Constrained Control and Optimization of Tubular Solid Oxide Fuel Cells for Extending Cell Lifetime

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Overview

Objective:

Perform load-following and disturbance rejection with tubular solid oxide fuel cells while operating within thermal stress-based constraints. Multi-input multi-output (MIMO) linear model predictive control combines controlled variables for power, thermal stress, and other failure modes into one performance index.

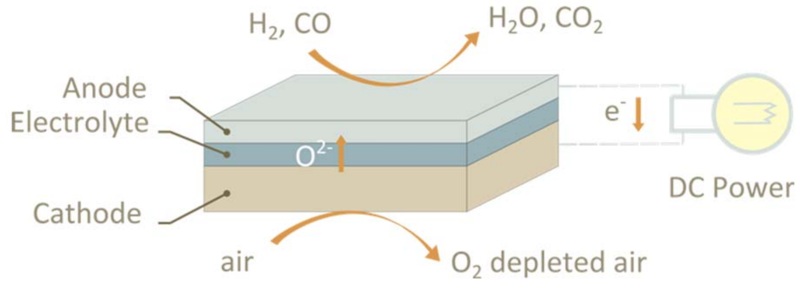
Agenda:

- Description and Motivation of SOFC Power Generation
- Dynamic Modeling of Thermal Stress Indicators
- Constrained Predictive MIMO Control of the SOFC
- Conclusion

Description and Motivation of SOFC Power Generation

Tubular Solid Oxide Fuel Cells

SOFC Operational Principles



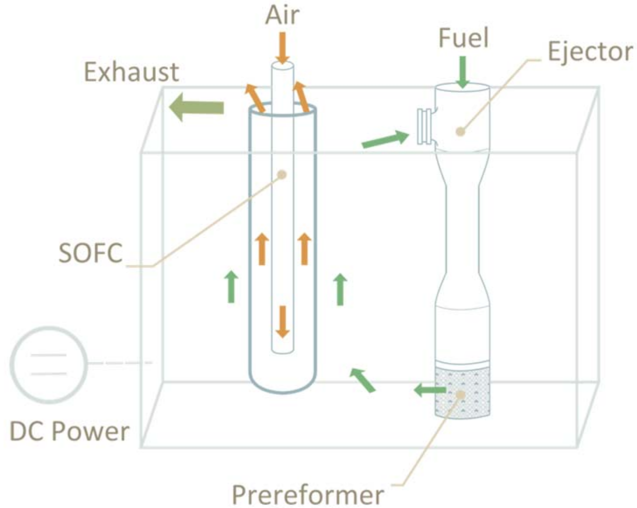
$$H_2 + O^{-2} \xrightarrow{r_{anode}} H_2O + 2\,e^-$$

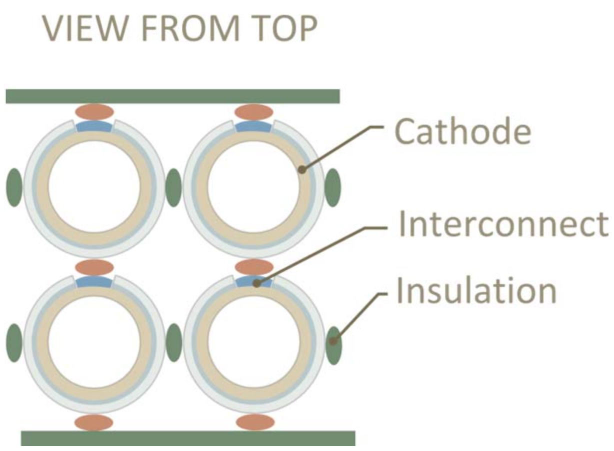
$$O_2 + 4e^- \xrightarrow{r_{cathode}} 2\,O^{-2}$$

$$2\,H_2 + O_2 \xrightarrow{r_{redox}} 2\,H_2O$$

Electricity is primarily produced through H_2 oxidation. CO oxidation also occurs.

Tubular SOFC Systems





Tubular cells are arranged in bundles and connected in series.

Methane is internally reformed given operating temperatures from 600-1000°C.

Tubular Solid Oxide Fuel Cells

Why the interest in SOFCs?

- High efficiencies over a wide power range (1 kW – 100 MW):
  40-50% (LHV) for SOFC, 60-70% for GT-SOFC, 80-90% for GT-SOFC + cogeneration.
- Fuel flexibility:
  - Natural gas, gasoline, diesel, coal
  - Hydrogen, methanol, ethanol, biomass
- Suitability for cogeneration with high exhaust temperatures
- Low noise and emission levels.

Why are SOFCs not in widespread use?

- Reported lifetimes have yet to reach goals – 40,000 h (DOE) – causing cost of electricity to be high.
- Microcracking, sulfur catalyst poisoning, carbon deposition, and air & fuel starvation decrease lifetime.

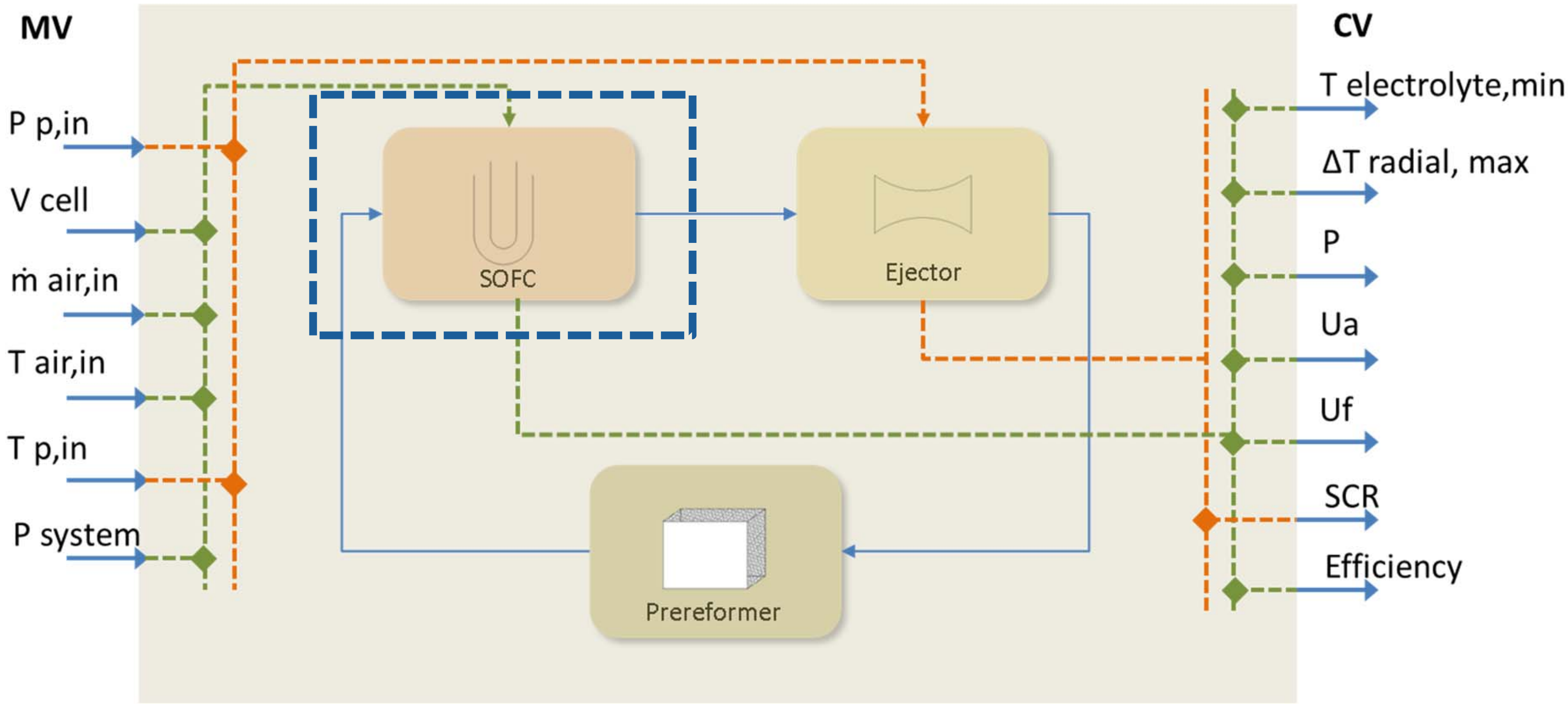
Dynamic Modeling of Thermal Stress Indicators

SOFC Performance and Operational Variables

Performance Requirement	Controlled Variable
DC Power Delivery	Power (W)
Thermal Stress Minimization	Minimum Cell Temperature (K)
	Radial Thermal Gradient (K/m)
Avoid Carbon Deposition	Steam-to-Carbon Ratio
Avoid Air and Fuel Starvation	Air and Fuel Utilization (%)

Fischer (2009) reports that minimum stack temperature and radial thermal gradient are the primary two contributors to high tensile thermal stresses. Conclusion agrees with Nakajo (2006).

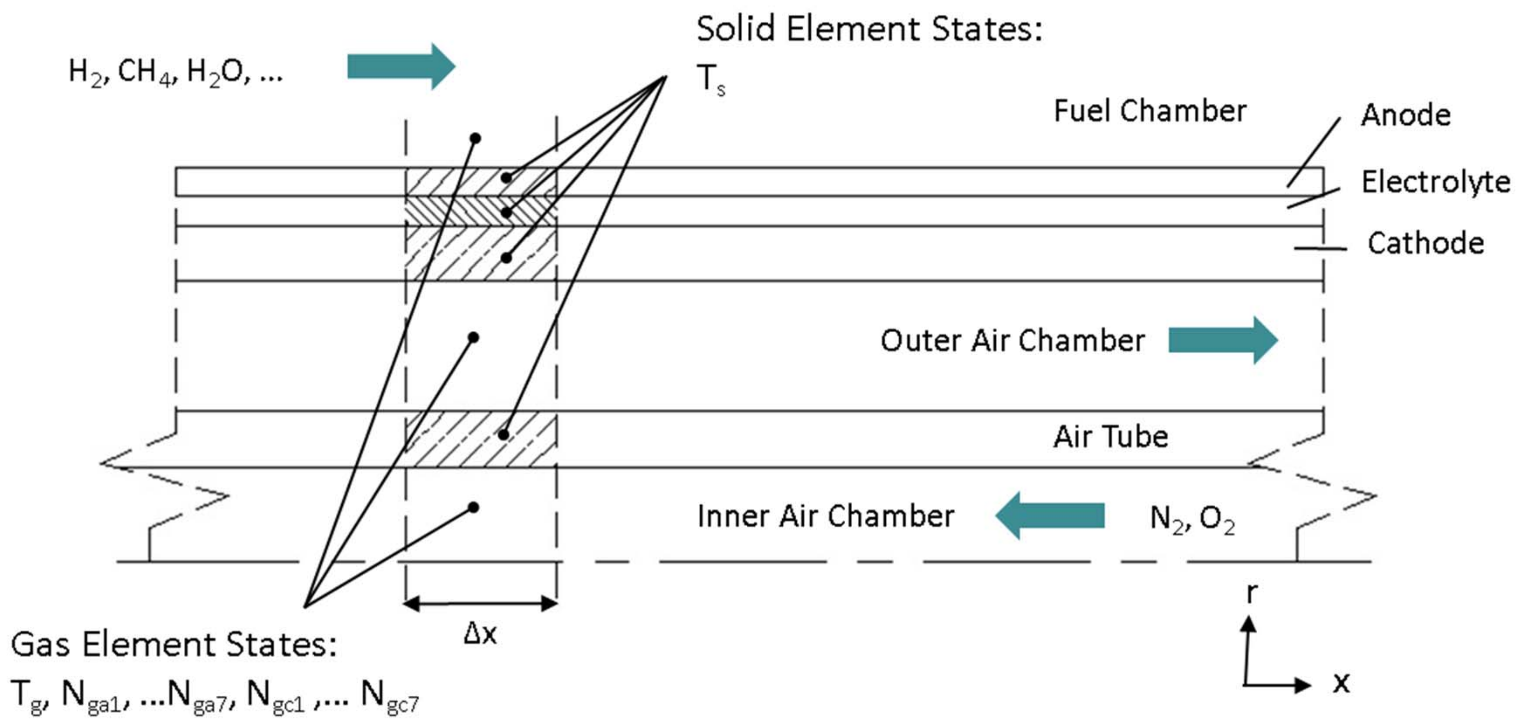
SOFC System Model in Simulink



Next Slides: SOFC model details

SOFC Submodel: 2D Model Discretization

SOFC Cross-Section in Radial (r) and Axial (x) Directions



Total DAE States per Radial Element = 65 : Temperatures, Molar Flows, Current, and Intermediate Variables

Total Nodes per Steady-State Model = 40, per Dynamic Model = 10

The distributed parameter model captures factors causing high thermal stresses

SOFC Submodel: First-Principles Equations

Electrochemical Model

$$V_{cell} = V_{oc} - \eta_{act} - \eta_{conc} - \eta_{ohm}$$

$$V_{oc} = V^0_{H_2} + \frac{RT}{2F} \ln\left(\frac{p_{H2}\, p^{0.5}_{O_2}}{p_{H_2O}}\right)$$

$$V^0_{H_2} = -\frac{\Delta G_0}{2F} + \frac{\Delta S_0}{2F}(T - 298)$$

$$\eta_{ohm} = I\, R_{ohm} \qquad \eta_{act} = \frac{R\,T\,i}{n\,F\,i_0}$$

$$i_{0,an} = \gamma_{an}\left(\frac{p_{H_2}}{p_{amb}}\right)\left(\frac{p_{H_2O}}{p_{amb}}\right)^m \exp\left(-\frac{E_{act,an}}{RT}\right)$$

$$i_{0,cat} = \gamma_{cat}\left(\frac{p_{O_2}}{p_{amb}}\right)^{0.25} \exp\left(-\frac{E_{act,an}}{RT}\right) A/m^2$$

Energy Conservation Model

$$\rho V c_{p,i} \frac{dT_{s,i}}{dt} =$$

$$h\,A\,(T_{s,surf,i} - T_{g_i}) + k\,A \frac{dT_{s,i}}{dx} + \varepsilon\, F_i\, \sigma\, A\,(T^4_{s,opp} - T^4_s)\,|_i + Q_{elec}$$

$$Q_{elec} = \left(\frac{\Delta H_{f,H_2O(g)}}{n\,F} - V_{cell}\right) \cdot i_i$$

$$\frac{c_{p,ig}}{R} = \alpha + \beta T + \gamma T^2 + \frac{\varsigma}{T^2}$$

Steam Methane Reforming Model

$$CH_4 + H_2O \xleftrightarrow{r_{CH_4}} CO + 3\,H_2$$

$$CO + H_2O \xleftrightarrow{r_{shift}} CO_2 + H_2$$

$$r_{CH_4} = A \exp\left(-\frac{E_a}{RT}\right) p_{CH_4}$$

$$r_{shift} = k\left(X_{H_2O}\, X_{CO} - \frac{X_{H_2}\, X_{CO_2}}{K_{eq}}\right)$$

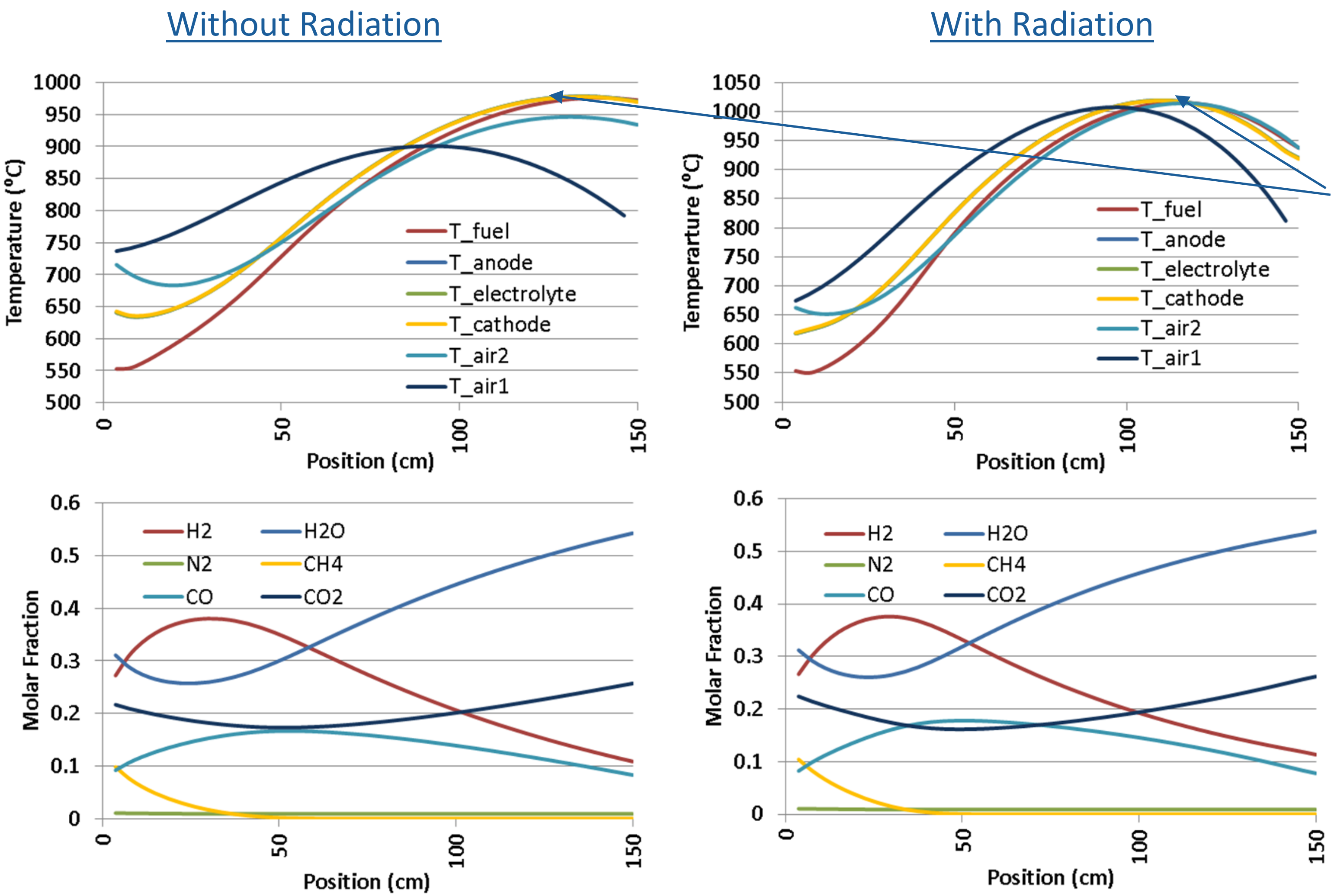
$$K_{eq} = \exp(-0.2935\,\zeta^3 + 0.635\,\zeta^2 + 4.1788\,\zeta + 0.3169)$$

$$\zeta = \frac{1000}{T} - 1.$$

Some past literature iterate b/t electrochemical and energy models for steady-state solutions **– here it is solved simultaneously and dynamically using APMonitor Modeling Language.**

SOFC Submodel: Radiation Sensitivity

Radiation Analysis for Plant B : Air channel radiation is significant

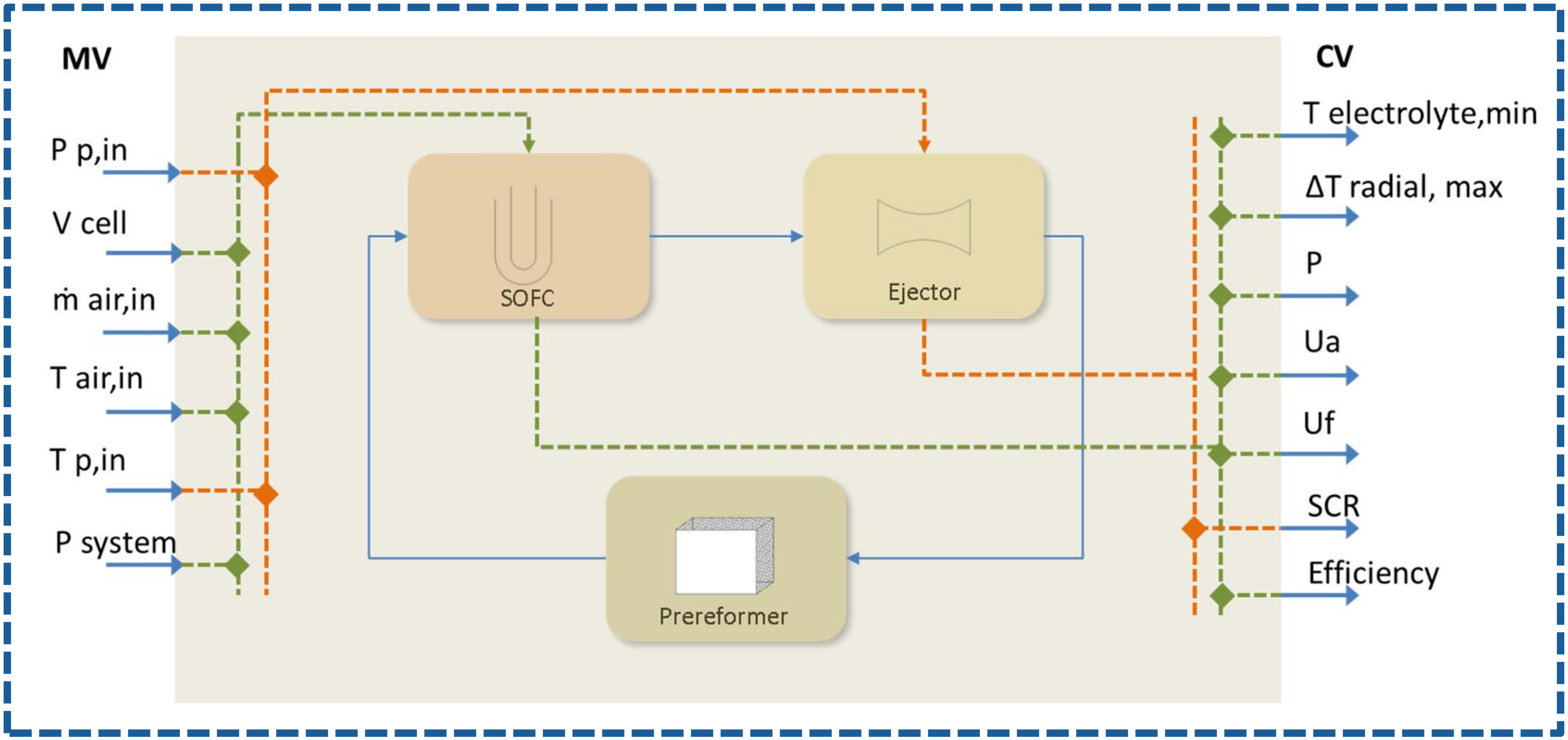


Radiation Effects:

- Increased peak temperature
- Inlet air and solid PEN is closer in temperature
- Molar flow exhibits negligible change.

Final Steady-State Model = Validated Campanari Model **+** Air Channel Radiation

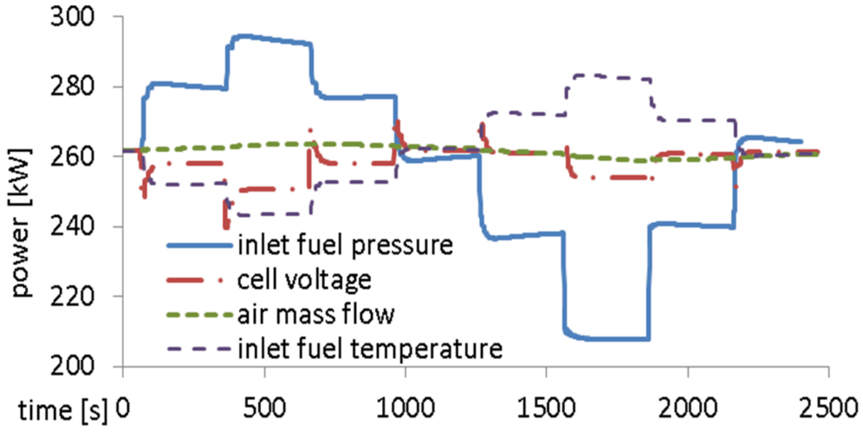
SOFC System Model in Simulink



Next Slides: Dynamic results for full SOFC system model

Dynamic Response of Controlled Variables

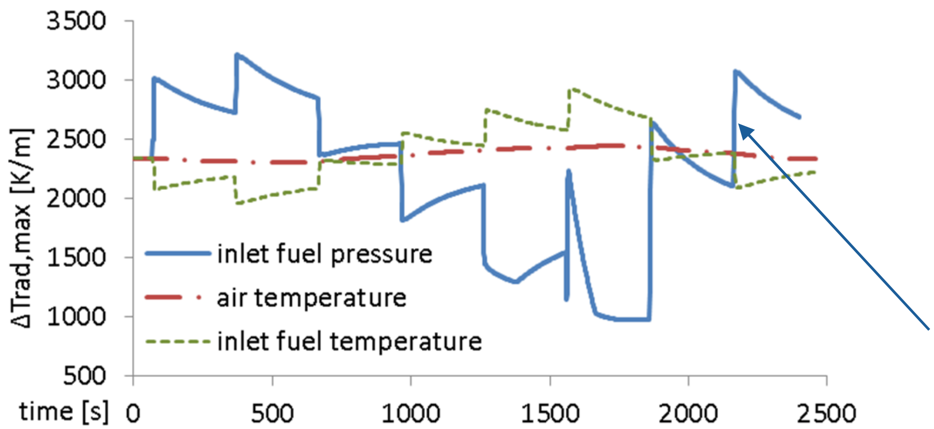
Power



- Power increases as fuel flow rate/density increases – with higher pressure and lower temperature.
- Voltage or current is not an effective MV for load-following near peak power.

Maximum Radial Thermal Gradient

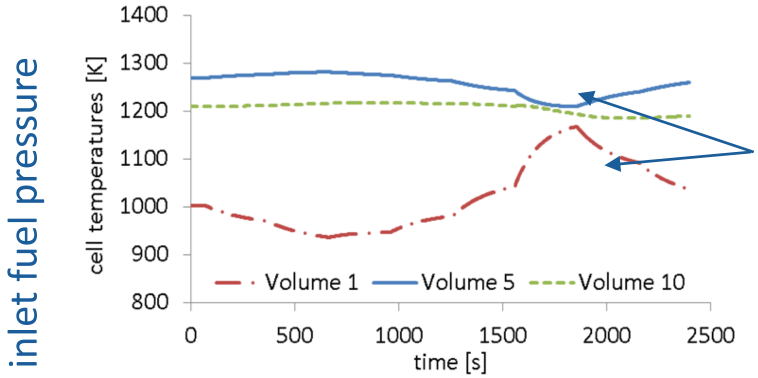
Thermal Stress Indicator

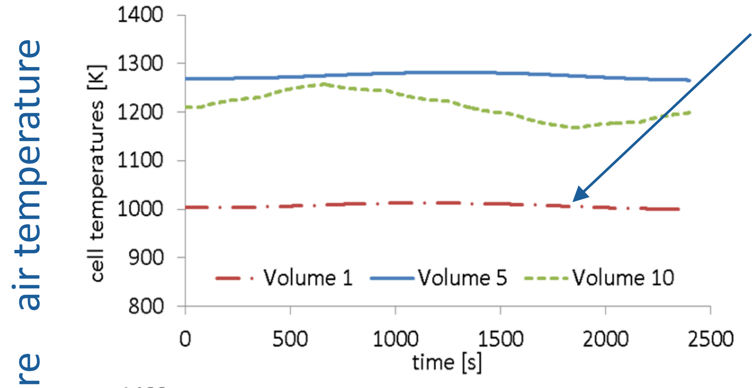


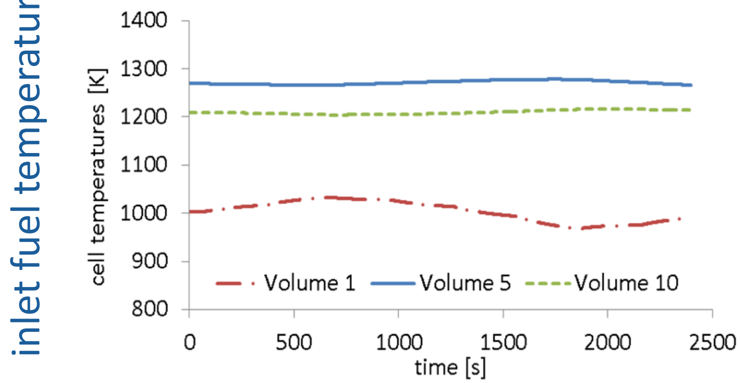
- Main MVs for controlling power also affect the thermal gradient significantly.
- Air temperature has little effect due to insulation from the thick cathode.
- The gradient responds on the same time scale as power due to numerator dynamics.

New Conclusion - thermal gradients should be controlled at the same time scale as the power

Dynamic Response of Controlled Variables







Axial Cell Temperatures

Thermal Stress Indicator

Fuel pressure and temperature effect on inlet cell temperature is twice or greater than middle or outlet temperature.

Air temperature effects outlet temp but not inlet. Relatively thick cathode (1 mm) insulates the anode inlet.

Key Conclusions:

1) The median temperature dynamics are unique from the minimum temperature dynamics.

2) Some variables may be disturbances to the minimum temperature if not set as MVs – inlet fuel temperature.

3) The primary MVs for load-following also affect the minimum temperature.

Constrained Predictive MIMO Control of the SOFC

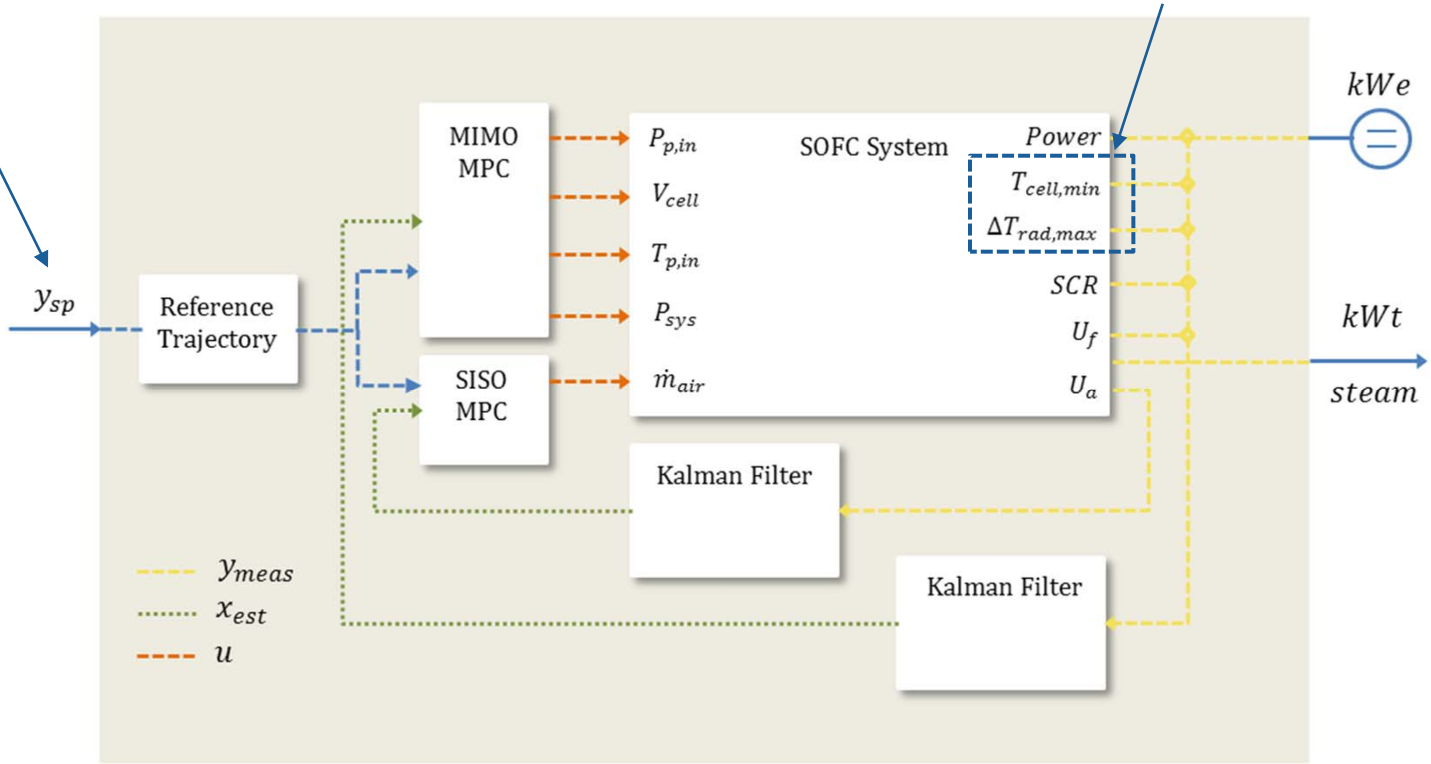
MIMO Control Structure

Decentralized MIMO + SISO Control

Tracked CVs
- Power
- Tcell,min

Constrained CVs
- dTrad,max
- Tcell,min
- SCR
- Uf
- Ua

Thermal Stress Indicators



Measurements or estimates of the thermal stress indicators are used directly as controlled variables.

Linear MPC Algorithm

MPC Formulation:

Constrained Nonlinear Programming Optimization

$$\min_{u(t)} J = \underbrace{\frac{1}{2}(\mathrm{x}-\mathrm{x}_{ref})^T \,\widetilde{\mathrm{Q}}\,(\mathrm{x}-\mathrm{x}_{ref})}_{\text{CV Tracking Error}} + \underbrace{\frac{1}{2}\Delta\mathrm{u}^T\mathrm{R}\Delta\mathrm{u}}_{\text{MV Move Suppression}} + \underbrace{\frac{1}{2}\xi^T\mathrm{V}\xi}_{\text{Slack Variables}}$$

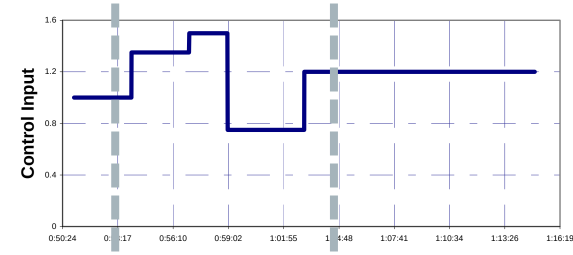
where

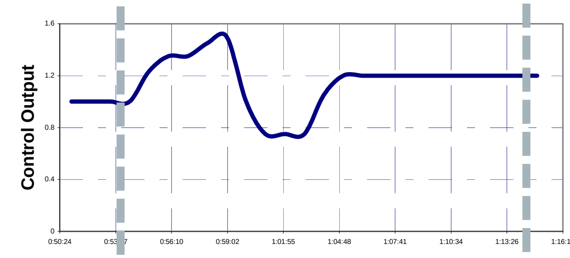
$$\mathrm{x}-\mathrm{x}_{ref} = (\Gamma\,\Delta\mathrm{u} + \Omega\,x_0) - \widetilde{\mathrm{C}}\,\mathrm{y}_{ref}$$

s.t.

$$\begin{array}{ccccc} u_{min} & \leq & u(k) & \leq & u_{max} \\ \Delta u_{min} & \leq & u(k)-u(k-1) & \leq & \Delta u_{max} \\ y_{min} & \leq & y(k)+\xi(k) & \leq & y_{max} \end{array}$$

MV horizon





CV horizon

Vectors represent variable values across the horizon

Unique Features

- Tracking and slack variable weights vary by variable and time step to control variables with very different dynamics and settling times.

- Minimum cell temperature has a time constant 100-1000x greater than the fast time constant of other CVs.

Linear MPC Algorithm

Reference Trajectory

$$y_{ref} = y_0 + y_{sp}\left(1 - \exp\left(-\frac{t}{\tau_r}\right)\right)$$

Reference trajectory converges to the CV target with first-order dynamics.

The time constant, τ_r, is defined as 1/5 of the acceptable time to reach steady-state.

Analytical Derivatives

$$\begin{aligned}
\frac{dJ}{d\tilde{u}} &= \left[\frac{dJ}{du}, \frac{dJ}{d\xi}\right] \\
\frac{dJ}{du} &= \left((\mathbf{x} - \mathbf{x}_{ref})^T \widetilde{\mathbf{Q}}\,\Gamma \; + \Delta\mathbf{u}^T\mathbf{R}\right)\frac{d\Delta u}{du} \\
\frac{dJ}{d\xi} &= \boldsymbol{\xi}^T\mathbf{V}
\end{aligned}$$

Analytical derivatives are used by the MATLAB *fmincon* solver to reduce computational time. Derivatives are calculated using matrix calculus.

Kalman Filter State Estimation

The Kalman filter provides the linear unbiased minimum variance estimate for the unmeasured states.

$$\begin{aligned}
X^+(k)_j &= X^-(k)_j + \Delta x(k)_j \\
\Delta x(k)_j &= K(k)_j\, \Delta y(k)_j \\
\Delta y(k)_j &= Y(k)_j - G(k)_j \\
G(k)_j &= C_j\, X^-(k)_j,
\end{aligned}$$

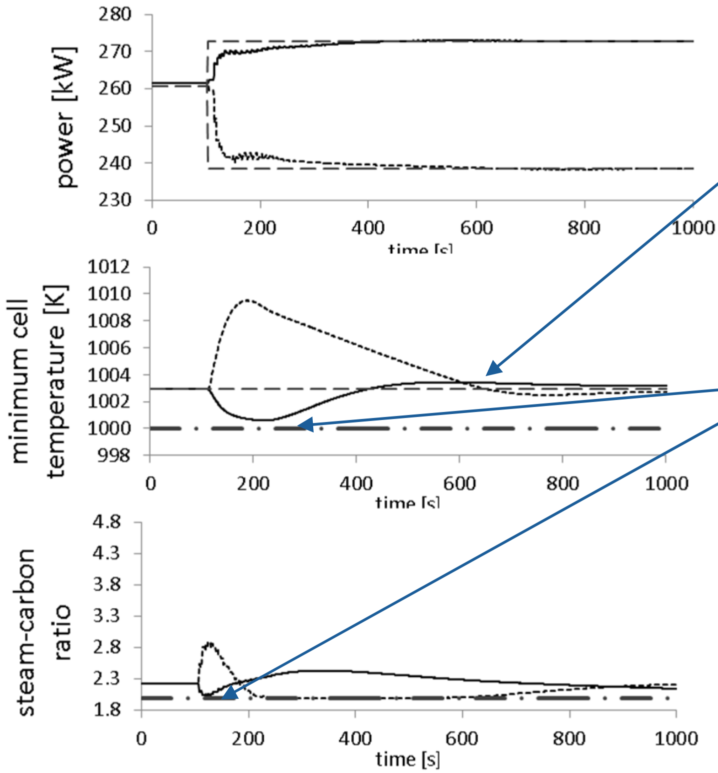
Kalman gain

$$\begin{aligned}
K_j &= \bar{P}(k)_j\, \widetilde{H}_j\left(\widetilde{H}_j \bar{P}(k)_j \widetilde{H}_j^T\right)^{-T} + R \\
\widetilde{H}_j &= C_j,
\end{aligned}$$

MPC Results: Reliability Control Study

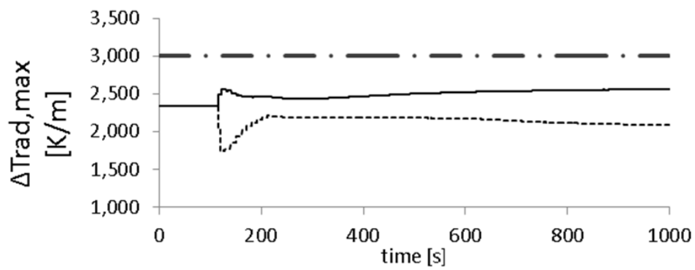
Objective: Determine whether controlling outlet gas temperatures or average cell temperature provides control of thermal stress indicators – common approach in literature.

Minimum Temperature Control



- Power output settles in 400 s.

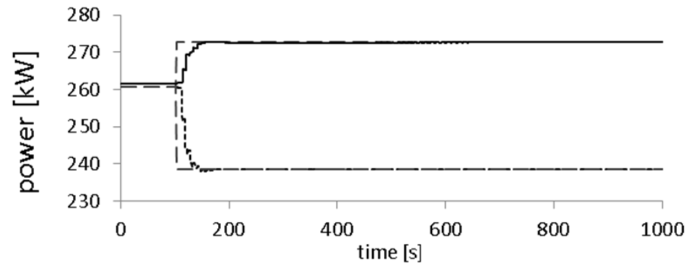
- The minimum cell temperature settles to the target in 700 s.
- Minimum cell temperature constraint prevents limit violation.
- The minimum cell temperature and steam-to carbon ratio limits affect the solution at t=150 s.

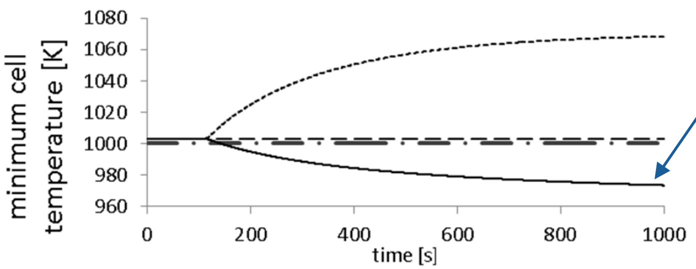


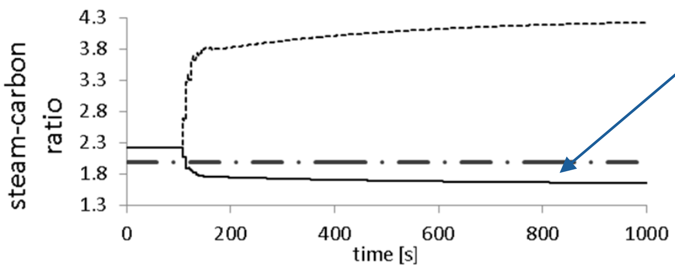
Load-following is achieved while maintaining thermal stress indicators in limits.

MPC Results: Reliability Control Study

Average Temperature Control



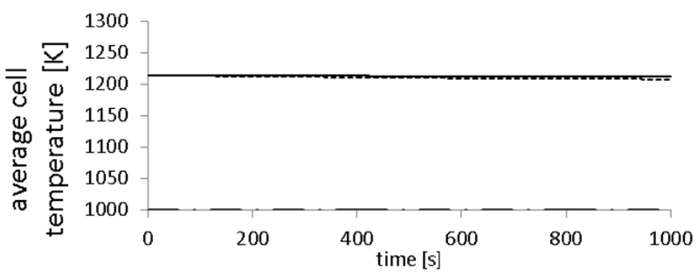




- Power and average temperature are tracked. No other CVs are constrained.

- The minimum temperature travels 30 K past the previous lower limit constraint. Outlet temperature control results are nearly identical.

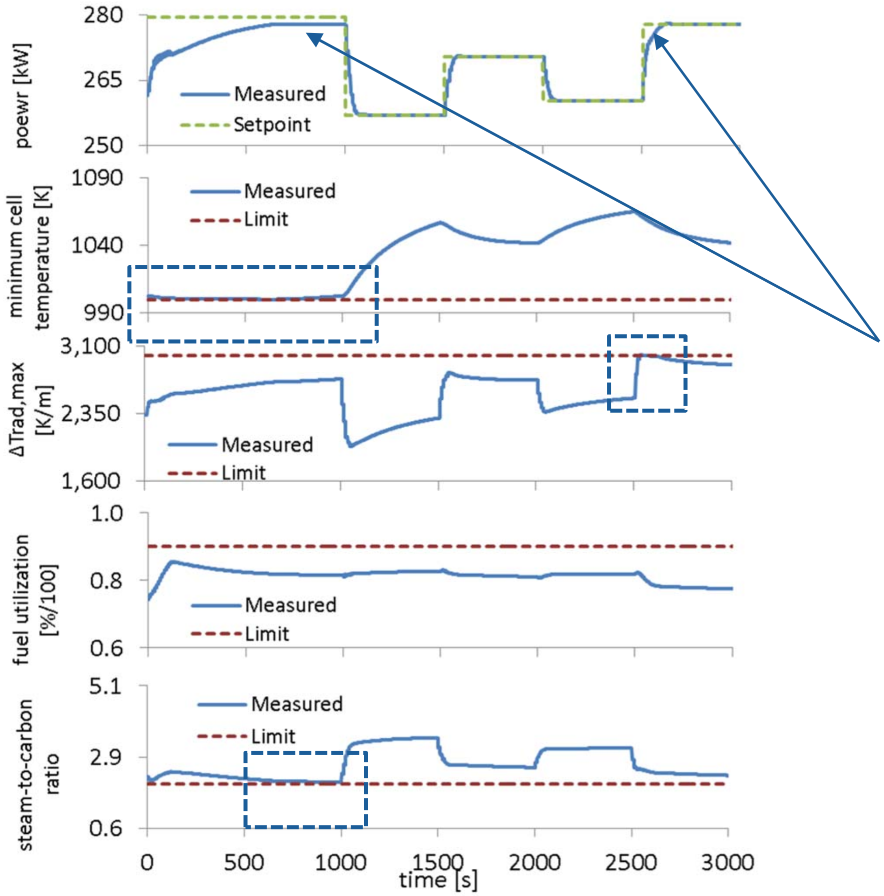
- Steam-to-carbon ratio would violate limits without constrained control.



Nearly identical results when outlet gas temperature is controlled.

MPC Results: Load-Following Study

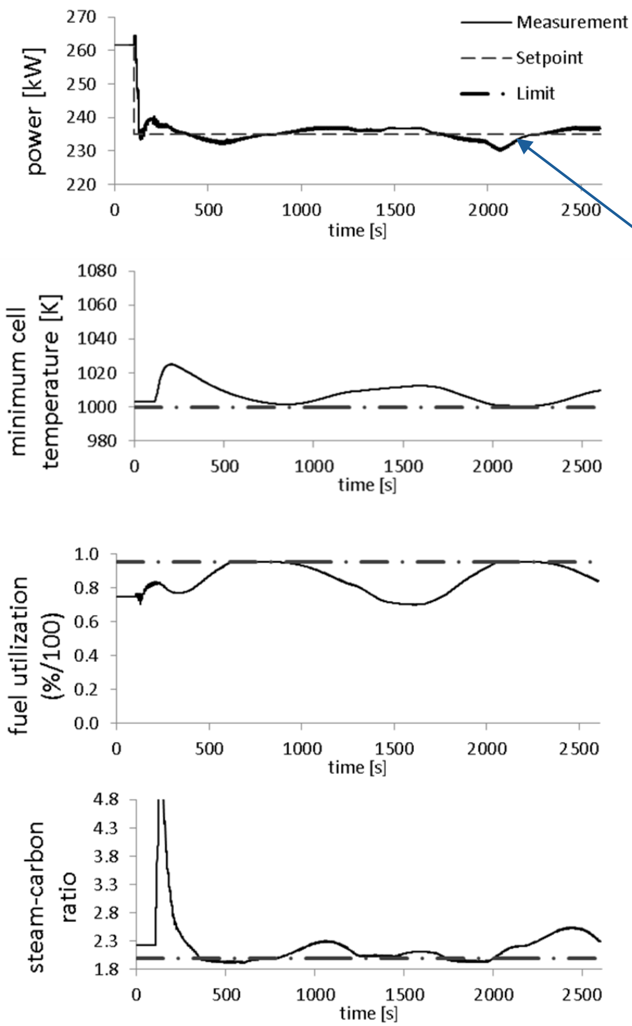
Objective: Test load-following while satisfying thermal-stress based constraints.



- Load-following is achieved between 250-280 kW with settling times between 50 – 750 s.
- Minimum cell temperature, thermal stress constraints, and stream-to-carbon ratio lengthen settling time at higher loads.

MPC Results: Disturbance Rejection Study

Objective: Investigate whether LMPC maintains power output in the presence of alternating fuel quality, relevant for biogas applications.



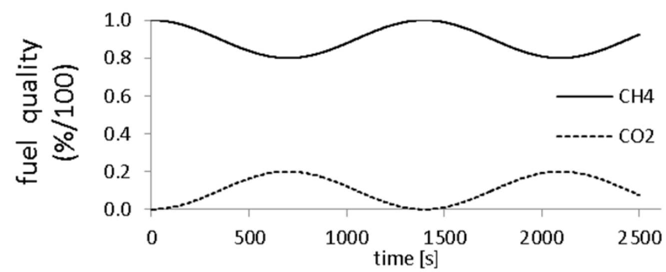
- An augmented MV variable is used to include disturbance measurements.

$$\Delta\tilde{u}(k) = \begin{bmatrix}\Delta u(k)\\ \Delta d(k)\end{bmatrix}$$

- Load demand is satisfied within 2% of the setpoint.

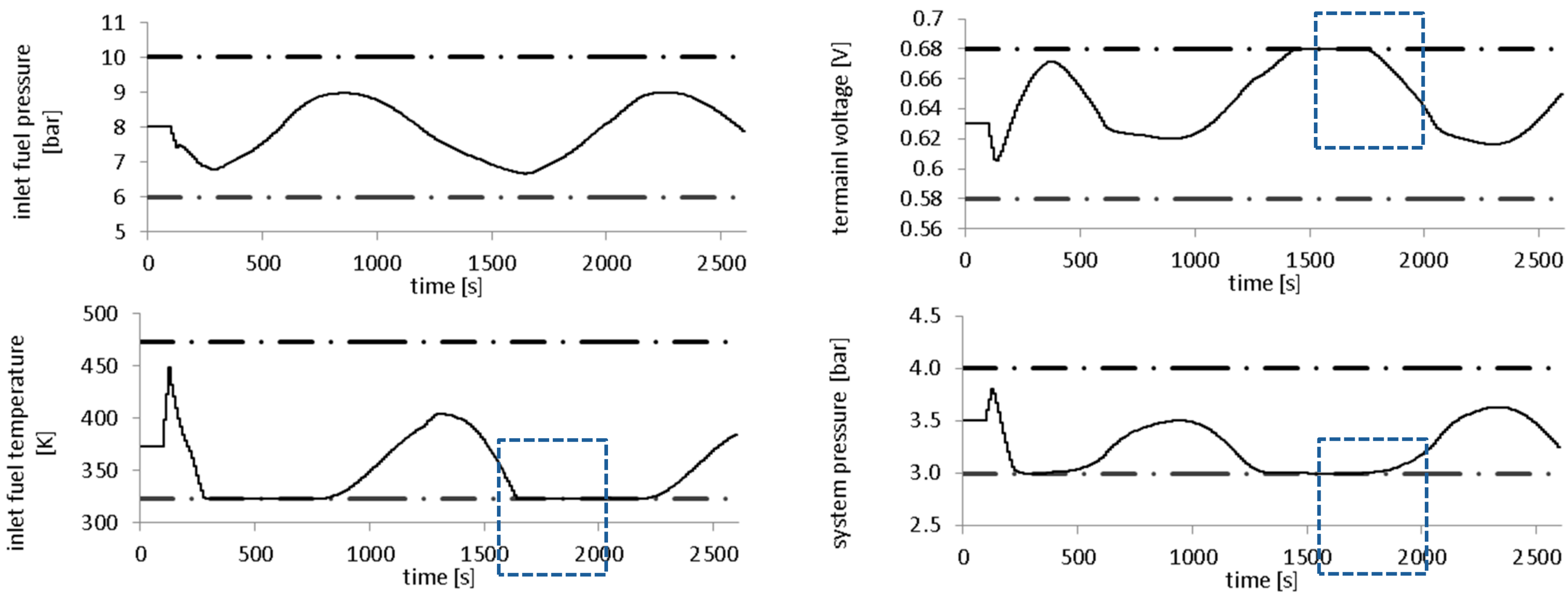
- Three CVs are riding constraints with negligible violations at low methane conditions.

Disturbance Variable: CH_4 mole %



MPC Results: Disturbance Rejection Study

Manipulated Variable Plots



3 of 4 manipulated variables are at constraint values as methane decreases from peak values.

Conclusions

Dynamic Modeling of Thermal Stress Indicators

- Investigated dynamics of minimum cell temperature and maximum radial thermal gradient for the tubular SOFC.
- Thermal stress should be controlled on same time scale as load due to numerator dynamics of thermal gradient.
- Demonstrated effect of radiation on tubular SOFC temperature and concentration profiles.

Constrained Predictive MIMO Control of the SOFC

- A distributed-parameter based model is recommended for controlling thermal stress indicator dynamics. Lumped models or outlet temperature measurements are not sufficient.
- Varying time constants of SOFC can be accommodated by using non-constant MPC tracking weights.
- LMPC is capable of rejecting measured fuel quality disturbances.

Acknowledgments

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- APMonitor Modeling Language
- ExxonMobil
- NSF IGERT Program
- Labmates

Questions ?

Appendix

Tubular Solid Oxide Fuel Cells

Problem Statement

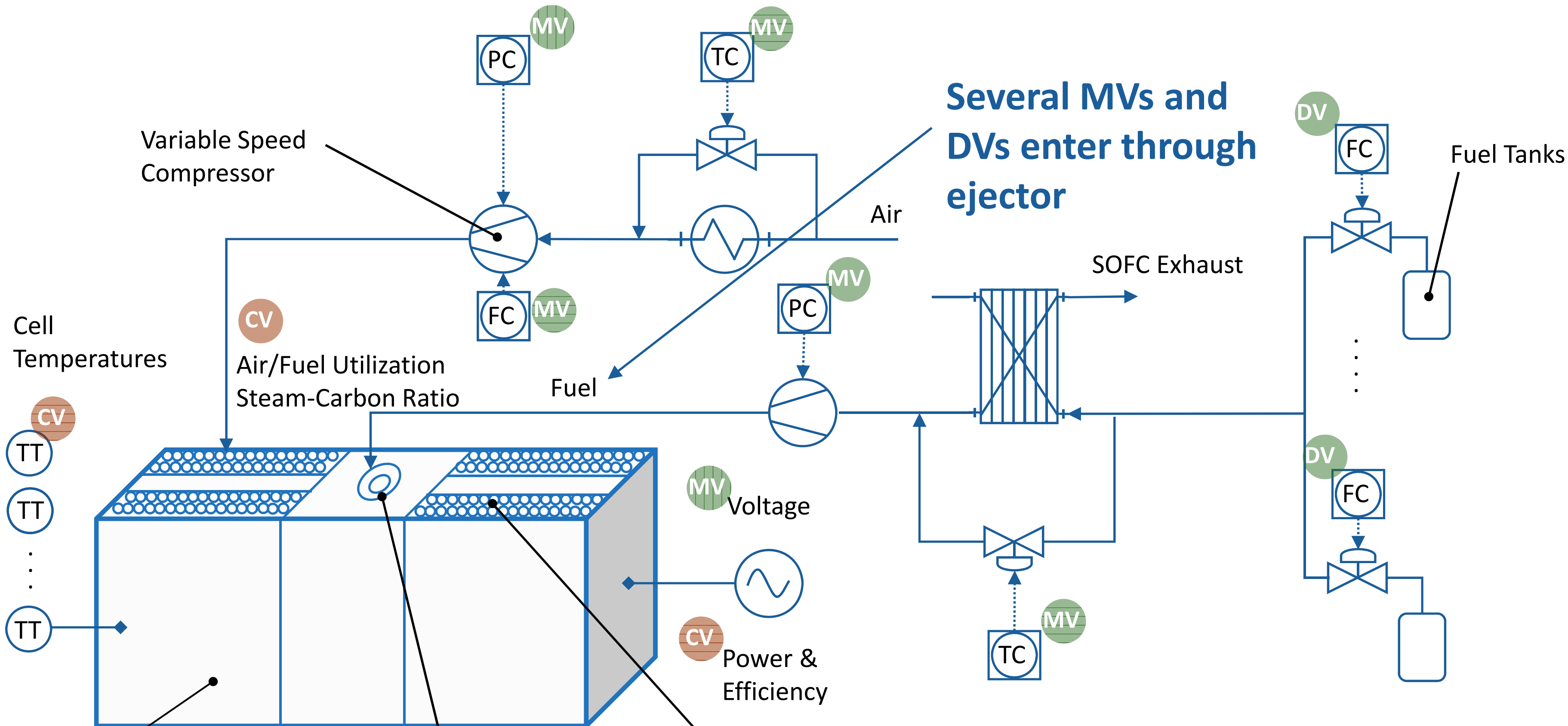
Research is needed to investigate the dynamics of factors causing the SOFC to experience shortened lifetimes, especially microcracking, and directly control these factors.

SOFC System Modeling Decisions

Feature	Description
7 Molar Gas Species	7 species (H_2, H_2O, N_2, O_2, CH_4, CO, CO_2) are needed to accommodate methane fuel and air oxidant. Some models may use 3 (H_2, H_2O, O_2).
Reformation Reactions	Steam-methane reformation, water-gas shift. Introduce nonlinearities and implicit equations – increased convergence difficulty. Unnecessary with H_2 fuel.
2D Discretization	Axial and radial discretization is required to capture **minimum cell temperature** and **maximum radial thermal gradient**. 0D (lumped) and 1D models capture neither and have less accurate performance prediction.
Voltage Losses	Includes ohmic, activation, and diffusion losses. Some models include only 1.
Material Properties	Temperature-dependent, nonlinear ohmic resistance and specific heat models.
Pressure Drop	Based on Darcy's law, compressible flow with < 10% pressure drop. Models may choose constant pressure drop.
Minimum/Maximum Functions	Variables may occur at different locations – maximum gradient, minimum temperature.
Multiple Submodels	SOFC, Ejector, Prereformer. Necessary for modeling real inputs.
Heat Transfer	Non-Isothermal. Convection, Radiation, and Two-Dimensional Conduction.
Time Delays	Transport time delays since molar transport is assumed at quasi-steady-state

Goal: accurate dynamic model directly applicable to real SOFC system operation.

SOFC and Balance of Plant



Prereformer:
Quasi-Steady-State
Algebraic Model
8 States
Matlab

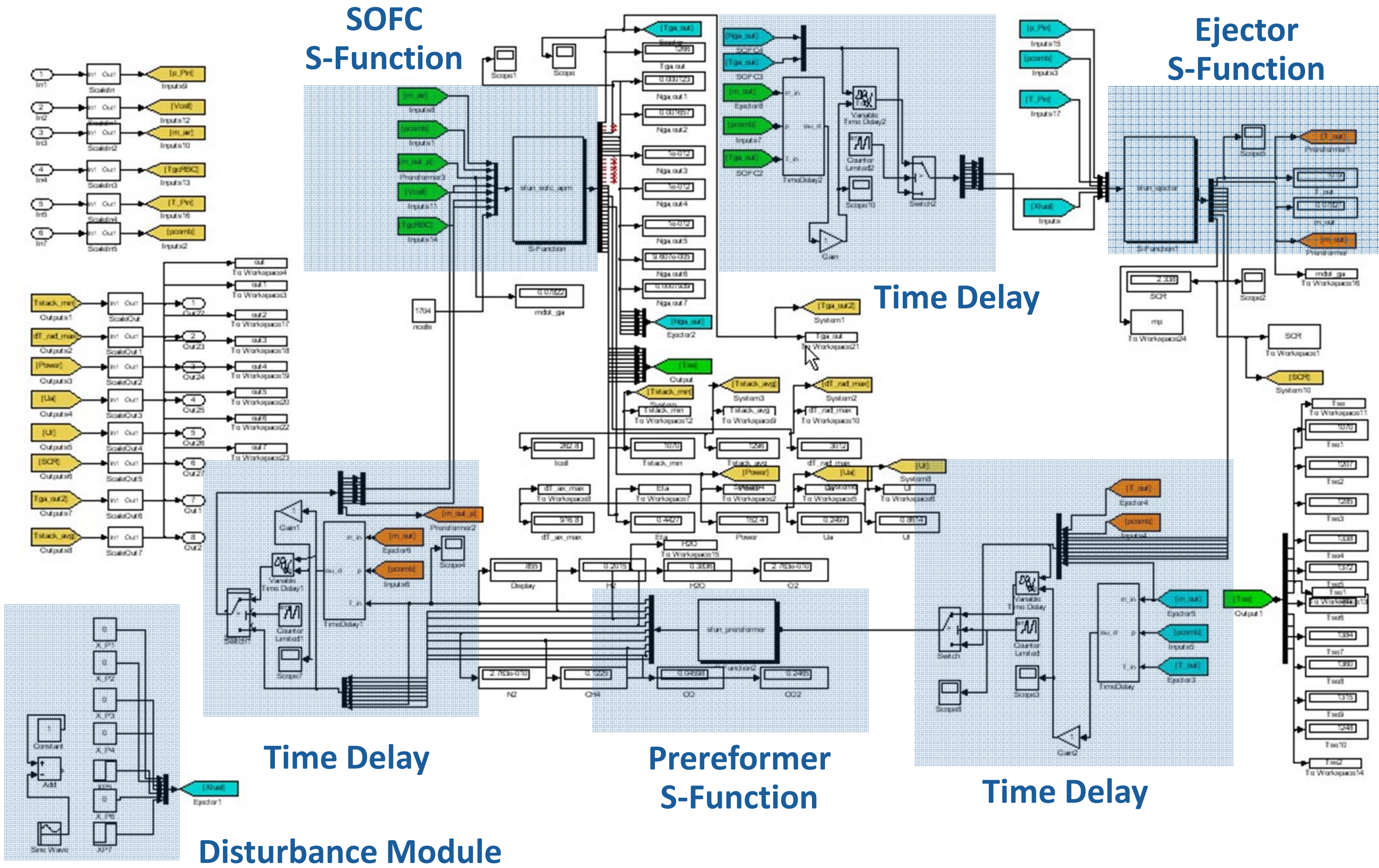
Ejector:
Quasi-Steady-State
Algebraic Model
9 States
Matlab

SOFC :
Dynamic
DAE Model
220 States
APMonitor

MV: manipulated variable
CV: controlled variable
DV: disturbance variable

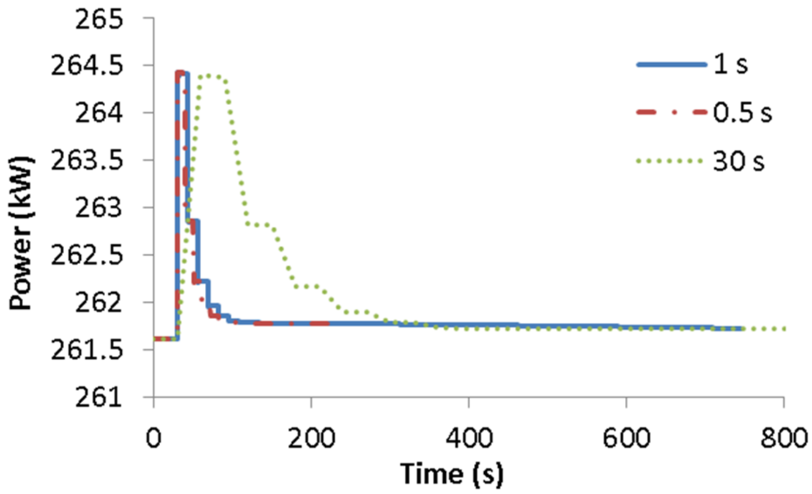
Ejector and prereformer models are necessary to accommodate realistic MVs

SOFC System Simulink Model



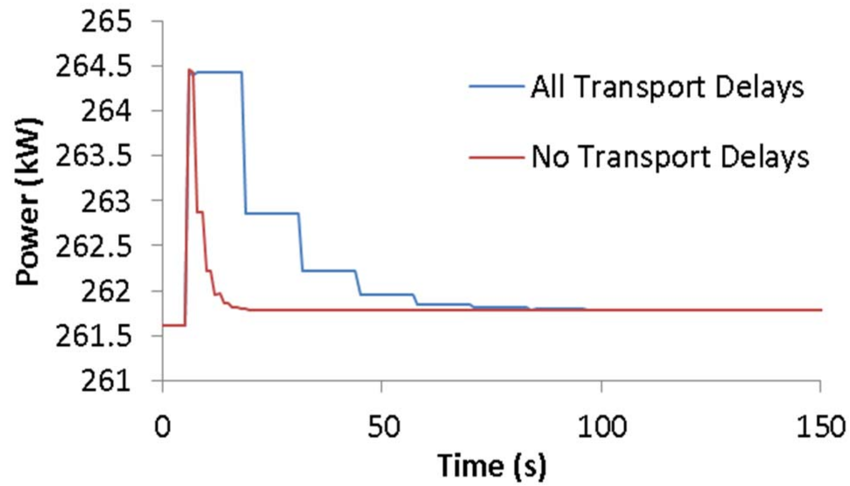
Simulink Dynamic Simulation Design

Simulation Time Discretization: Power Response to Voltage Step



- Decreasing time steps below 1 s yields little change in dynamic response.
- The QSS gas transport assumption is valid to 1s time steps.

Transport Time Delays



- **Delays are important for sub-60 s response.**
- Transport delay is a function of mass flow.

Model Validation and Verification

Validation Process

Steady-State Model

1) **Ensure credibility of model equations published in literature.** Model is sourced from many authors due to incomplete or inaccurate models in literature.

2) **Literature search for design parameters.** 2D model requires many specific parameters from many authors.

3) **Match model output directly to empirical and simulation data.** Only used 3 tuning parameters – heat transfer coefficient, cell outer diameter, and contact resistance. Authors may not describe theirs.

Steady-state model validation is consistent with the leading SOFC models in literature (Campanari, 2004; Stiller, 2006).

Verification Process

Dynamic Model

1) **Add energy balance dynamics to account for thermal time constant.**

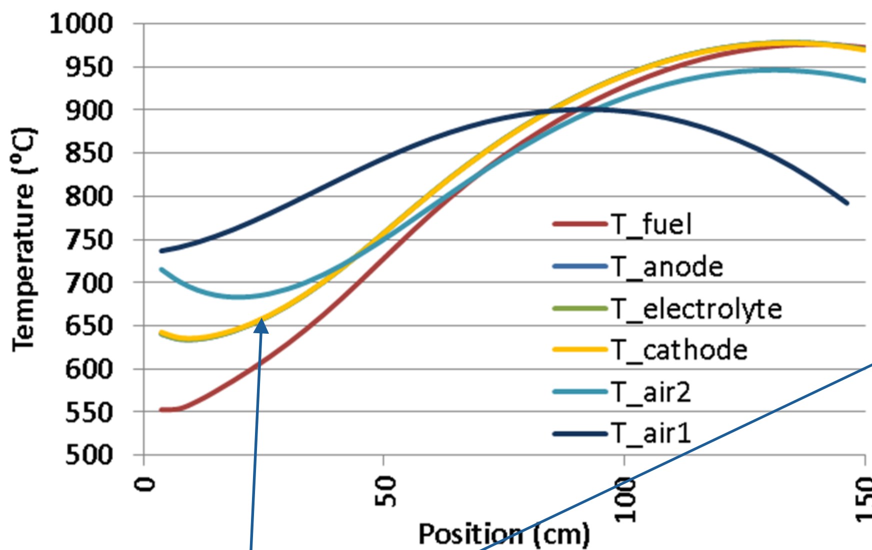
2) **Compare open-loop settling time, dynamic characteristics, and MV-CV gains to other SOFC models.** Results seen in both single-step test and staircase test.

Verification is challenging because public validation data is scarce. Noted by other authors (Bhattacharrya, 2010).

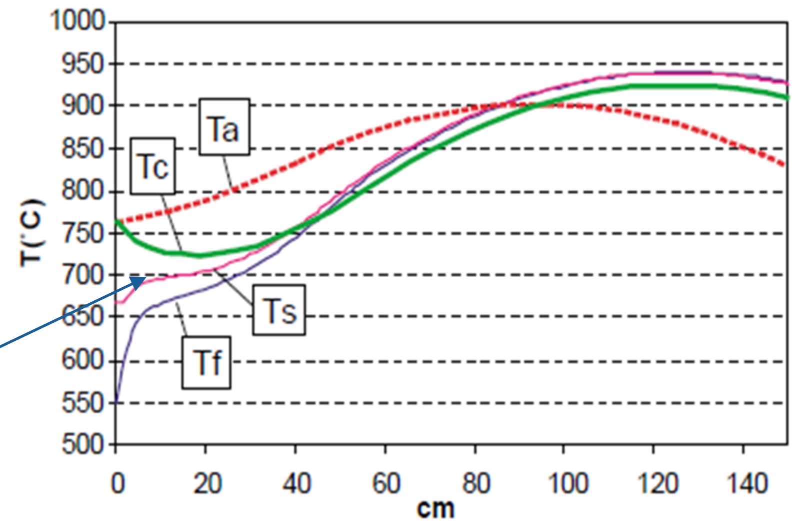
SOFC Submodel: Steady-State Validation

Validation: Match to Simulation Data

Spivey Model



Campanari Model



The mean absolute percentage (MAP) error is used to compare the models.

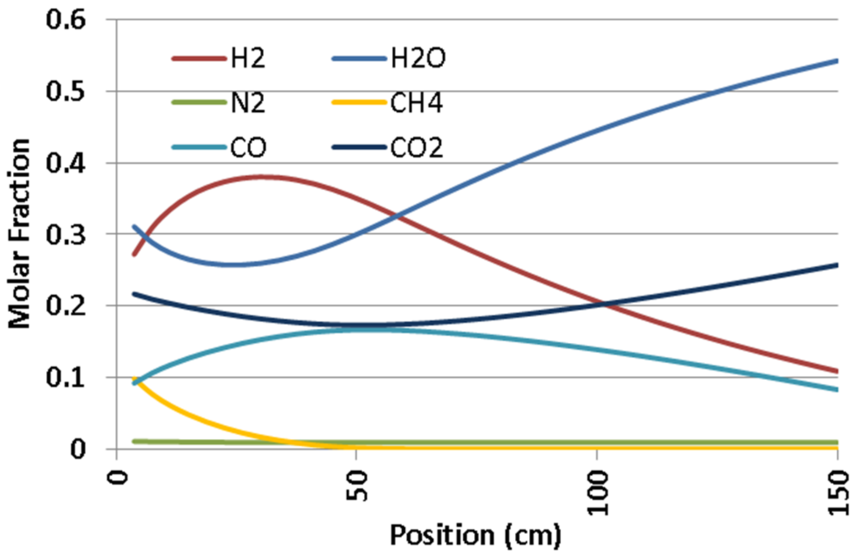
MAP for Electrolyte Temperature = 3.85%

$$MAP = \frac{1}{n}\sum_{t}\left|\frac{A_t - P_t}{A_t}\right|$$

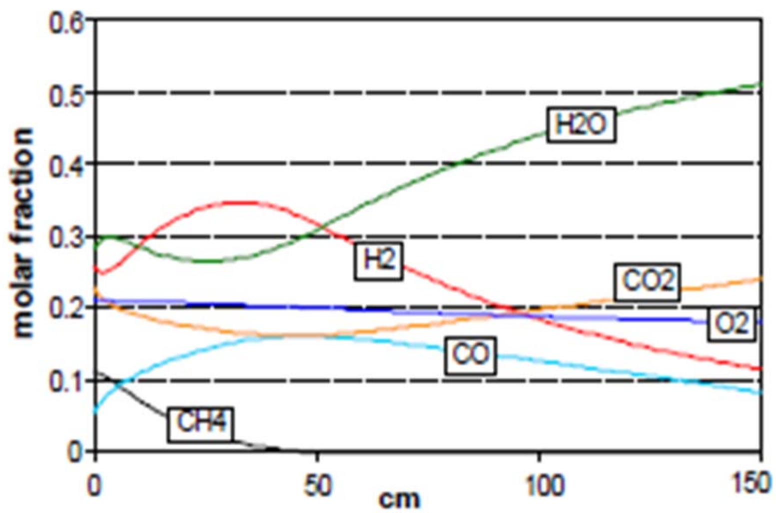
SOFC Submodel: Steady-State Validation

Validation: Match to Simulation Data

Spivey Model



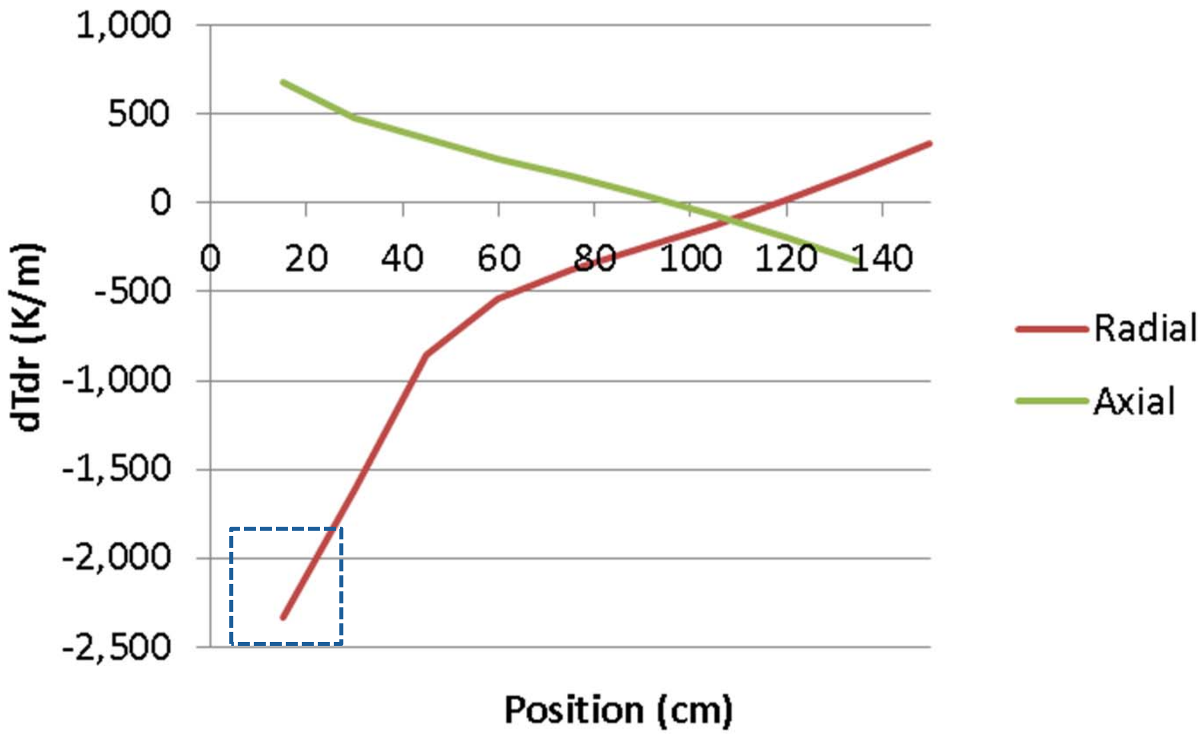
Campanari Model



Comparison of the concentration profiles also indicates that the steady-state model matches well versus the standard models used for tubular, high-temperature SOFC modeling.

Radial versus Axial Temperature Gradient

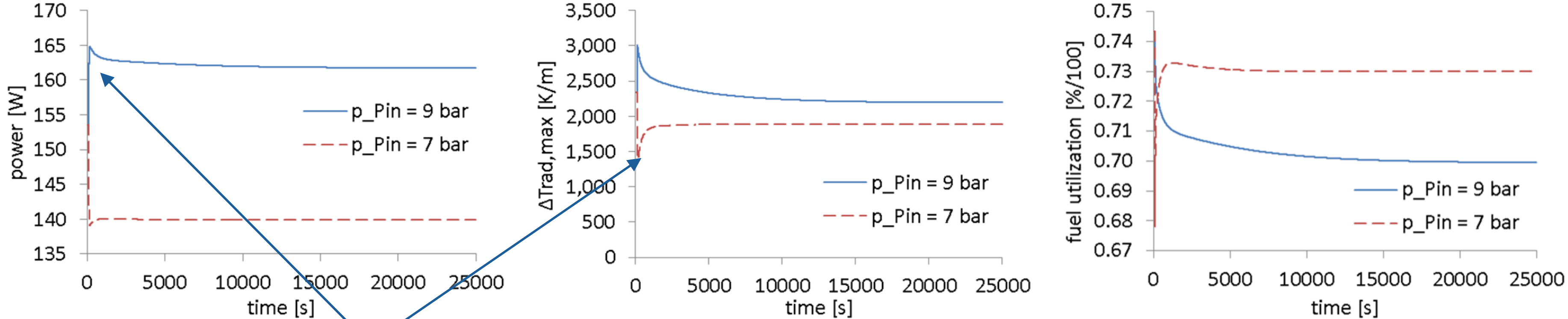
The radial gradient is negative near the fuel inlet placing the anode in tension. The radial gradient is several times the axial gradient.



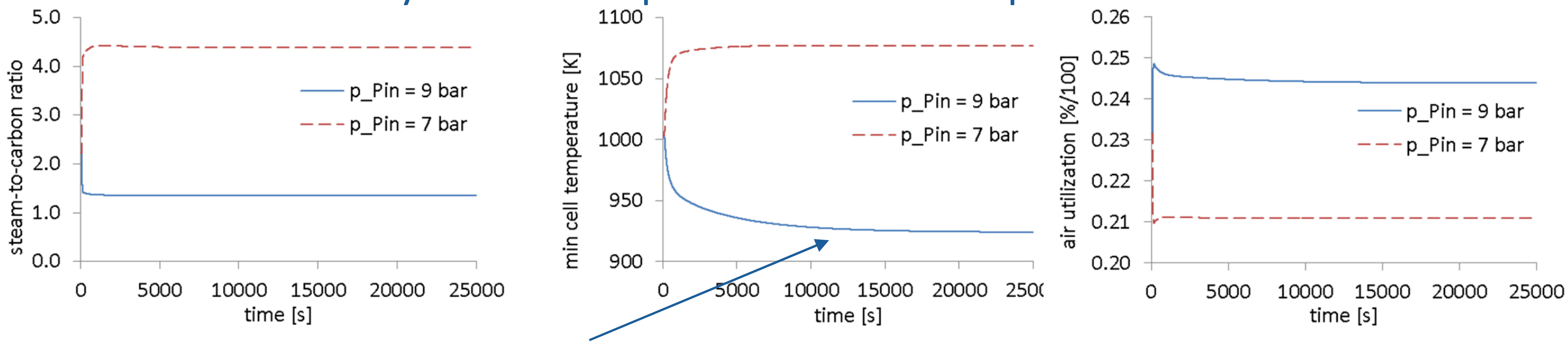
Simulation results agree with prior studies indicating that radial thermal gradients are most significant.

SOFC System Model: Dynamic Model Verification

Open-loop response to fuel pressure step



Numerator dynamics is expected due to multiple time constants.

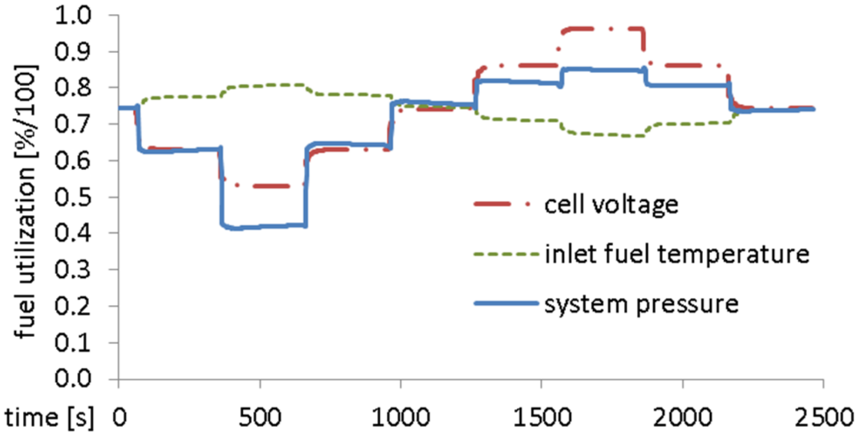


OL settling time of 2500-12000 s is consistent with literature (Hall, 1999).

Higher fuel flow increases power but decreases minimum temp – a higher reaction rate of steam-methane reformation

Dynamic Response of Controlled Variables

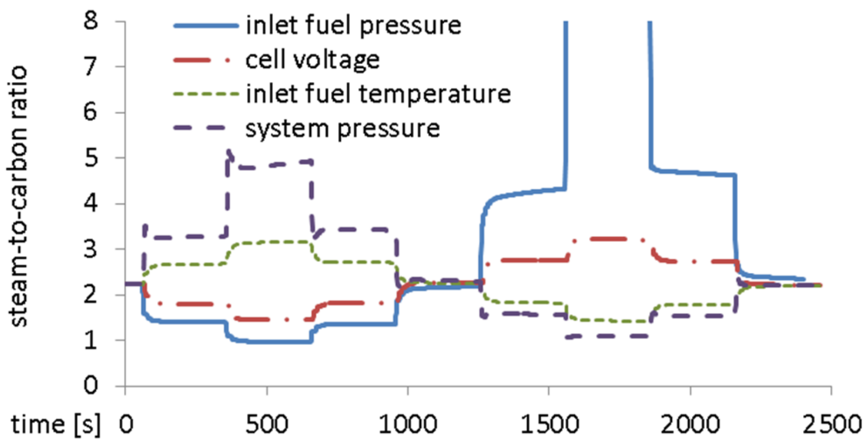
Fuel Utilization



Voltage has linear effect on fuel utilization – voltage changes current directly, thereby changing fuel consumption.

Changing fuel flow rate (pressure or temperature) does not affect fuel utilization greatly because it also affects power.

Steam-to-Carbon Ratio (SCR)



Adding fuel (increasing pressure or decreasing temperature) causes the steam-to-carbon ratio to decrease.

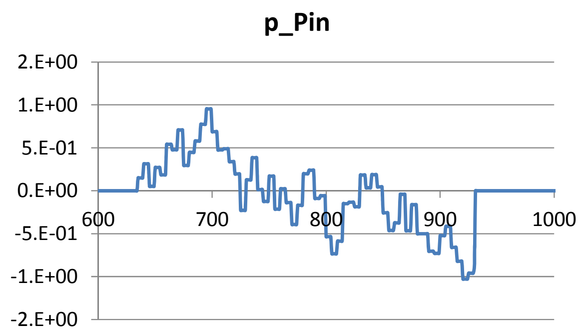
Increasing system pressure increases SCR – more recycle flow.

Decreasing voltage increases SCR – higher rate for electrochemical reaction with H_2O product.

Linear MIMO Control Model Identification

Test Signals for Dynamic Excitation

- Generated a restricted and variable length random walk signal.
- MVs and CVs are normalized by bias and slope.



Transfer Function Model

$$
\begin{aligned}
Y(s) &= G(s)U(s) \\
G(s) &= \begin{bmatrix} \frac{K(\tau_a s+1)}{(\tau_1 s+1)(\tau_2 s+1)} & \cdots & \frac{K(\tau_a s+1)}{(\tau_1 s+1)(\tau_2 s+1)} \end{bmatrix}
\end{aligned}
$$

Staircase tests used to constrain model parameter estimation – sign of gain, presence of numerator dynamics.

State-Space Model

$$
\begin{aligned}
x_{n_x}(k+1) &= A_{n_x} x_{n_x}(k) + B_{n_x} u(k) \\
y(k) &= C_{n_x} x_{n_x}(k).
\end{aligned}
$$

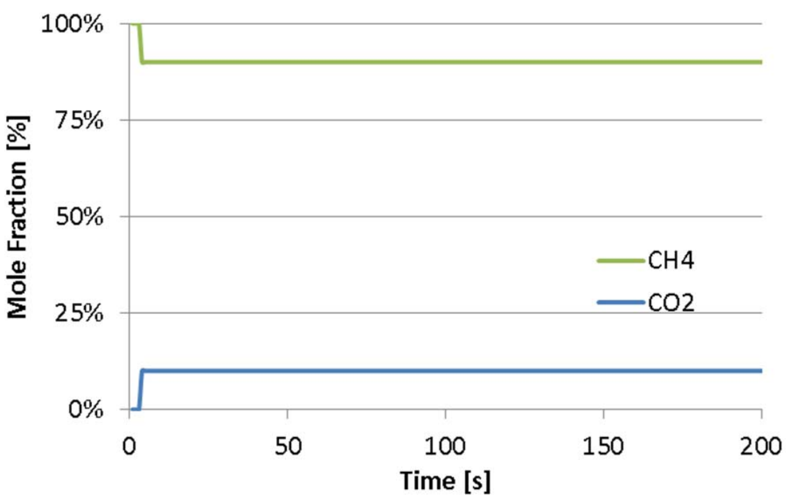
Conversion from transfer function to state-space is necessary for efficient MPC matrix calculations

Process knowledge + numerical parameter estimation → model identification

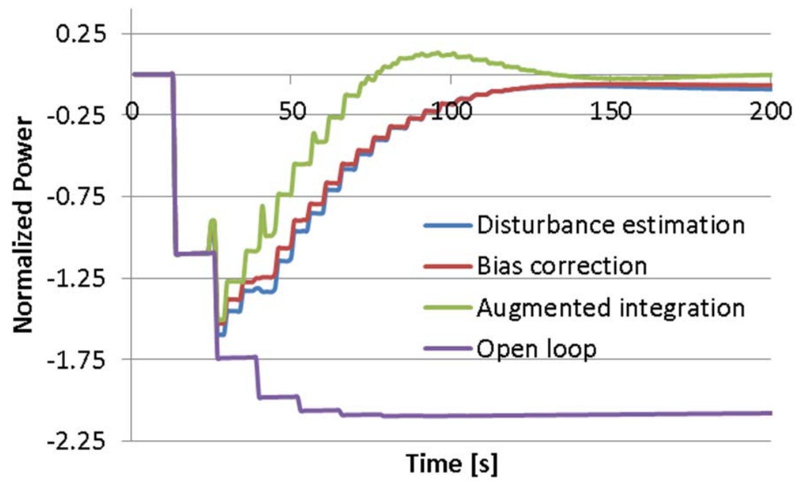
Eliminating Steady-State Offset

An unmeasured fuel quality step disturbance is applied at t = 5s.

Disturbance Variable



Controlled Variable



Augmented State-Space Model with Integration

$$\begin{bmatrix} \Delta x_{n_x}(k+1) \\ y(k+1) \end{bmatrix} = \begin{bmatrix} A_{n_x} & 0_{n_x}^T \\ C_{n_x} A_{n_x} & I_{n_y} \end{bmatrix} \begin{bmatrix} \Delta x_{n_x}(k) \\ y(k) \end{bmatrix} + \begin{bmatrix} B_{n_x} \\ C_{n_x} B_{n_x} \end{bmatrix} \Delta u(k)$$

$$y(k) = \begin{bmatrix} 0_{n_x} & I_{n_y} \end{bmatrix} \begin{bmatrix} \Delta x_{n_x}(k) \\ y(k) \end{bmatrix}.$$

Augmented State Vector

Measurement feedback is key to eliminate offset

The augmented model with integration produces a negligible steady-state offset.

MPC Results: Reliability Control Study

Reliability Study Implications:

- A control model based on distributed parameters is necessary since controlling an average SOFC temperature does not sufficiently constrain minimum temperature dynamics.

- Control based on a thermocouple measuring the outlet gas temperature would not be sufficient for containing thermal stress indicators.

- Constrained control is necessary for ensuring that the CVs do not exceed operability limits.

MPC Results: Disturbance Rejection Study

Disturbance Rejection Study Implications:

- Load-following is achieved despite 3 CVs and 3 MVs riding constraints at different times due to ± 10% fuel quality variation.

- The controller is capable of reacting to prevent temperature excursions even though the thermal settling time is 2500s +.

- Constrained MVs suggest improvements for system design given these disturbances – sizing an air compressor to handle lower pressures.

SOFC Optimization Subject to Operability Constraints

Steady-State Constrained Design Optimization

Objective

Find a minimal cost design and set of operating conditions for a given power demand profile of a load-following system.

Economic Optimization Model

$$C_{tot} = C_{cap} + C_{op},$$

$$C_{op} = c_f V_f N_h,$$

$$C_{cap} = C_{fin} + C_{mai} + C_{ins},$$

$$C_{pur} = C_{sofc} + C_{inv} + C_{pre} + C_{aux}.$$

$$C_{sofc} = n_{cells} \pi D_{outer} L \, (2.96 \, T_{sofc} - 1907)$$

$$C_{inv} = 10^5 \left(n_{cells} \frac{P_{max}}{500} \right)^{0.7}$$

$$C_{pre} = 130 \left(\frac{A}{0.093} \right)^{0.78} + 3240 \, V_{pr}^{0.4} + 21280.5 \, V_{pr},$$

Optimality defined as minimum annual system cost

$$\min_{u(t)} J = C_{tot}$$

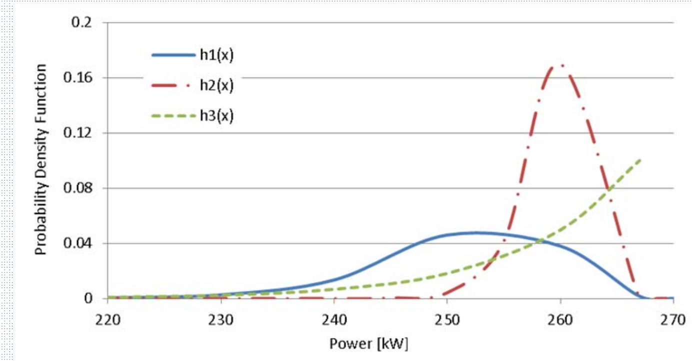
$$\begin{aligned} s.t. \quad g(x,u) &= 0 \\ u_{min} \le & \; u(k) \le u_{max} \\ y_{min} \le & \; y(k) \le y_{max} \end{aligned}$$

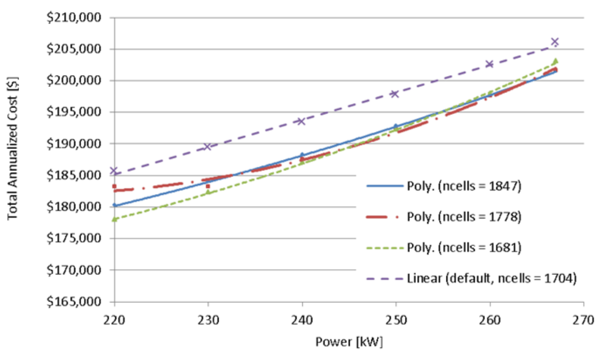
The first-principles SOFC system model with 2000+ states and intermediate variables permits inclusion of real CV limits.

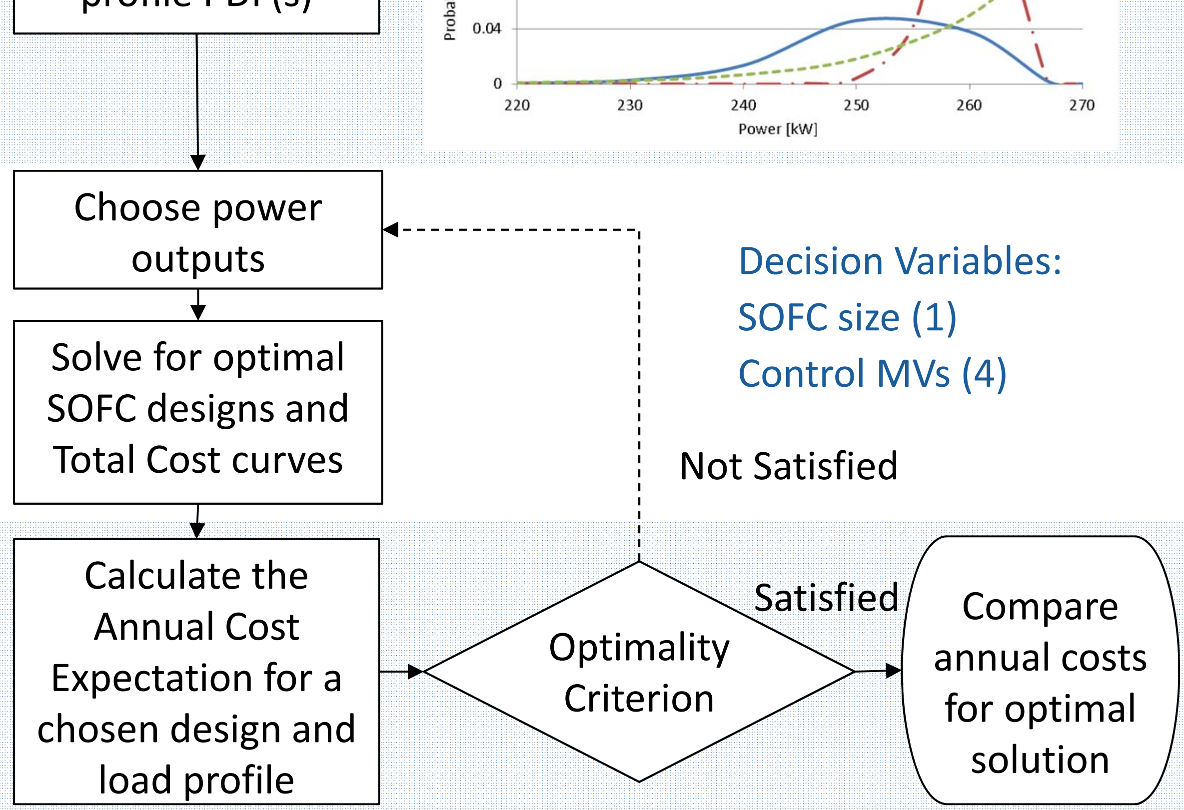
Optimization Algorithm for Load-Following

$$h_{weibull}(x) = \frac{\beta}{\delta}\left(\frac{x}{\delta}\right)^{\beta-1} \exp\left[-\left(\frac{x}{\delta}\right)^{\beta}\right],$$

$$h_{exp}(x) = \lambda \exp\left[\lambda\left(x - 267\right)\right],$$





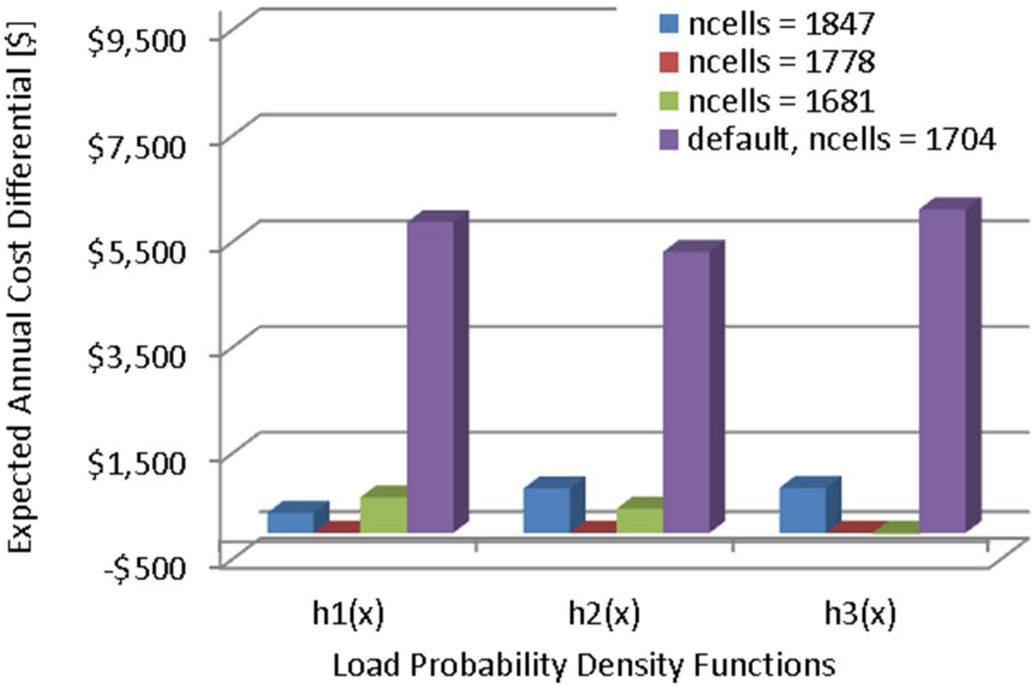


Decision Variables:
SOFC size (1)
Control MVs (4)

$$E_j\left[f_i(x)\right] = \int_{220}^{267} h_j(x) \cdot f_i(x)\, dx$$

Power demand is probabilistic for load-following applications and requires calculation of expectation values for optimization.

Design Optimization Results



- Optimization results in cost savings of $5300-6100 or 5% of operating costs.

- Majority of cost savings is achieved through finding optimal operating conditions for load following.

Design optimization is achieved simultaneously with constraint satisfaction

Summary of Contributions

Contributions

SOFC Optimization Subject to Operability Constraints

- Using a detailed, first-principles system model for optimization ensures operational feasibility of optimum.
- Demonstrated a probabilistic approach for load-following system optimization.
- Design optimization reduces operating costs by five-percent at the steady-state value while satisfying control constraints.

Publications and Conferences

- Spivey, Hedengren, Edgar. Constrained Nonlinear Estimation of Industrial Process Fouling. *Industrial & Engineering Chemistry Research.* 2010.

  Published September 2010
- Spivey, Edgar. Dynamic Modeling, Simulation, and MIMO Predictive Control of a Tubular Solid Oxide Fuel Cell. *Journal of Process Control.*

  Submitted for Review in June 2011
- Spivey, Edgar. First-Principles-Based NMPC for a Tubular Solid Oxide Fuel Cell.

  To be submitted

- Spivey, Edgar. Dynamic Modeling of Reliability Constraints in Solid Oxide Fuel Cells and Implications for Advanced Control. *2010 AIChE Annual Meeting.* Salt Lake City, UT. November 7-12, 2010.
- Spivey, Edgar. Advanced Control for Solid Oxide Fuel Cell Power Plants. *2011 TWCCC Spring Meeting.* Austin, TX. February 7, 2011.
- Spivey, Edgar. Modeling and Analysis of Solid Oxide Fuel Cell Dynamics. *2010 TWCCC Fall Meeting.* Madison, WI. September 28, 2011.

SOFC Submodel: Modeling Challenges

- Distributed parameter approach produces a large number of states: 650 states and intermediates for 10 finite volumes.
- Dynamic system of differential and algebraic equations to be solved simultaneously (without algebraic loops).
- Algebraic equations are in an implicit form.
- Nonlinearities introduced by reaction and electrochemical terms.
- Multiple time scales varying from milliseconds to hours.

The complete SOFC model is solved simultaneously via constrained NLP using the **APMonitor** Modeling Language.

$$
\begin{aligned}
&\min_{x \in \Omega} \quad J(x,u) \\
&s.t.\ \dot{x} = f(x,u) \\
&\qquad 0 = g(x,u) \\
&\qquad h(x) \geq 0
\end{aligned}
$$

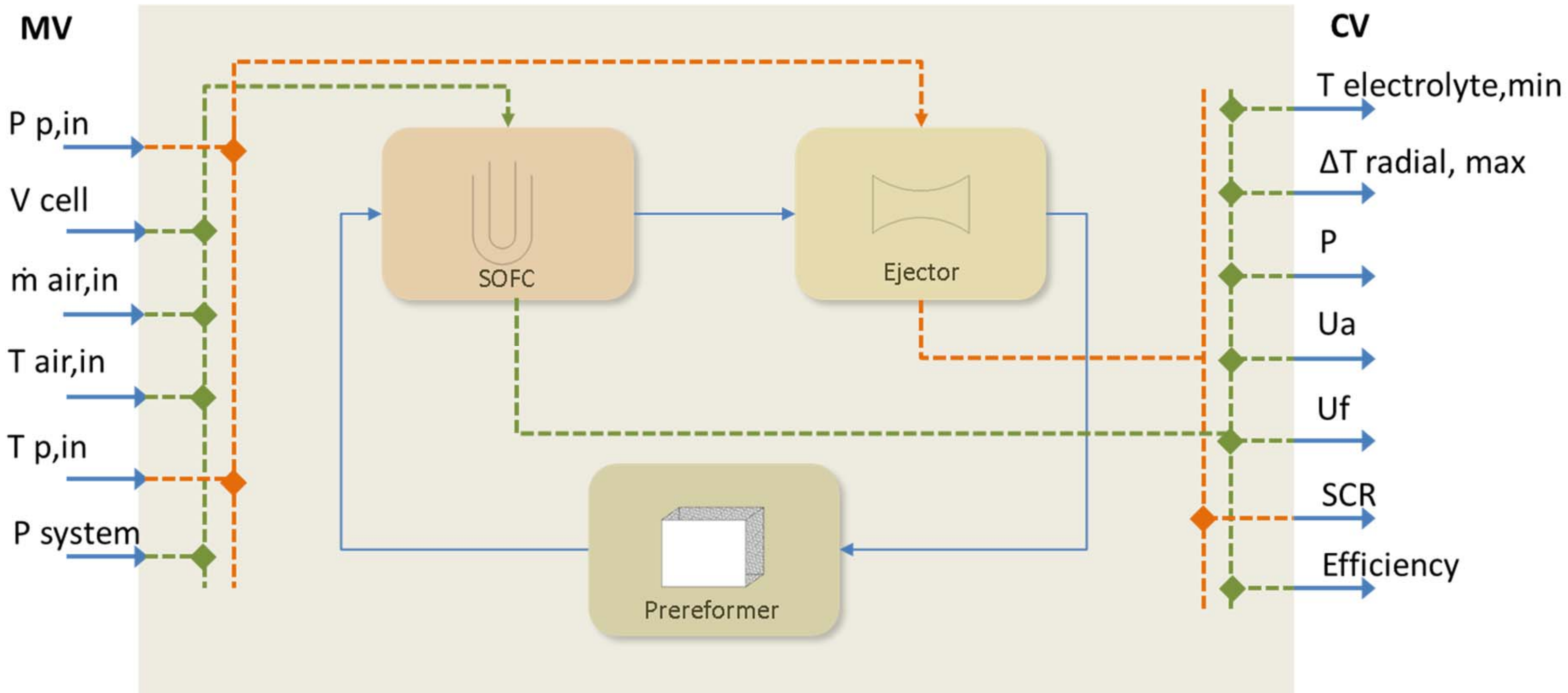
SOFC Steady-State Model Validation

The SS SOFC model results (model) are compared to the actual plant data (expected). The model error is also compared to the Campanari model error.

Plant A				
	Model	Expected	Error	Campanari Error
Single cell power output (W)	109.0	104.8	4.0	1.6
Current density (A/m^2)	1792.0	1800.0	0.4	0.4
Voltage (V)	0.7294	0.6981	4.5	1.6
Fuel utilization (%)	68.4	69.0	0.8	0.6
Air utilization (%)	17.3	17.8	2.6	1.7
Plant B				
	Model	Expected	Error	Campanari Error
Single cell power output (W)	158.0	157.0	0.6	3.0
Current density (A/m^2)	3000.0	3000.0	0.0	1.1
Voltage (V)	0.6315	0.6275	0.6	3.0
Fuel utilization (%)	70.1	69.0	1.6	2.9
Air utilization (%)	23.8	23.8	0.1	1.7

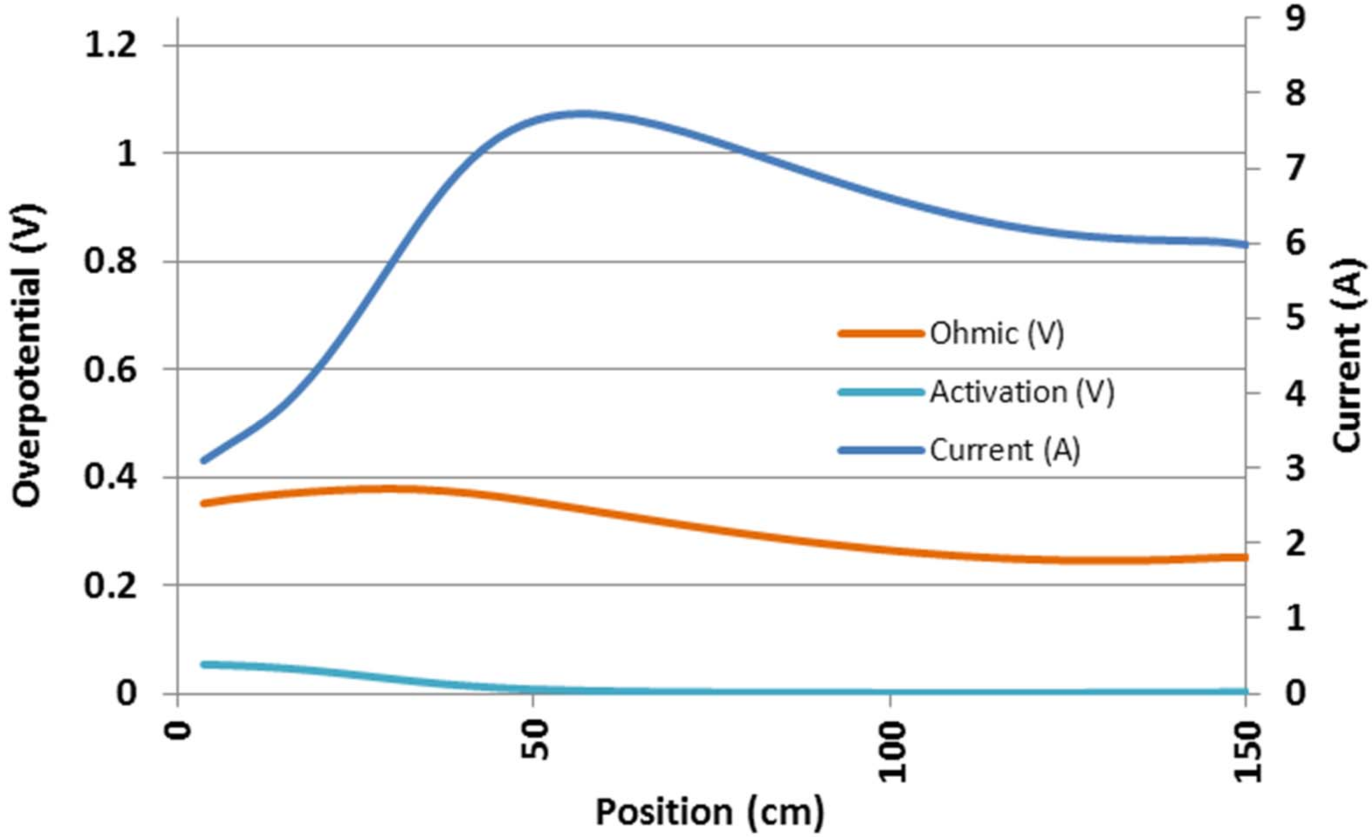
The model validation error is comparable to the Campanari model error.

SOFC System Model in Simulink

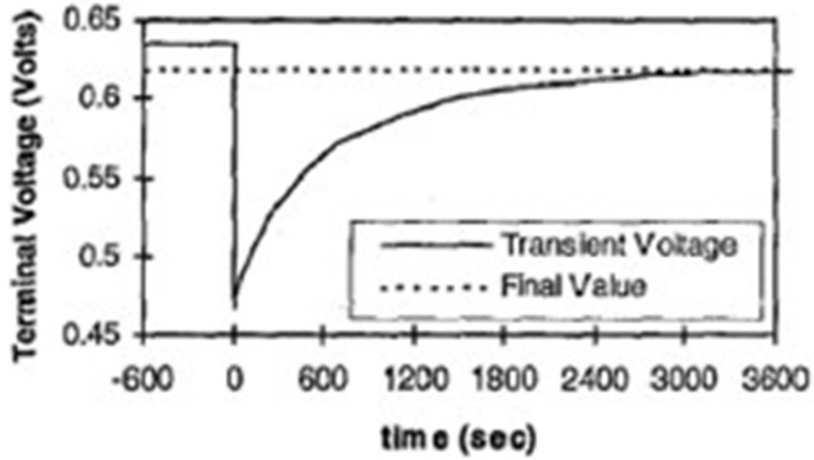


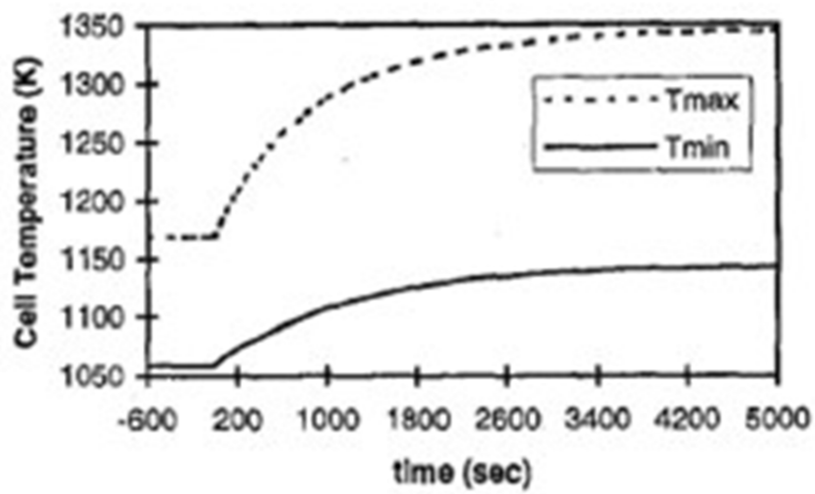
SOFC, ejector, and prereformer models are solved at each time step to investigate MV-CV relationships

Current and Overpotential Plot



Hall – Tubular SOFC Thermal Time Constant

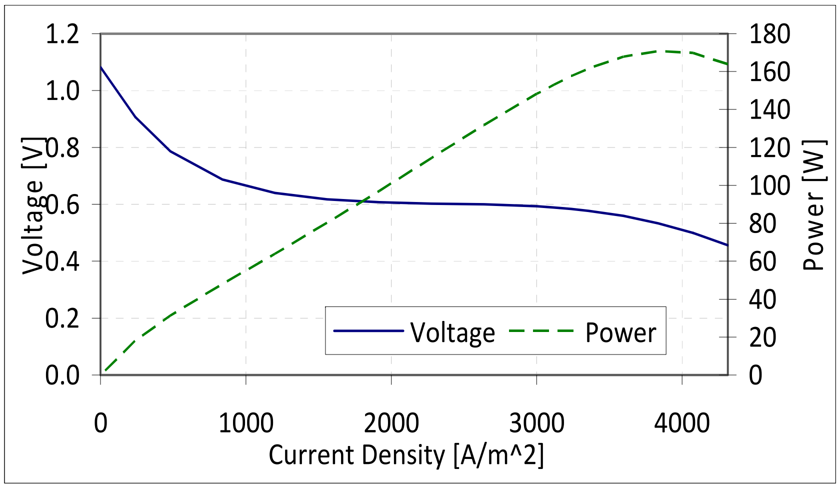


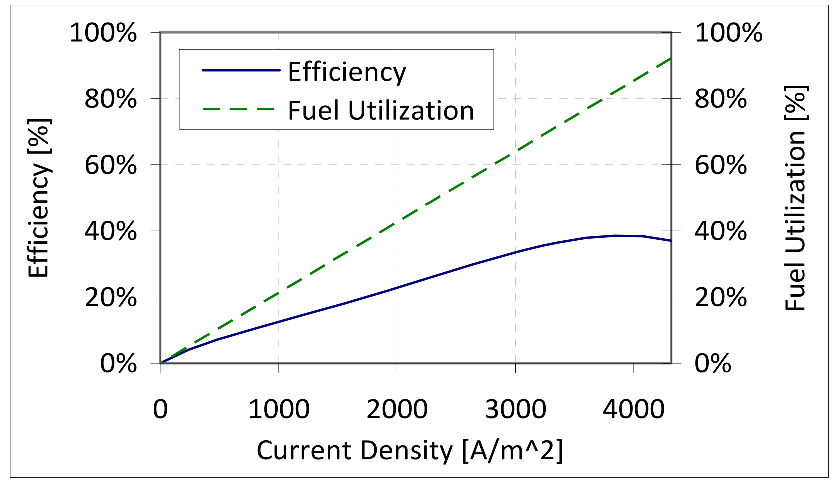


SOFC Electrical Characterization

SS Electrical Characterization with Fixed Fuel Flow Rate (Plant B)

Plant B : 267 kW, 3.50 bar

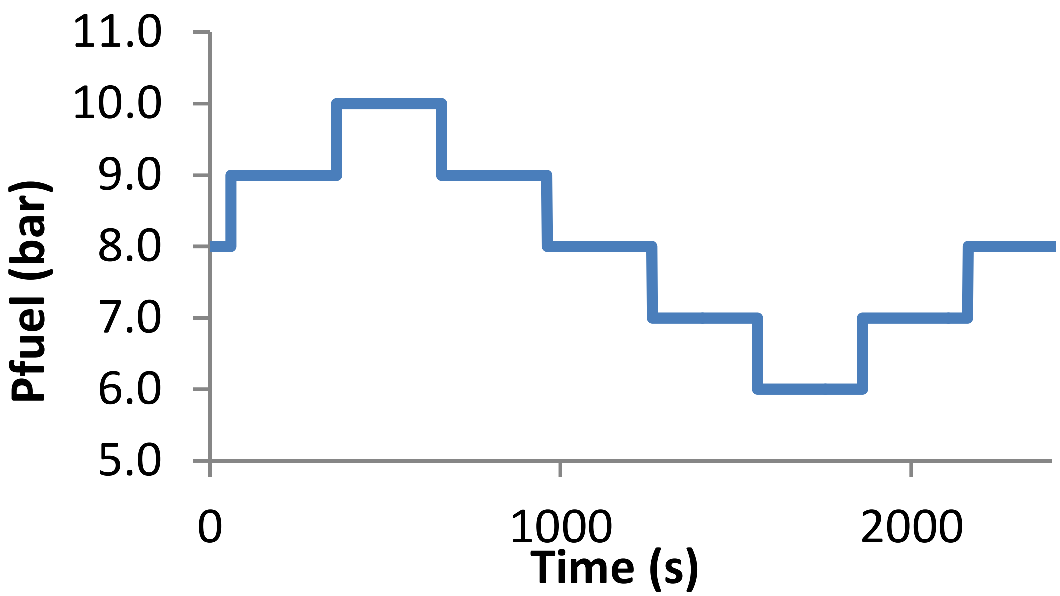




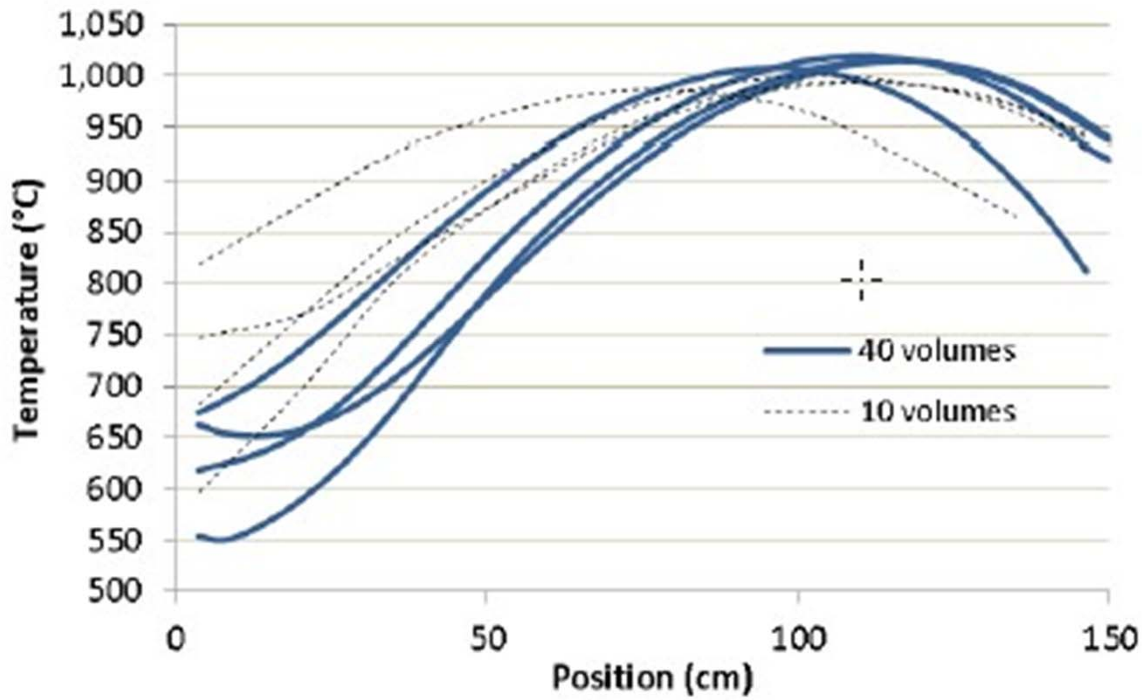
- LHV efficiencies are 45% and 38% for Plants A and B respectively - typical for 100-300 kW SOFC.
- Nominal efficiency is based upon provided inputs, not plant modeling.

$$\eta = \frac{I \cdot V}{LHV_{H2O} \cdot N_{H2O,in} + LHV_{CO} \cdot N_{CO,in} + LHV_{CH4} N_{CH4,in}}$$

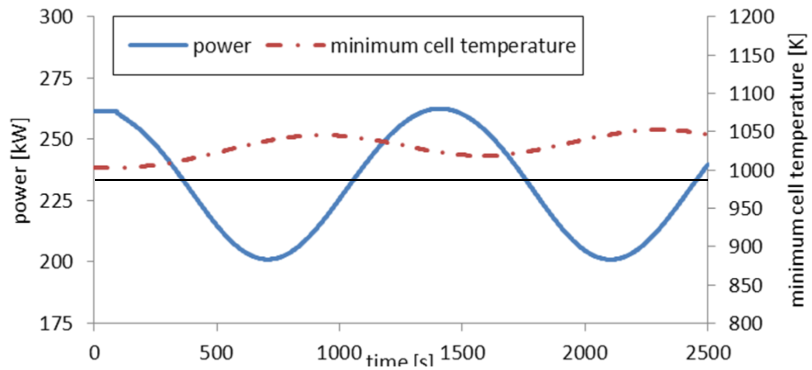
Example Staircase MV Profile

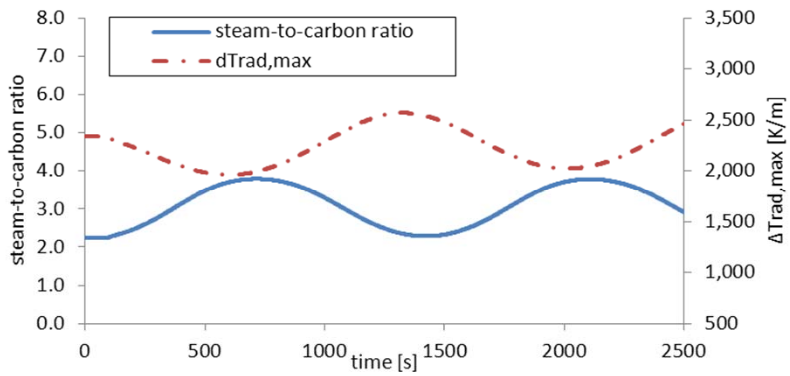


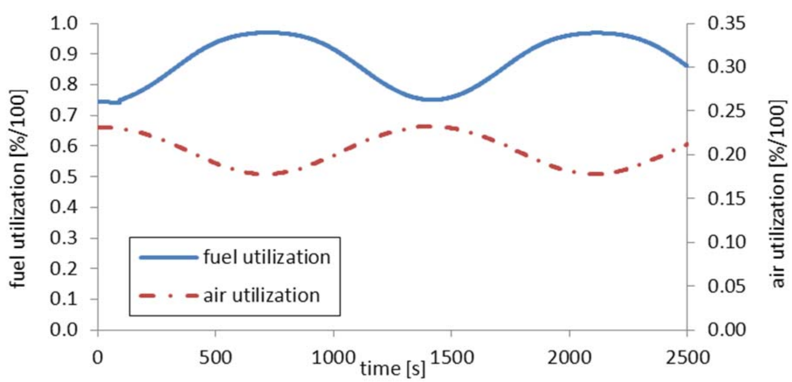
Discretization Comparison



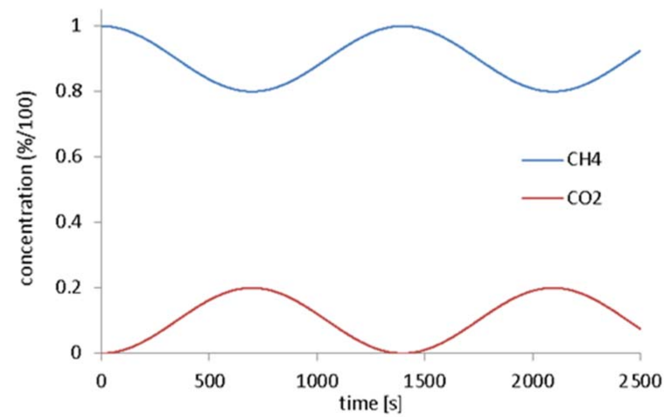
Fuel Quality Disturbance







+/- 15% variation in power



MPC Results: Reliability Control Study

Outlet Temperature Control