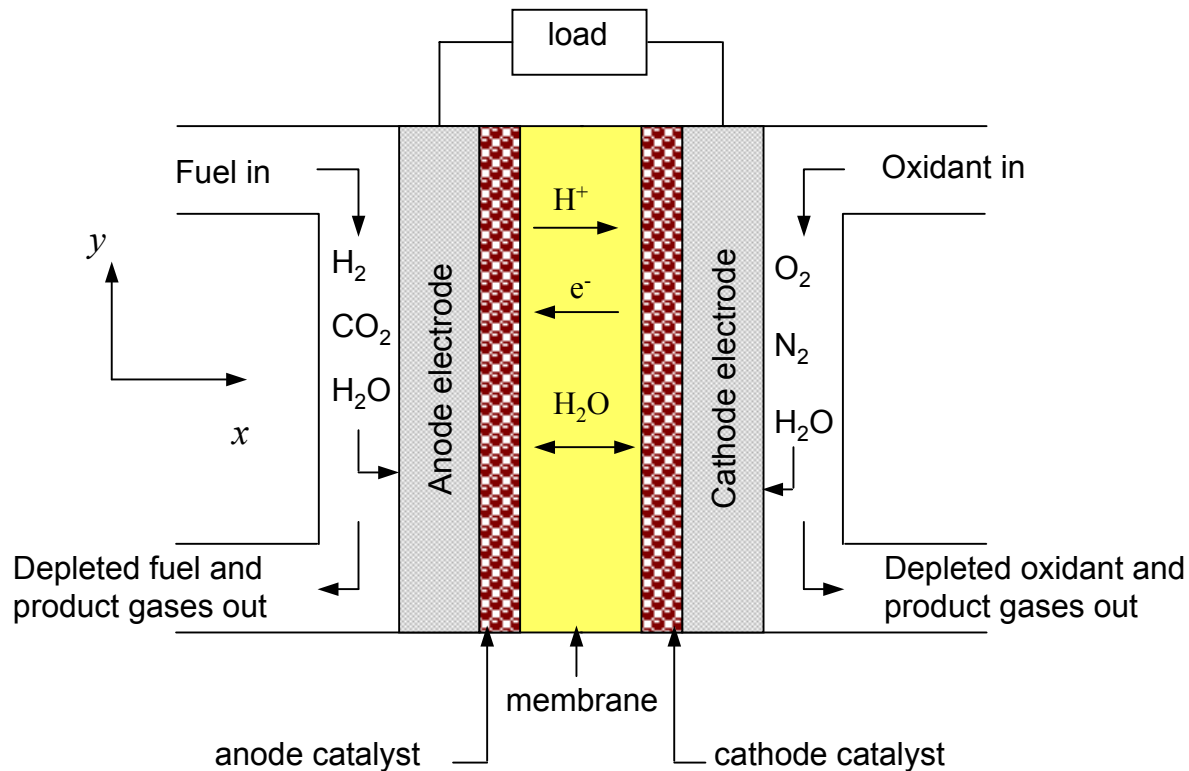
Outline

Objective: To develop a physics-based model for a PEM fuel cell and to illustrate a methodology for model-assisted cell design and optimization

- ❖ Transport and Electrochemical Phenomena Modeling
- ❖ Model Validation
- ❖ Parametric Analysis
- ❖ Operating Window Development
- ❖ Optimum Design



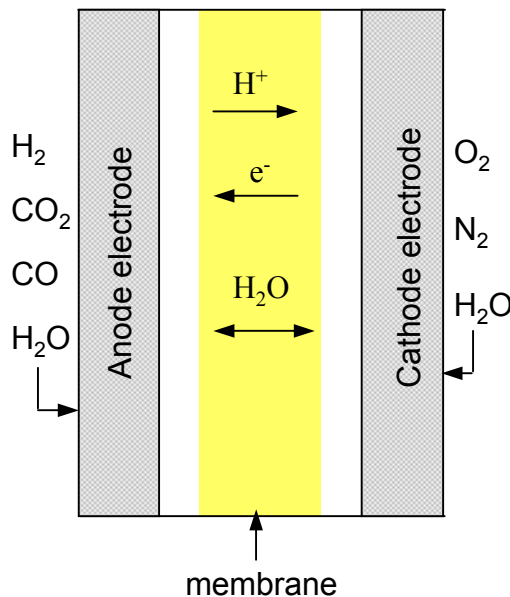
Modeling Considerations



- One-dimensional description
- Steady state operation
- Nonisothermal effects
- CO poisoning effects



Governing Equations: Electrodes and Membrane



□ Electrodes:

$$\text{Energy: } -k^{\text{eff}} \frac{d^2 T}{dx^2} + \left[\left(\frac{I}{nF} \right) W_1 C_{p,1} + N_3 W_3 C_{p,3} + N_4 W_4 C_{p,4} \right] \frac{dT}{dx} + h_{\text{vap}} W_3 - \frac{I^2}{\sigma^{\text{eff}}} = 0$$

$$\text{Species: } \frac{dN_i}{dx} = \frac{w_i}{W_i} \quad \text{Stefan-Maxwell: } \frac{dx_i}{dx} = \frac{RT}{P} \sum_{j=1}^N \left[\frac{x_i N_j - x_j N_i}{D_{ij}^{\text{eff}}} \right] \quad \text{Potential: } \frac{d\Phi_s}{dx} = -\frac{I}{\sigma^{\text{eff}}}$$

Unknowns: T, N_i, x_i, Φ_s

Anode Species: $i=1 \rightarrow 4, 1=H_2, 2=CO_2, 3=H_2O(g), 4=CO$

Cathode Species: $i=1 \rightarrow 3, 1=O_2, 2=N_2, 3=H_2O(l)$

□ Membrane:

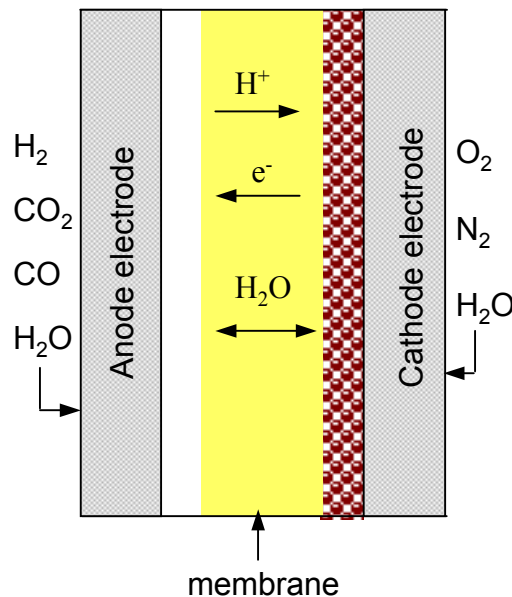
$$\text{Energy: } -k^{\text{eff}} \frac{d^2 T}{dx^2} + N_3 W_3 C_{p,3} \frac{dT}{dx} - \frac{i_m^2}{\kappa} = 0 \quad \text{Species: } \frac{dN_i}{dx} = 0$$

$$\text{Potential: } \frac{d\Phi_m}{dx} = -\frac{i_m}{\kappa} + \delta \frac{RT}{F} \left(\frac{3}{1+\delta\lambda} \right) \frac{d\lambda}{dx} + \frac{FN_i}{\kappa\lambda}$$

Unknowns: T, N_i, Φ_m Membrane Species: $i=2 \rightarrow 3, 2=H^+, 3=H_2O(l)$



Governing Equations: Cathode Catalyst



$$\text{Energy: } -k^{\text{eff}} \frac{d^2 T}{dx^2} + [N_1 W_1 C_{p,1} + N_3 W_3 C_{p,3}] \frac{dT}{dx} + \left| \frac{j_{O_2}(x)}{nF} \right| (T \Delta \bar{s}) - j_{O_2}(x) (\Phi_s - \Phi_m) - \frac{i_m^2}{\kappa^{\text{eff}}} = 0$$

$$\text{Species: } \frac{dN_i}{dx} = -\frac{\nu_i j_{O_2}(x)}{nF} \quad \text{Nernst Planck } c_1: D_1^{\text{eff}} \frac{d^2 c_1}{dx^2} - \frac{N_3}{c_3} \frac{dc_1}{dx} - \frac{c_1}{c_3} \frac{dN_3}{dx} + \frac{dN_1}{dx} = 0$$

$$\text{Nernst Planck } \Phi_m: \frac{d\Phi_m}{dx} = -\frac{i_m}{\kappa^{\text{eff}}} + \frac{F}{\kappa^{\text{eff}}} \frac{c_2}{c_3} N_3 \quad \text{Potential: } \frac{d\Phi_s}{dx} = -\frac{i_s}{\sigma^{\text{eff}}}$$

Where $j_{O_2}(x)$ is governed by the Butler-Volmer equation

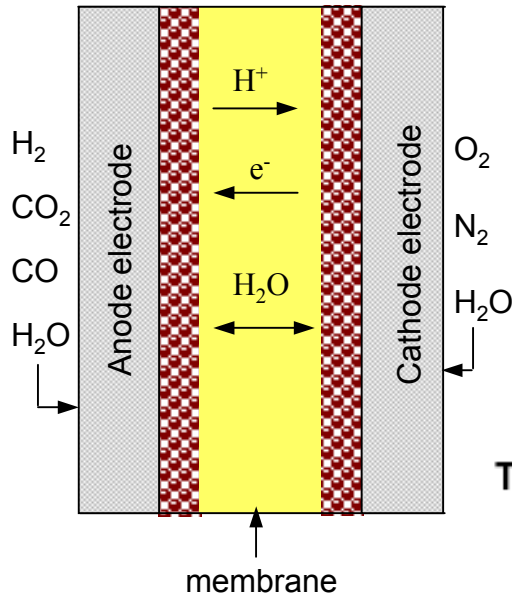
$$j_{O_2}(x) = a i_0^{\text{ref}} \left(\frac{c_1}{c_1^{\text{ref}}} \right)^{\gamma_1} \left[\exp\left(\frac{\alpha_a F}{RT} (\Phi_s - \Phi_m) \right) - \exp\left(\frac{\alpha_c F}{RT} (\Phi_s - \Phi_m) \right) \right]$$

Unknowns: $T, N_i, c_1, \Phi_m, \Phi_s$

Cathode Catalyst Species: $i=1 \rightarrow 3, 1=O_2, 2=H^+, 3=H_2O(l)$



Governing Equations: Anode Catalyst



$$\text{Energy: } -k^{\text{eff}} \frac{d^2 T}{dx^2} + \sum_{\substack{i=1 \\ i \neq 2}}^5 [N_i W_i C_{p,i}] \frac{dT}{dx} + \left| \frac{j(x)}{nF} \right| (T \Delta \bar{s}) - j(x) (\Phi_s - \Phi_m) - \frac{i_m^2}{\kappa^{\text{eff}}} = 0$$

$$\text{Species: } \frac{dN_1}{dx} = -\frac{j_{H_2}(x)}{2F}, \quad \frac{di_m}{dx} = j_{H_2}(x) + j_{CO}(x) = j(x),$$

$$\frac{dN_3}{dx} = -\frac{j_{CO}(x)}{2F}, \quad \frac{dN_4}{dx} = -\frac{j_{CO}(x)}{2F}, \quad \frac{dN_5}{dx} = \frac{j_{CO}(x)}{2F}$$

$$\text{Nernst Planck } c_4: D_4^{\text{eff}} \frac{d^2 c_4}{dx^2} - \frac{N_3}{c_3} \frac{dc_4}{dx} - \frac{c_4}{c_3} \frac{dN_3}{dx} + \frac{dN_4}{dx} = 0$$

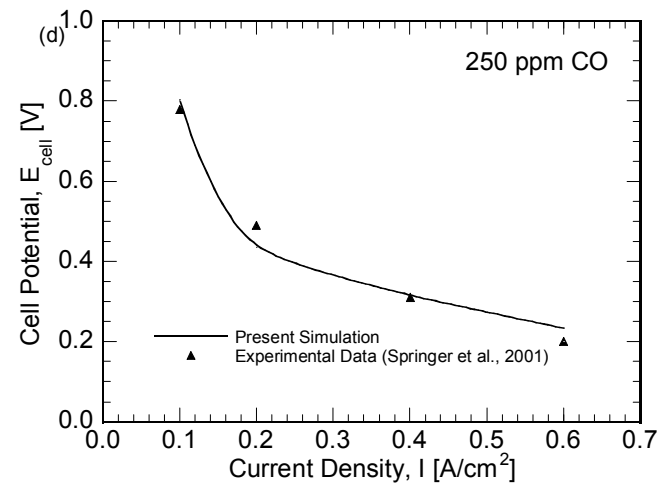
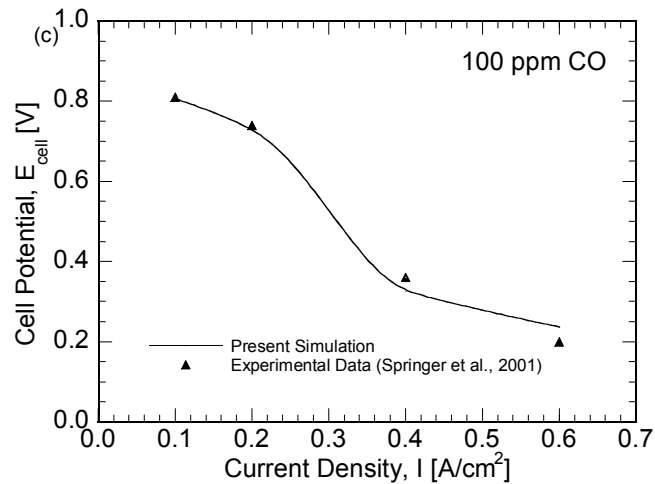
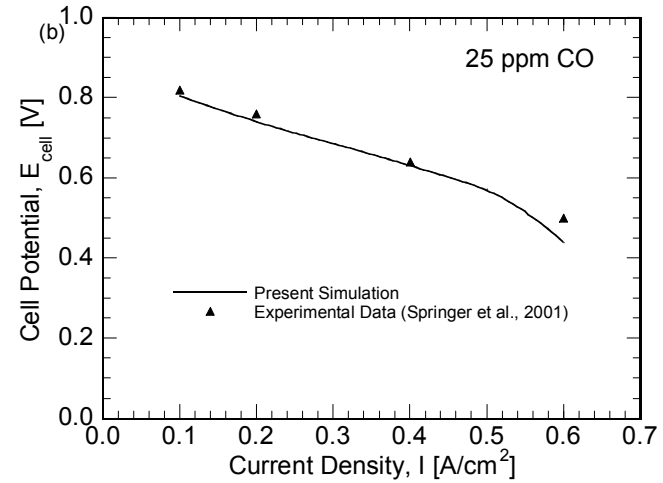
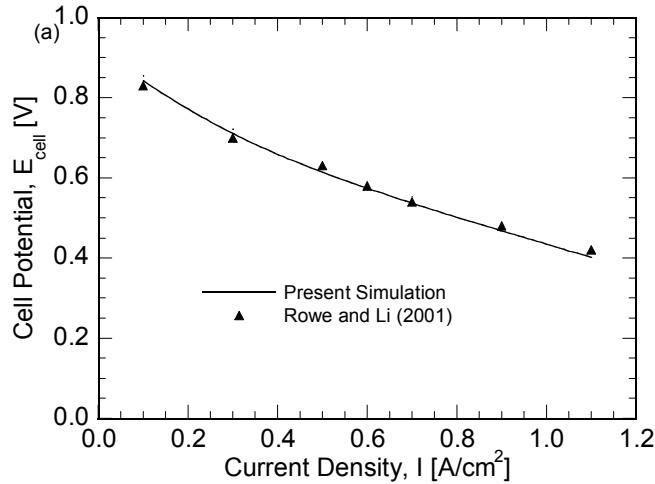
The Nernst-Planck equation for c_1 and Φ_m , and the potential equation for Φ_s follow those in the cathode catalyst region

Unknowns: $T, N_i, c_1, c_4, \Phi_m, \Phi_s$

Anode Catalyst Species: $i=1 \rightarrow 5, 1=H_2, 2=H^+, 3=H_2O(l), 4=CO, 5=CO_2$



Model Validation



Parametric Runs

Design Parameters:

- Platinum Loading
- Thickness of each cell layer
- Void fraction in catalyst layer
- Porosity
- Tortuosity

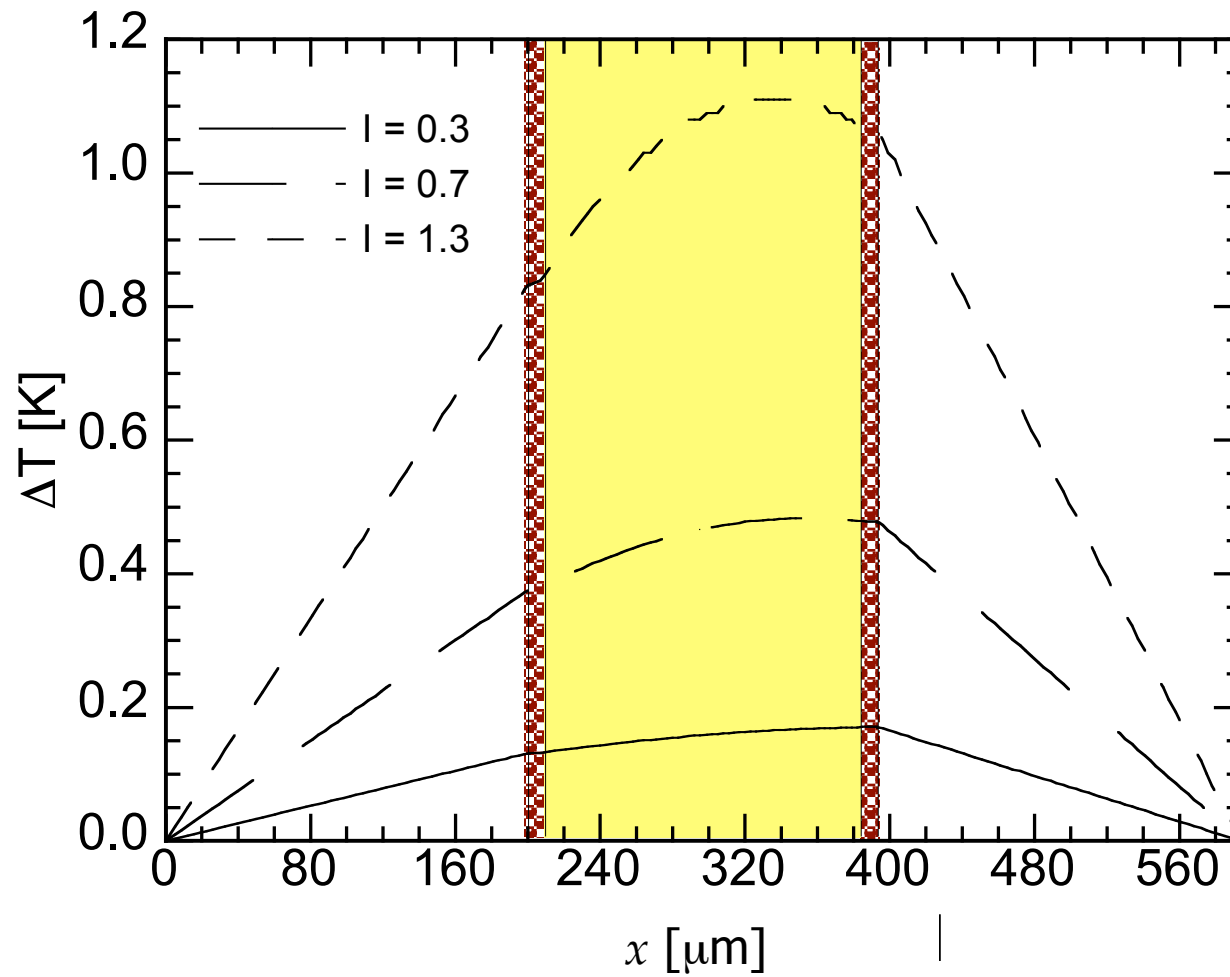
Operating Parameters:

- Cell Operating Temperature
- Pressure on the anode and cathode side
- Dry gas mole fraction on anode and cathode side
- Relative Humidity of anode and cathode stream
- Stoichiometry of anode and cathode feed

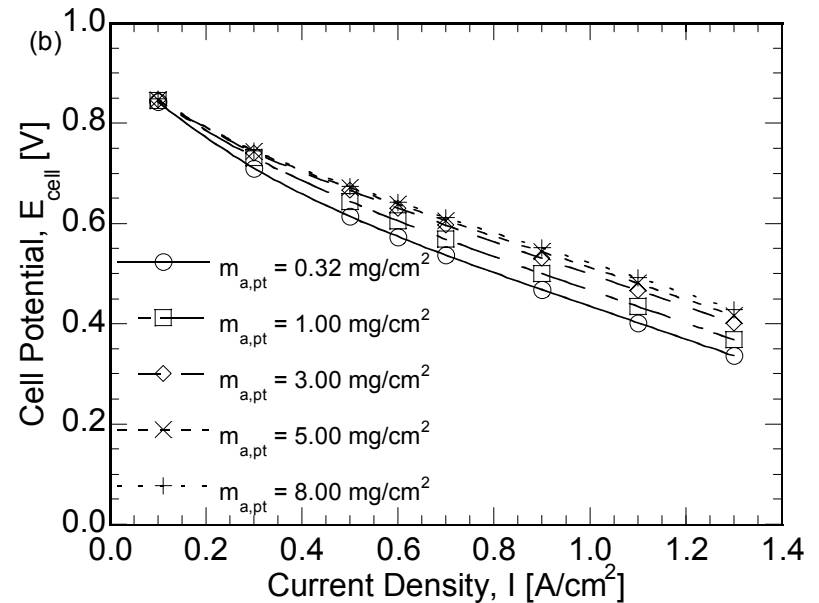
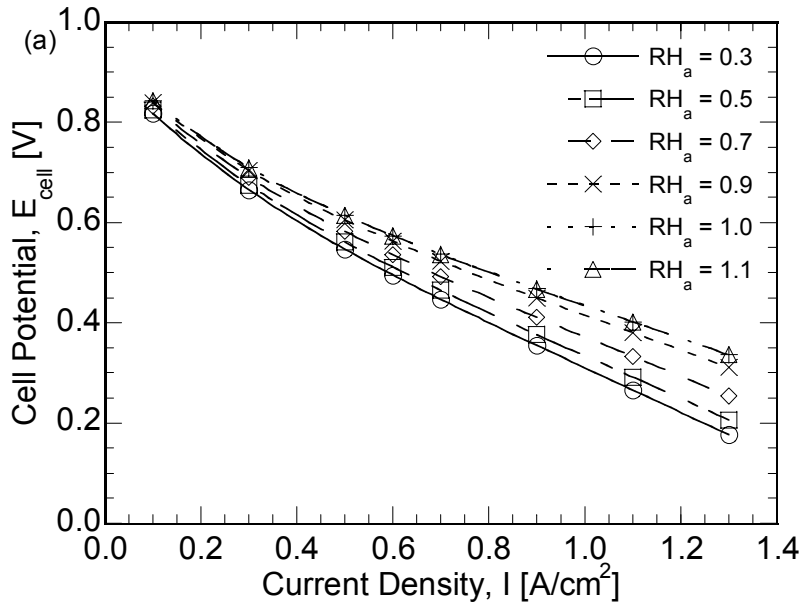


Sample Profile Across the Cell

V. Mishra, F. Yang, R. Pitchumani, *Journal of Power Sources* (2004)



Operating and Design Parameters



- ❑ Fig. (a) shows the effect of the relative humidity in the anode feed stream. An increase in the relative humidity results in increased water content and smaller resistive losses; however for a supersaturated stream, the heat of condensation adds to the losses.
- ❑ Fig. (b) shows the effect of the performance increases with increasing platinum loading owing to the increase in the number of reaction sites..



Operating Considerations

Objective function:

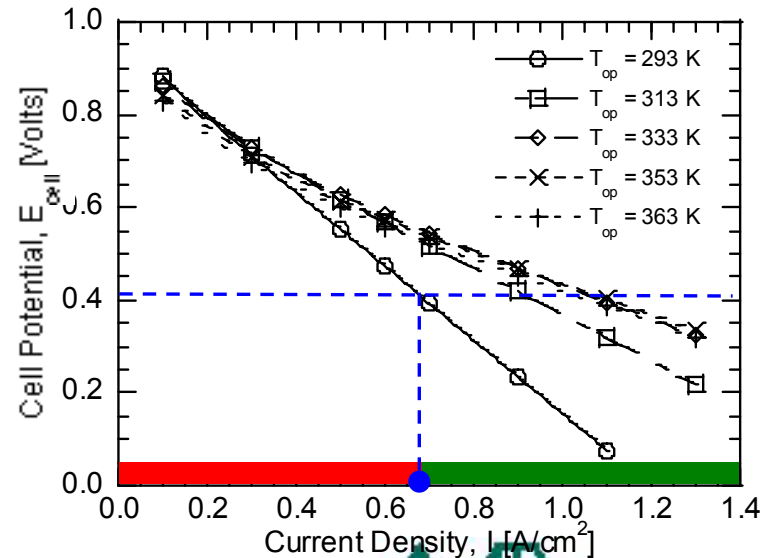
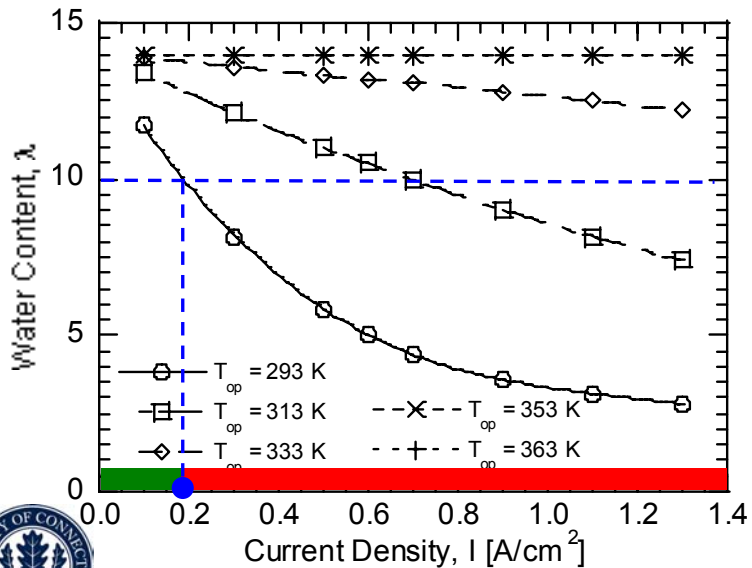
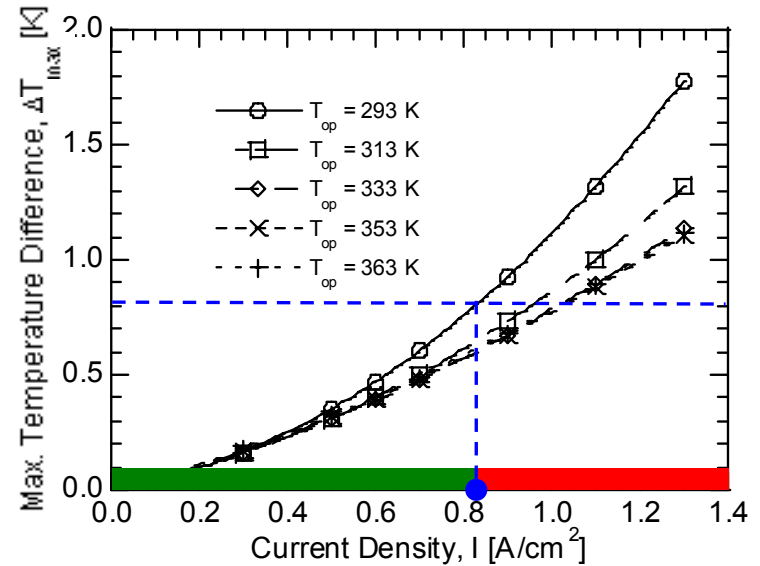
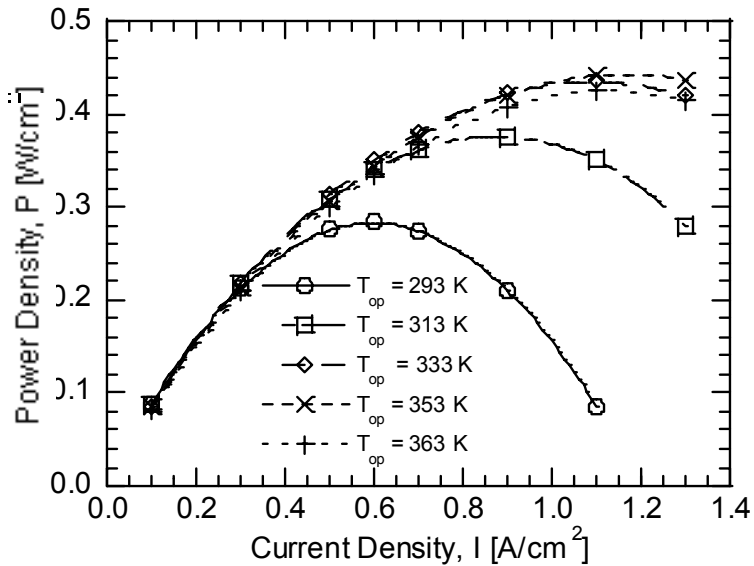
Maximize power density, P_d

Constraints:

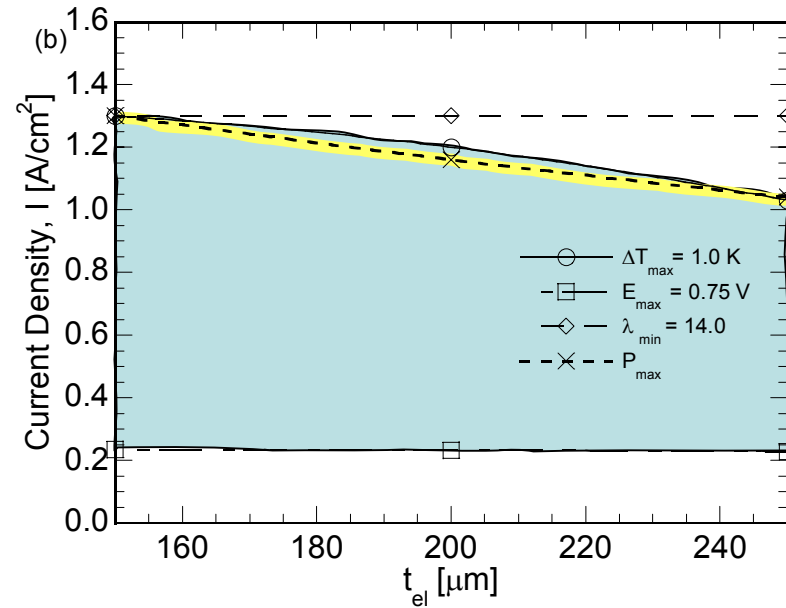
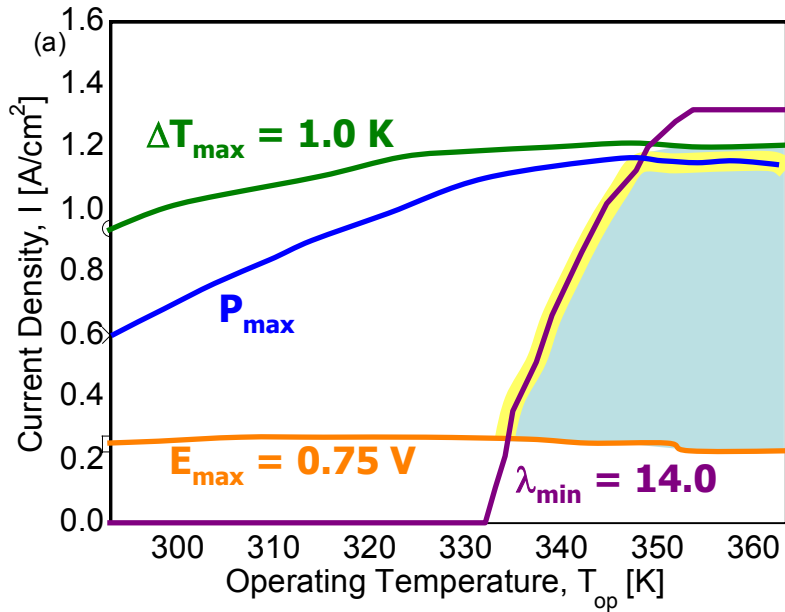
- temperature difference, $\Delta T < \Delta T_{\max}$
- hydration, $\lambda > \lambda_{\min}$
- potential, $E_{\text{cell}} < E_{\max}$



Unconstrained Optimum; Upper and Lower Bounds



Operating and Design Window



- Optimal solutions are obtained for various parameters.



Optimum Combination of Parameters

OPERATING PARAMETERS										DESIGN PARAMETERS									
I [A/cm ²]	T (K)	P _a [atm]	P _c [atm]	Rh _a	Rh _c	X _{CO2/H2}	X _{N2/O2}	ζ _a	ζ _c	m _{pt,ca} (mg/cm ²)	m _{pt,an} (mg/cm ²)	t _{el} (μm)	t _{cl} (μm)	t _{me} (μm)	e ^{cl} _m	e ^{cl} _s	e _e	τ	P _{d,max}
0.22	353.0	4.9	3.0	0.90	1.00	0.13	3.76	1.37	3.0	0.32	0.32	200	7	180	0.45	0.50	0.40	7.0	0.170
0.30	335.0	4.7	3.0	0.91	1.00	0.09	3.76	1.53	3.0	0.32	0.32	200	7	180	0.45	0.50	0.40	7.0	0.210
0.50	337.0	4.4	3.0	0.93	1.00	0.06	3.76	2.01	3.0	0.32	0.32	200	7	180	0.45	0.50	0.40	7.0	0.308
0.60	338.0	4.3	3.0	0.93	1.00	0.05	3.76	2.27	3.0	0.32	0.32	200	7	180	0.45	0.50	0.60	7.0	0.358
0.70	340.0	4.1	3.0	0.94	1.00	0.03	3.76	2.52	3.0	0.32	0.32	200	7	180	0.45	0.50	0.58	7.0	0.375
0.90	343.0	3.8	1.2	0.95	1.00	0.01	3.76	3.05	3.0	0.32	0.32	200	7	180	0.45	0.50	0.56	10.7	0.420
1.00	345.0	3.7	1.8	0.96	1.00	0.00	3.76	4.39	2.0	0.32	0.32	250	15	180	0.45	0.50	0.52	9.1	0.442
1.10	347.0	3.3	2.6	0.97	1.00	0.00	3.76	4.62	2.4	0.32	0.32	216	10	180	0.45	0.50	0.48	7.7	0.452
1.15	353.0	2.0	2.8	0.99	1.00	0.00	3.76	4.75	3.0	0.32	0.32	200	7	180	0.45	0.50	0.46	7.2	0.443
1.20	353.0	3.0	3.7	1.10	0.38	0.00	3.61	1.50	4.0	2.08	1.00	185	7	158	0.17	0.40	0.40	6.3	0.536
1.25	353.0	3.0	6.8	1.00	1.00	0.00	1.76	1.50	3.0	3.26	3.00	172	7	147	0.30	0.30	0.40	5.0	0.592
1.30	353.0	3.0	15.0	1.00	1.00	0.00	0.00	1.50	3.0	0.32	0.32	150	7	51	0.45	0.50	0.40	7.0	0.621



Summary

- ❑ A one-dimensional steady state model of a PEM fuel cell was presented.
- ❑ The model was used as basis for analysis of the effects of design and operating parameters on the cell performance parameters
- ❑ A methodology for simulation-assisted development of operating windows and optimum conditions was illustrated; the methodology applies to multi-dimensional models as well.

- ❑ Looking ahead...
 - ❖ Interfacing a numerical optimizer with the cell model
 - ❖ Integration of the cell model with system level simulations



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