Dynamic Modeling of Reliability Constraints in Solid Oxide Fuel Cells and Implications for Advanced Control

AIChE Fall 2010 Annual Meeting

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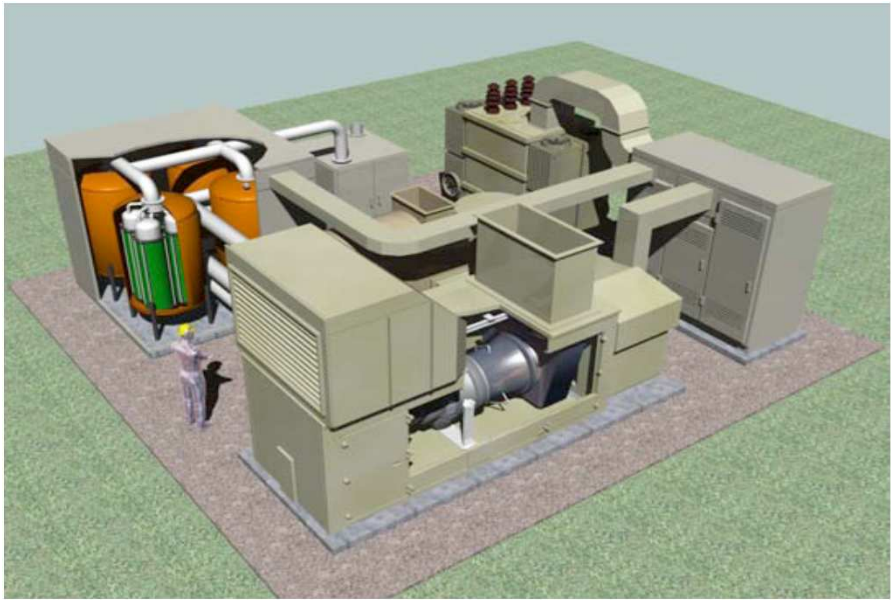


*GE, 2007

Overview

Modeling and Controls Objective:

Maintain solid oxide fuel cell (SOFC) performance and operational integrity subject to load-following, efficiency maximization, and disturbances using advanced process control.

Agenda:

- Motivation and Overview of Tubular SOFC System
- Distributed-Parameter SOFC Modeling
- SS and Dynamic Simulations of Fuel Cell Operation
- Conclusion

Research Motivation

Benefits

- High efficiencies at full and partial load:

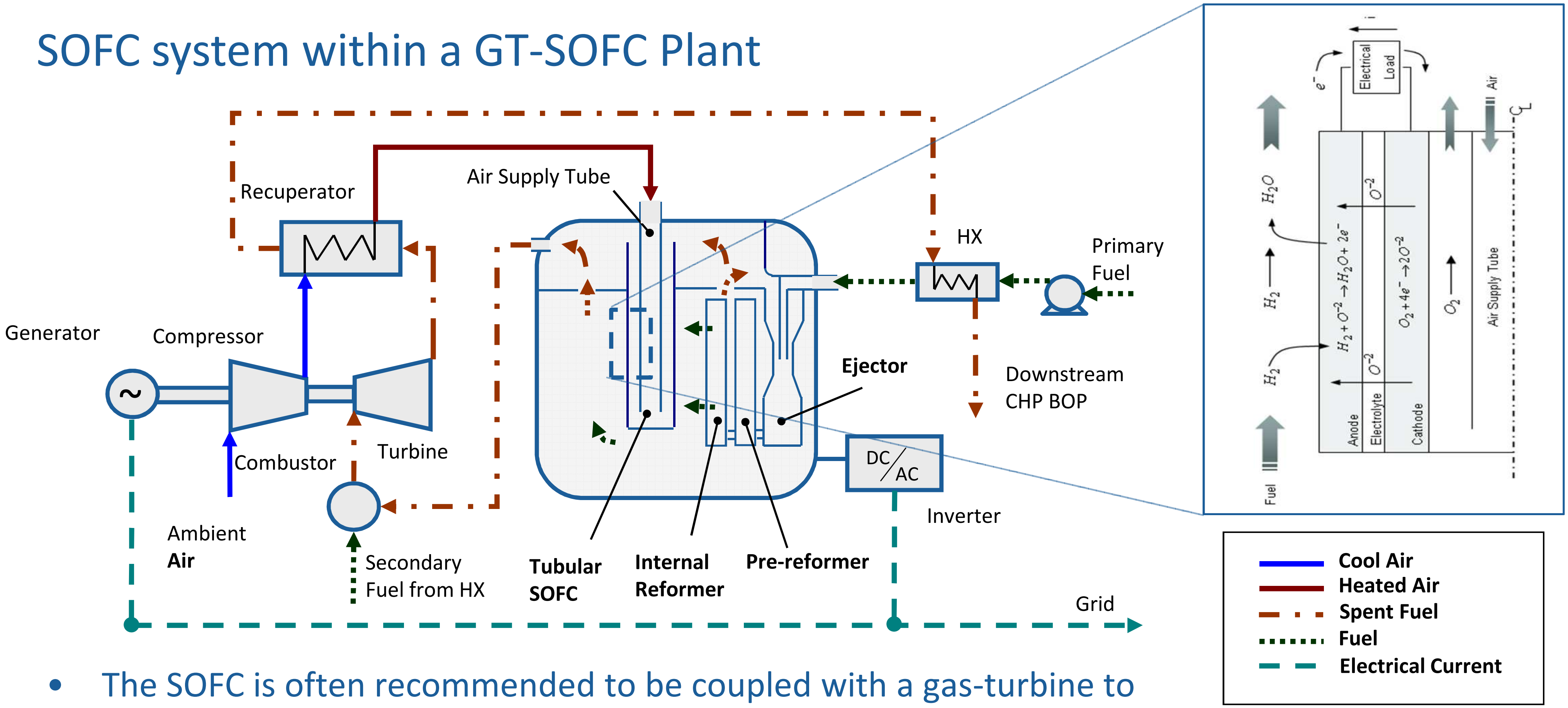
  40-50% (LHV) for SOFC for 200 kW, 60-70% for GT-SOFC, 90%+ for cogeneration.
- Fuel flexibility:
  - Hydrogen, natural gas, propane
  - Alcohols, biomass, coal gas
- Suitability for cogeneration with high exhaust temperatures
- Low noise and emission levels

Operational Challenges

- Micro-cracking, catalyst poisoning, and air & fuel starvation decrease the lifetime and increase cost of electricity.
- Majority of real plants have used SISO PID and PLC control – operations experience with advanced control is limited.

SOFC System Overview

SOFC system within a GT-SOFC Plant



- The SOFC is often recommended to be coupled with a gas-turbine to utilize waste heat, maximize efficiencies, and supplement power production.
- Model of manipulated variables assumes an external variable speed compressor and recuperators.

Distributed-Parameter SOFC Modeling

Tubular SOFC Modeling

Tubular Solid Oxide Fuel Cell Assembly

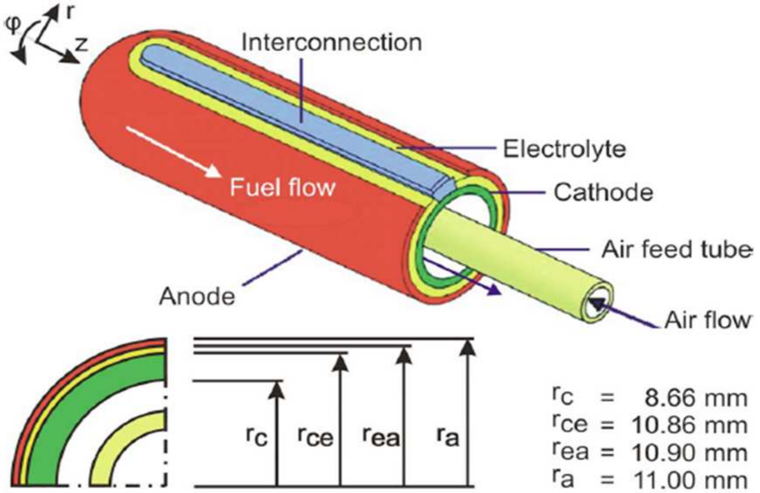


*Image from Singhal, S.C., 2006.

Type: high-temperature tubular SOFC

Structure: cathode-supported

Fuel: prereformation and direct internal reformation of methane

Balance of Plant in Model: ejector and prereformer

Pressurized to 3 bar

Based on a Siemens-Westinghouse plant at National Fuel Cell Research Center.

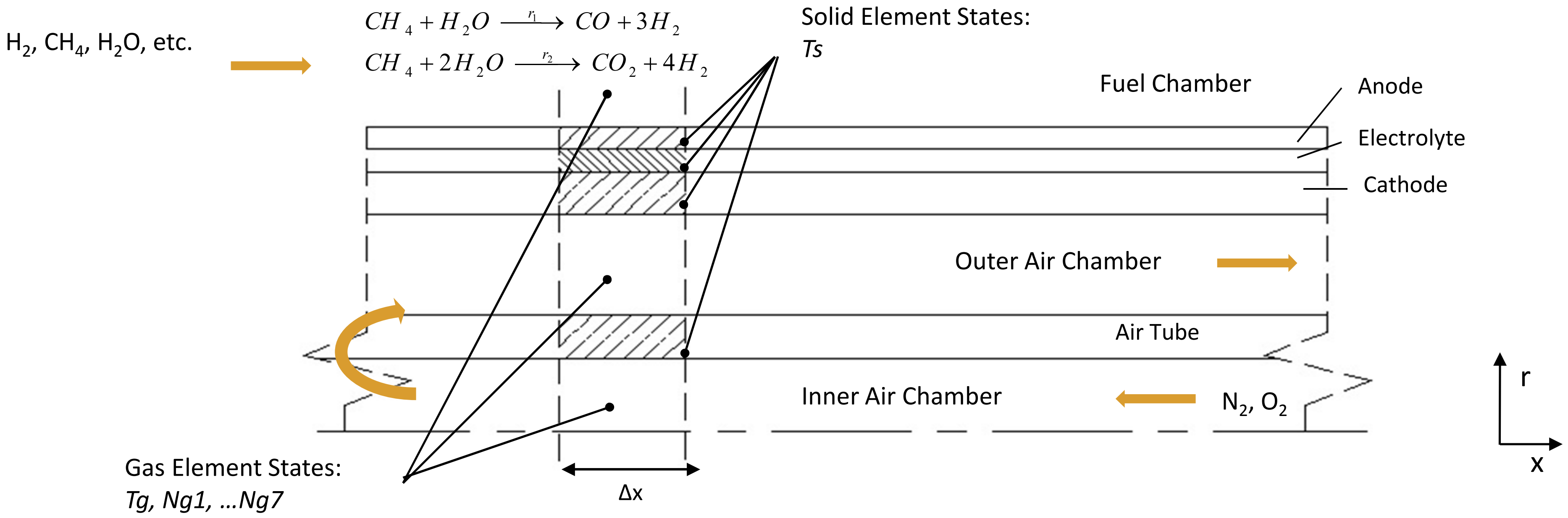
Parameters and inlet conditions are well known in literature versus other SOFC designs

Dynamic Modeling Challenges

- Distributed parameter approach produces a large number of states: 220 states for 10 finite volumes in the axial direction.
- 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.

Quasi-2D SOFC Model Discretization

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



$$CH_4 + H_2O \xrightarrow{r_1} CO + 3H_2$$

$$CH_4 + 2H_2O \xrightarrow{r_2} CO_2 + 4H_2$$

- Total States per Element = 22 : Tga, Tsa, Tse, Tsc, Tgc2, Tsat, Tgc1, Nga1-Nga7, Ngc21-Ngc27, I (current)
- Total States per SS Model = 878
- Total States per Dynamic Model = 220

Key SOFC Model Equations

Electrochemical Model

$$V_{cell} = E - \eta_a - \eta_c - \eta_r$$

$$E = E_0 + \frac{RT_{avg}}{2F} \ln\left(\frac{p_{H_2} p_{O_2}^{1/2}}{p_{H_2O}} \right)$$

$$E_0 = -\frac{\Delta G^r}{2F}$$

$$\eta_a = \frac{RT_{a,j}}{\alpha 2F} \ln\left({}^{i}/_{i_0} \right) + \frac{RT_{c,j}}{\alpha 4F} \ln\left({}^{i}/_{i_0} \right)$$

$$\eta_c = \frac{RT_{a,j}}{2F} \ln\left(1 - {}^{i}/_{i_{l,a}} \right) + \frac{RT_{c,j}}{4F} \ln\left(1 - {}^{i}/_{i_{l,c}} \right)$$

$$\eta_r = iR_{eff}$$

Species and Energy Balances

$$\dot{n}_{out} = \dot{n}_{in} + \sum_i \sum_j v_i r_{ij}$$

$$0 = \dot{m} c_p \frac{dT}{dx} + \sum_i h_i A_i \left(T_{s_i} - T_g \right) + Q_{r,rxn}$$

$$\rho V c_p \frac{dT_s}{dt} = \sum_i h_i A_i \left(T_{g_i} - T_s \right) + k \frac{dT_s}{dx} + \varepsilon F \sigma A \left(T^4_{s,opp} - T^4_s \right) + Q_{e,rxn}$$

Anode Steam Reformation Model

$$CH_4 + H_2O \xrightarrow{r_1} CO + 3H_2$$

$$CH_4 + 2H_2O \xrightarrow{r_2} CO_2 + 4H_2$$

$$r_1 = A \exp\left(-{}^{E_a}/_{RT_{sa}} \right) p_{CH_4} \cdot Area$$

$$r_2 = k \left(X_{CO} X_{H_2O} - \frac{X_{H_2} X_{CO_2}}{K_{ps}} \right) \cdot Vol$$

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

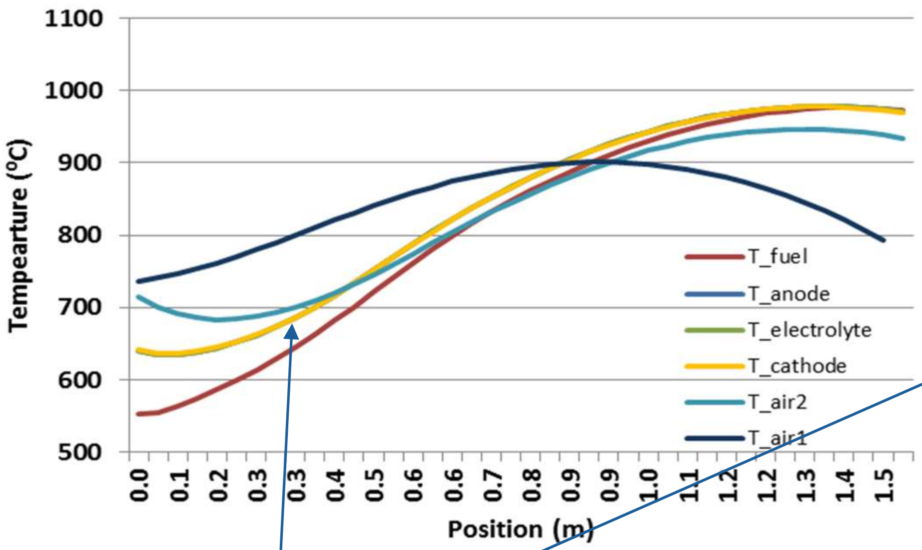
$$\min_{x \in \Omega} \; J(x, u)$$

$$\begin{aligned} s.t.\; \dot{x} &= f(x, u) \\ 0 &= g(x, u) \\ h(x) &\geq 0 \end{aligned}$$

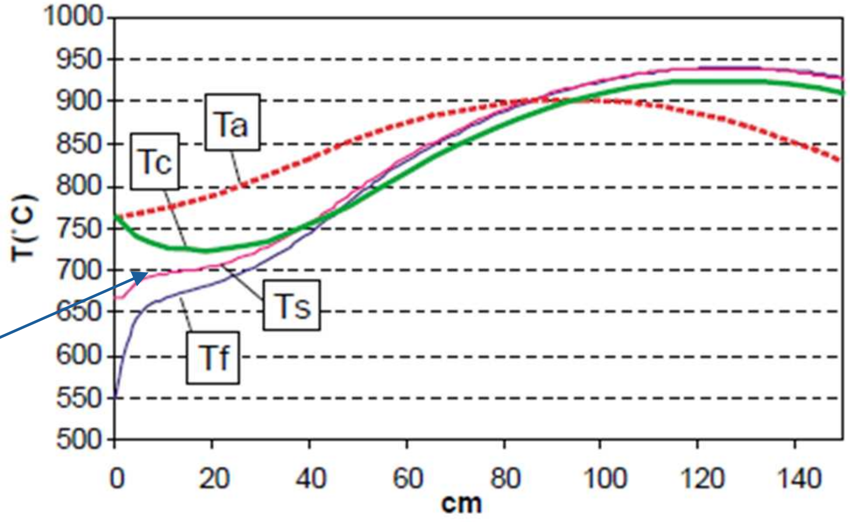
SOFC Steady-State Model Validation

The tubular SOFC steady-state model is validated based upon experimental data and model data from standard practice (Campanari, 2004; Seume, 2009).

Model Results



Campanari Model



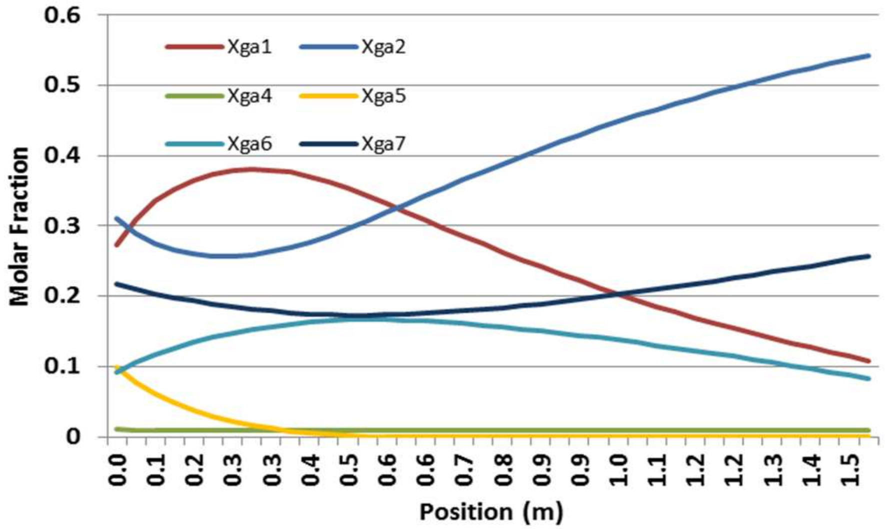
The mean absolute percentage (MAP) error is used to compare the models.

MAP for Electrolyte Temperature = 3.85%

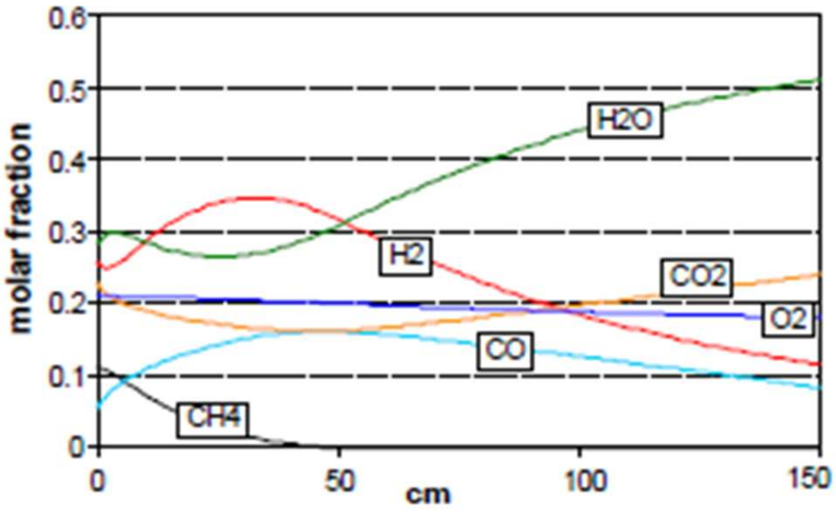
$$MAP = \frac{1}{n}\sum_{t}\left|\frac{A_t - P_t}{A_t}\right|$$

SOFC Steady-State Model Validation

Model Results



Campanari Model

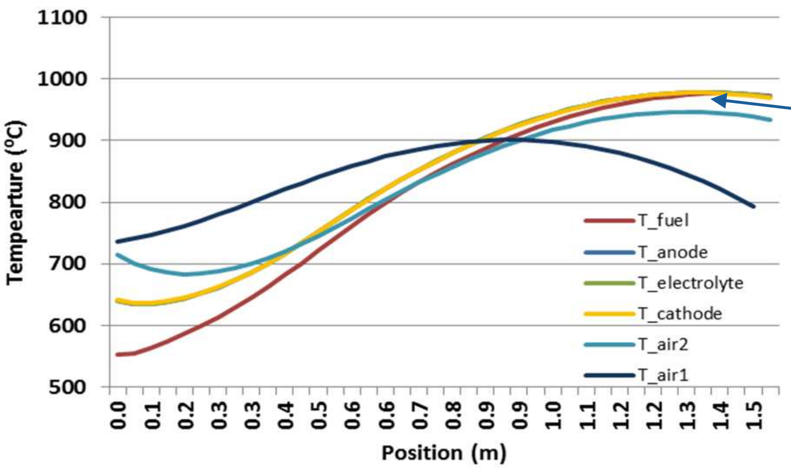


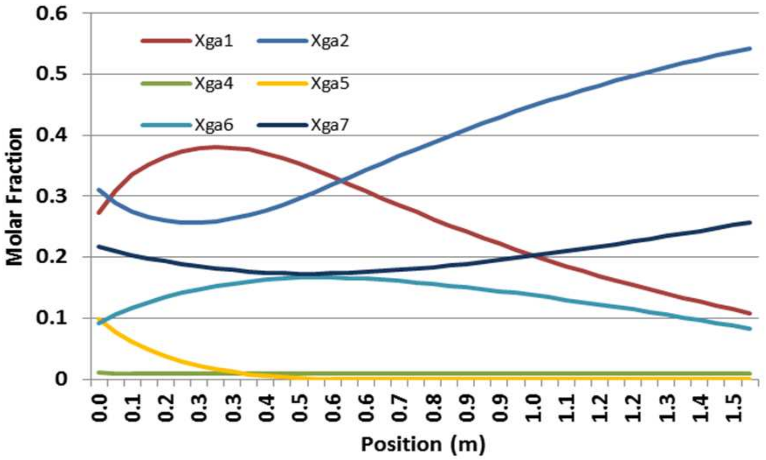
Comparison of the concentration profiles also indicates that the steady-state model matches well versus the standard models used for tubular, high-temperature SOFC modeling.

SOFC Radiation Sensitivity

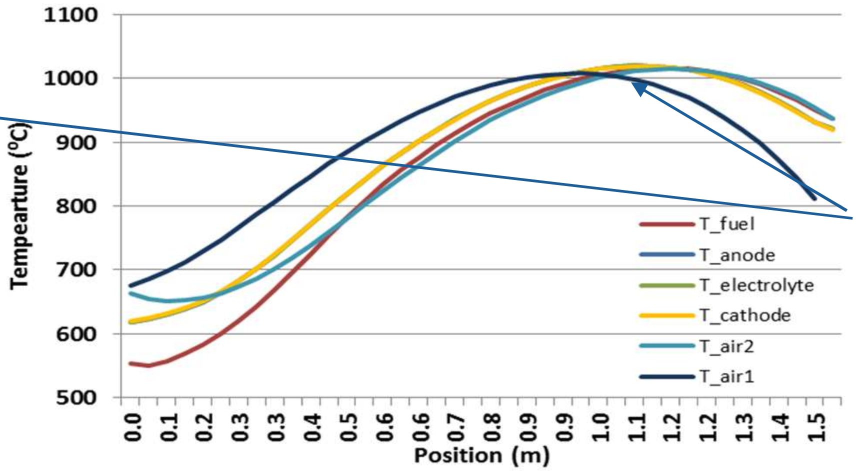
Radiation Analysis for Plant B : Air channel radiation is significant

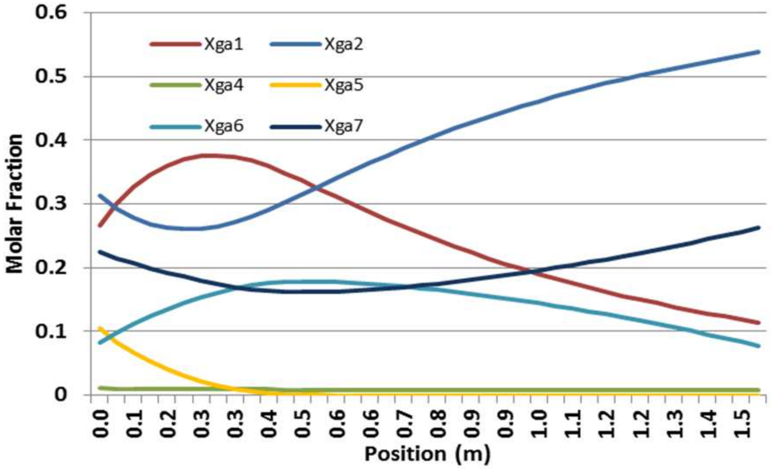
Without Radiation





With Radiation





Radiation Effects:

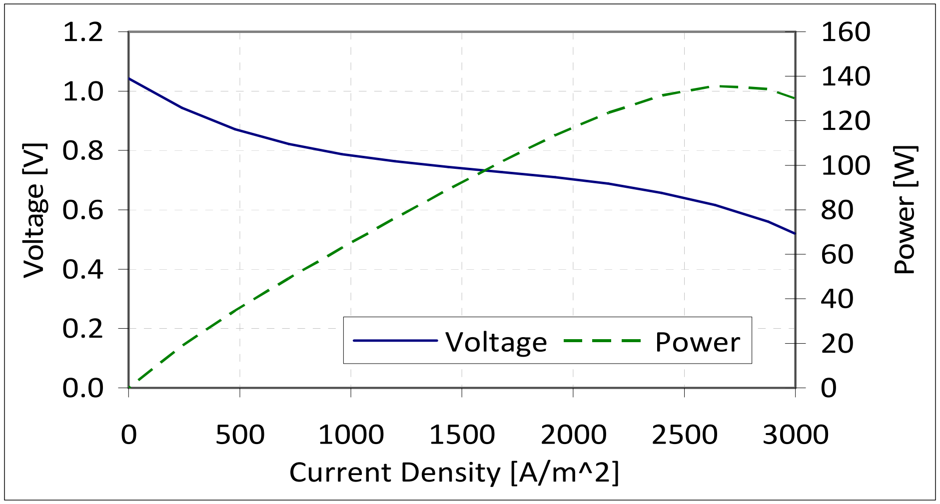
- Increased peak temperature
- Inlet air and solid PEN is closer in temperature
- Higher T gradients at outlet

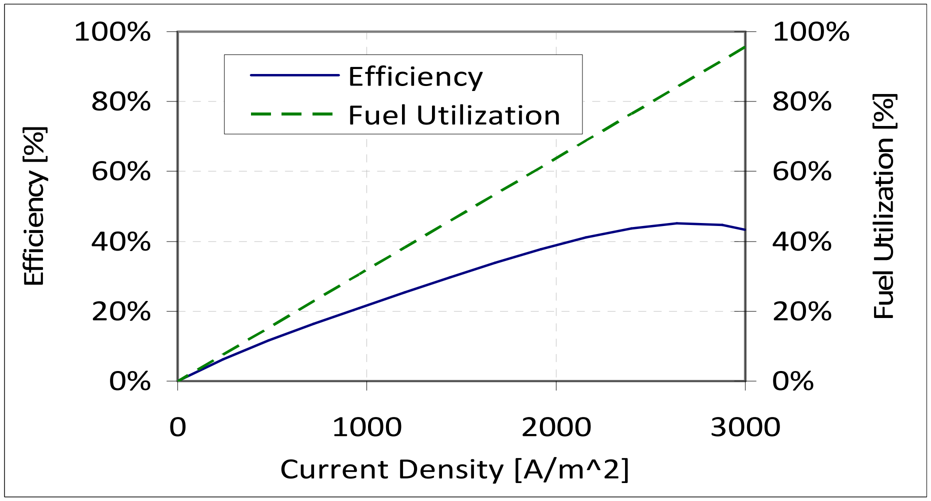
- Molar flow exhibits no noticeable change.

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

SOFC Electrical Characterization

SS Electrical Characterization for Plant A: 120 kW, 1.05 bar



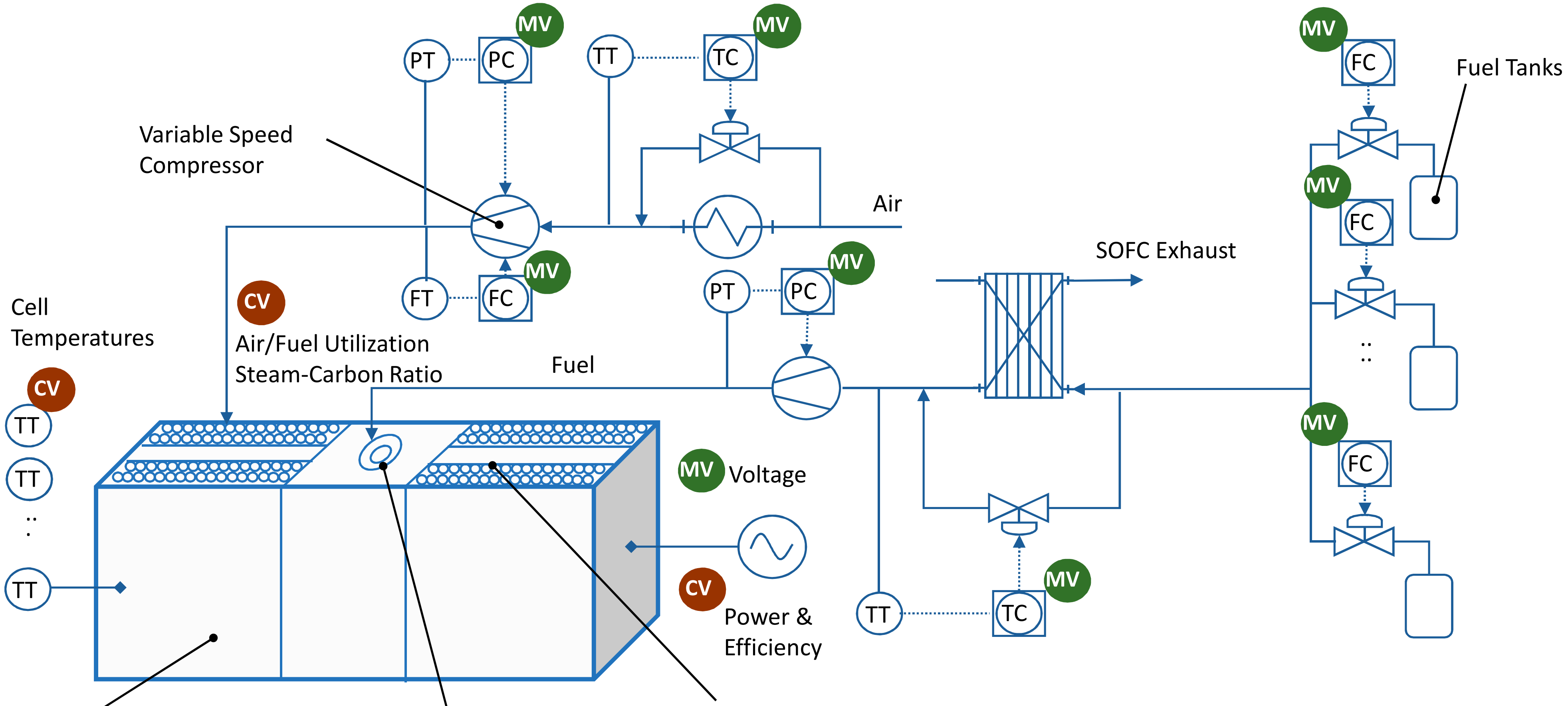


- LHV efficiencies are 45% and 38% for Plants A and B respectively - typical for 100-300 kW SOFC.
- Nominal efficiency is based upon provided inputs, not plant modeling.
- Fixed fuel flow rate condition

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

SS and Dynamic Simulations of Fuel Cell Operation

SOFC and Balance of Plant (BOP) System



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

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

SOFC :
Dynamic
DAE Model
220 States
APMonitor

Manipulated and controlled variables are chosen based upon the SOFC+BOP system

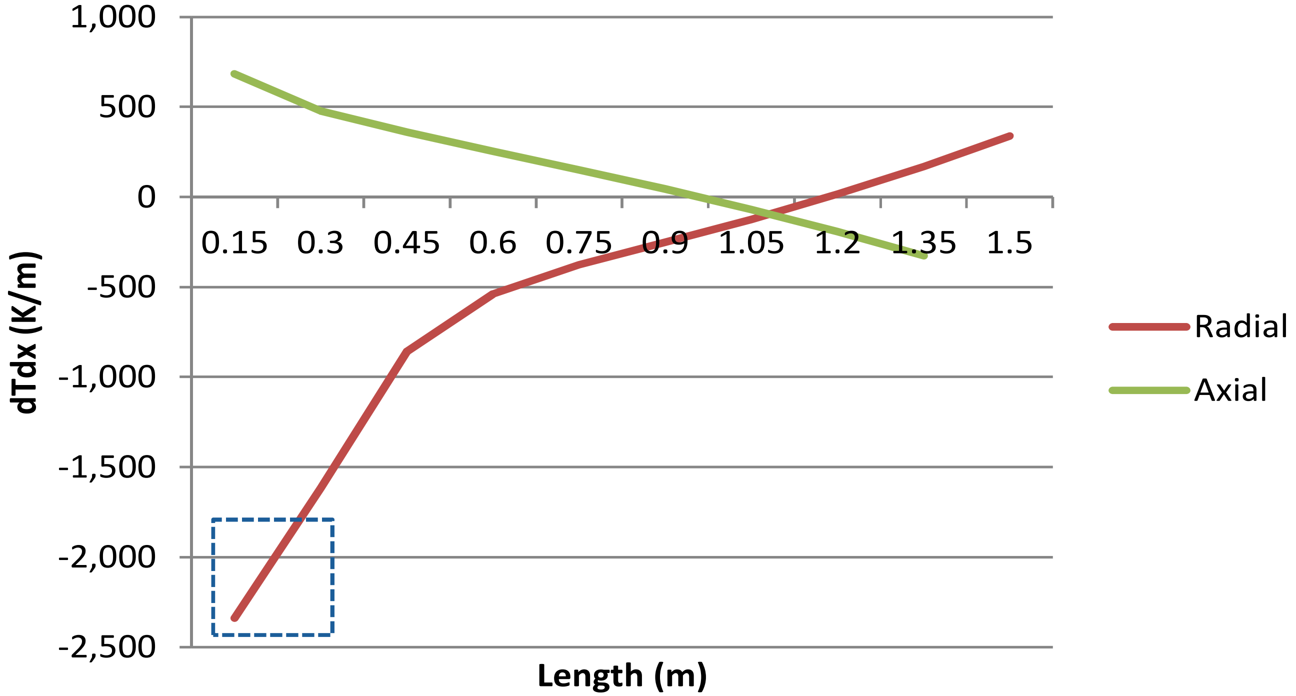
Relevance of Controlled Variables

Objective or Risk	Controlled Variable
DC Power Delivery	Power (W) Efficiency (%)
Thermal Stress Minimization	Minimum Stack Temperature (K) Radial Thermal Gradient (K/m)
Avoid Catalyst Poisoning	Steam-to-Carbon Ratio
Avoid Air and Fuel Starvation	Air and Fuel Utilization (%)

Recent studies report that the minimum stack temperature and radial thermal gradient are responsible for the highest and second-highest thermal stress levels (Seume, 2009).

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.

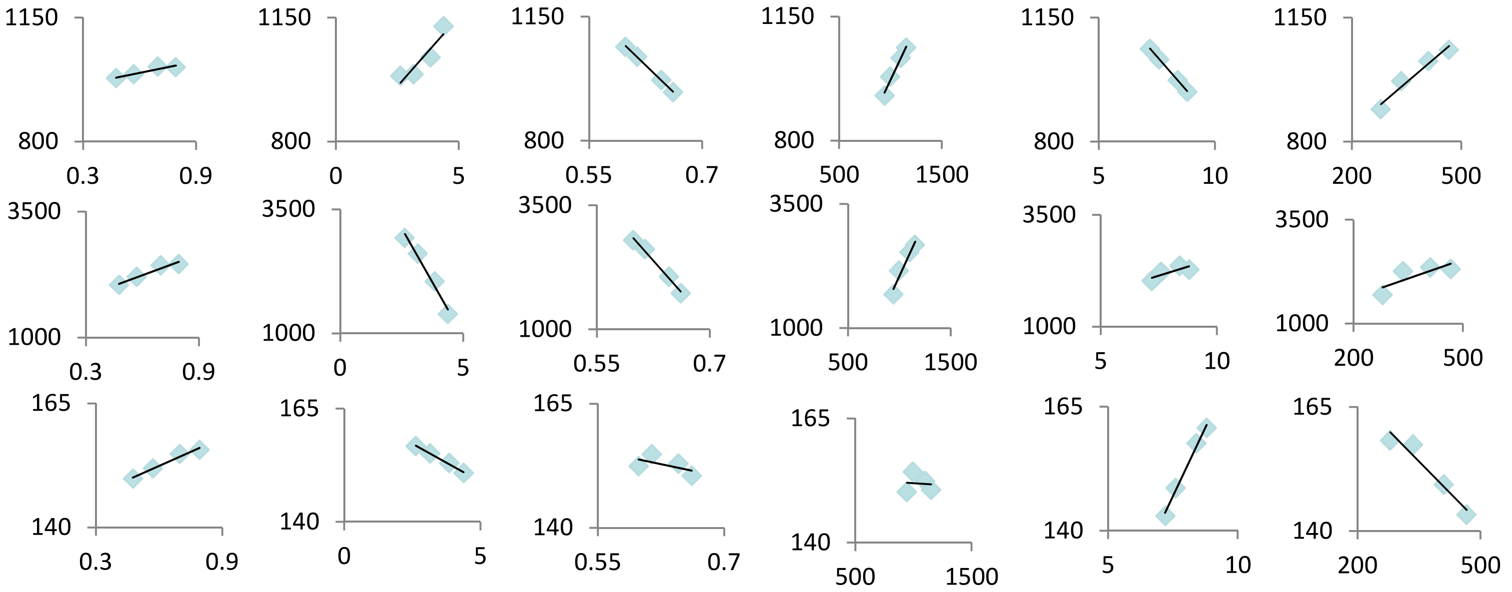


Simulation results agree with prior studies indicating that radial thermal gradients are most significant.

Variable Steady-State Gains

MVs: Air Mass Flow (kg/s) | System Pressure (bar) | Voltage (V) | Air Inlet Temperature (K) | Fuel Inlet Pressure (bar) | Fuel Inlet Temperature (K)

CVs: Tstack, min (K) | Radial ΔT/L, max (K/m) | Power (W)

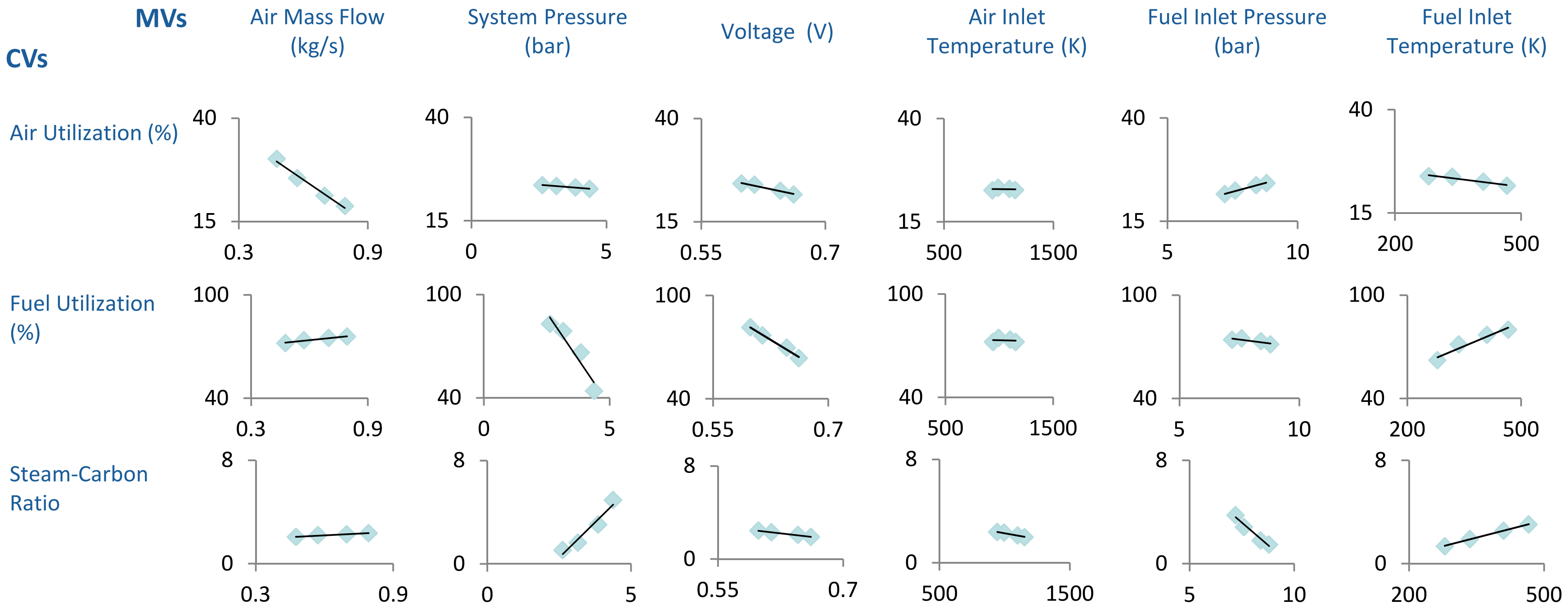


All scales are consistent for a given CV to compare slopes.

- Most MVs affect the minimum stack temperature.
- Air temperature and voltage affect the radial gradient significantly.
- Fuel pressure and temperature have most affect on power in this operating region.

Manipulated variables (MVs) are adjusted 10-20% of nominal on both sides of the nominal value. Nominal is close to Plant B conditions.

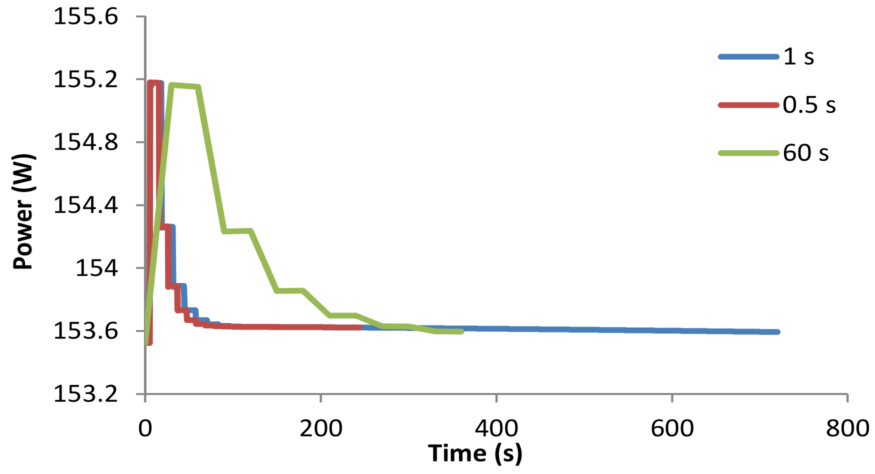
Variable Steady-State Gains



- Air mass flow is a key MV for managing air utilization.
- Fuel temperature and system pressure manage fuel utilization.
- Fuel pressure and temperature and system pressure significantly affect the steam-to-carbon ratio.

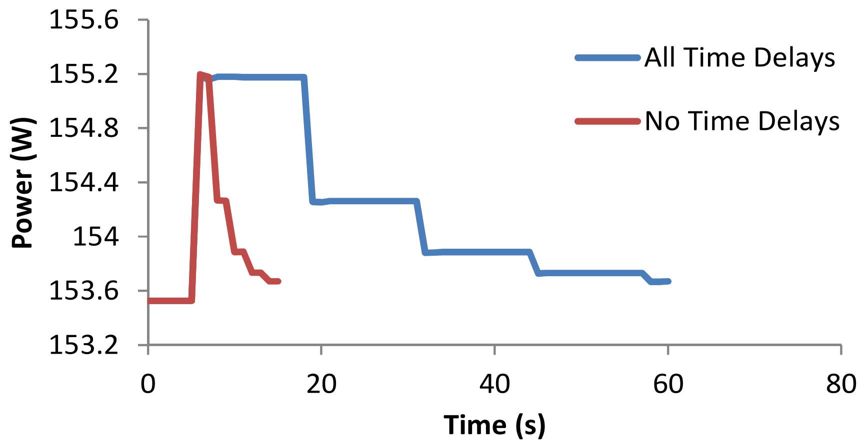
Dynamic Simulation Design

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 only valid to 1s time steps.

Transport Time Delays

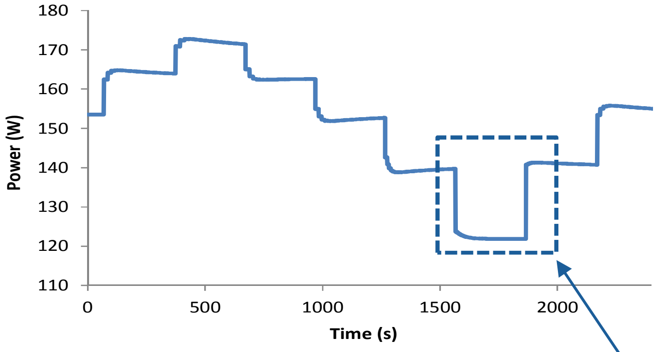


- Three transport time delays are added to the QSS gas transport models to improve dynamic accuracy.
- **Delays are important for sub-60 s response.**
- Delays are updated by mass flows

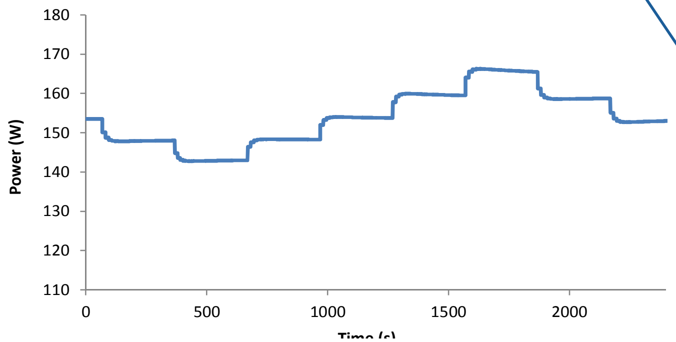
Staircase Dynamic Simulations: Power Plots

MV:

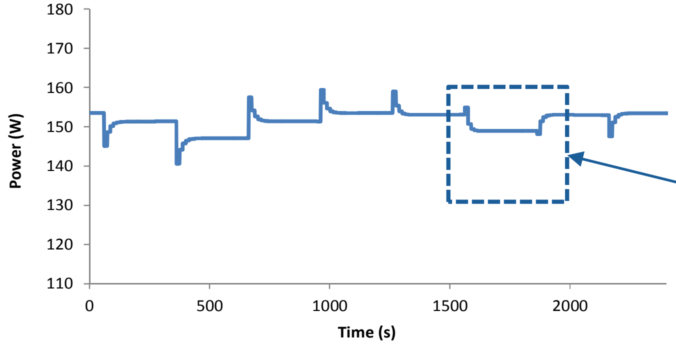
Fuel Pressure



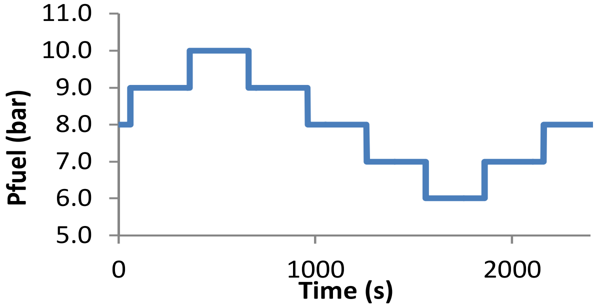
Fuel Temperature



Voltage



Example of staircase input:

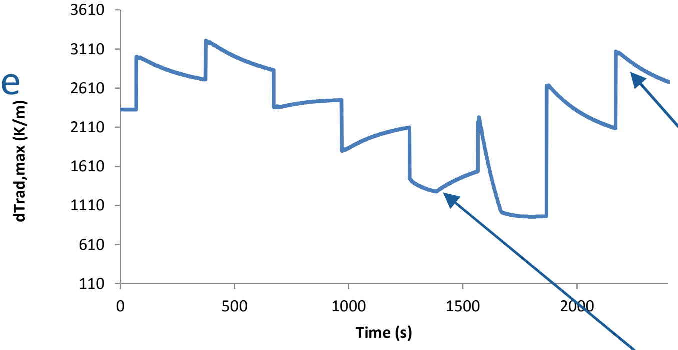


- Staircase tests are run over 5 minutes in response to MV steps over 1 s.
- Increasing gains further from the nominal illustrate non-linearity.
- Decreasing the voltage to 0.55 V reduces power output – crossed peak voltage and shows nonlinear V-P relationship.

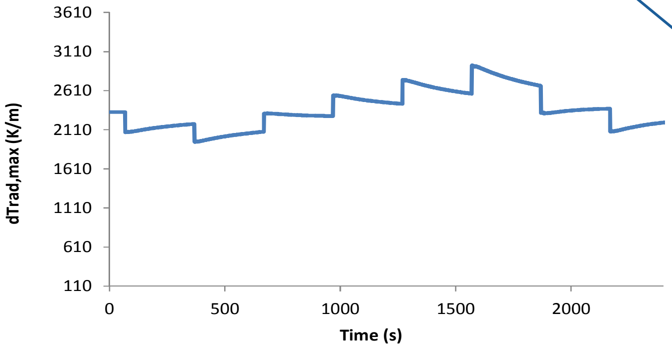
Staircase Dynamic Simulations: Max Radial dTdr Plots

MV:

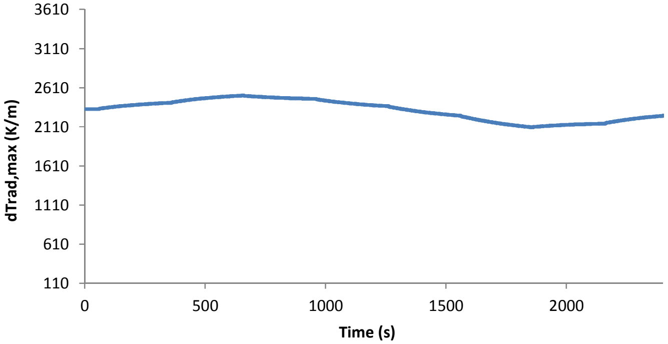
Fuel Pressure



Fuel Temperature

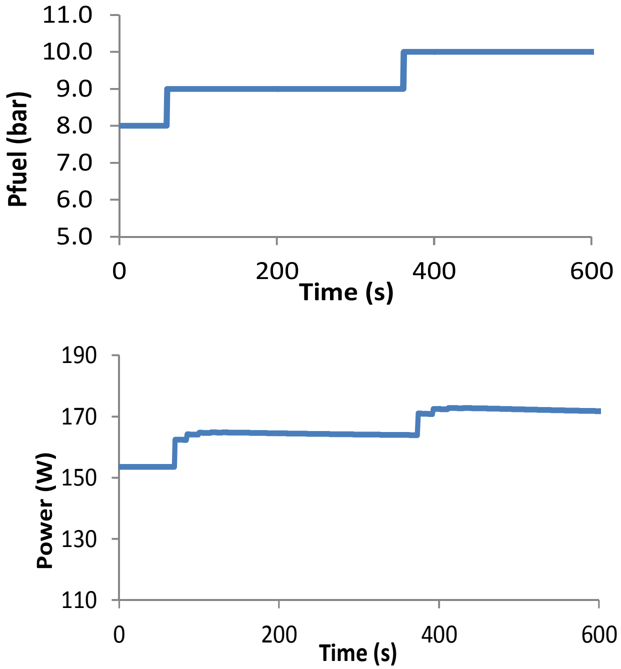


Air Mass Flow

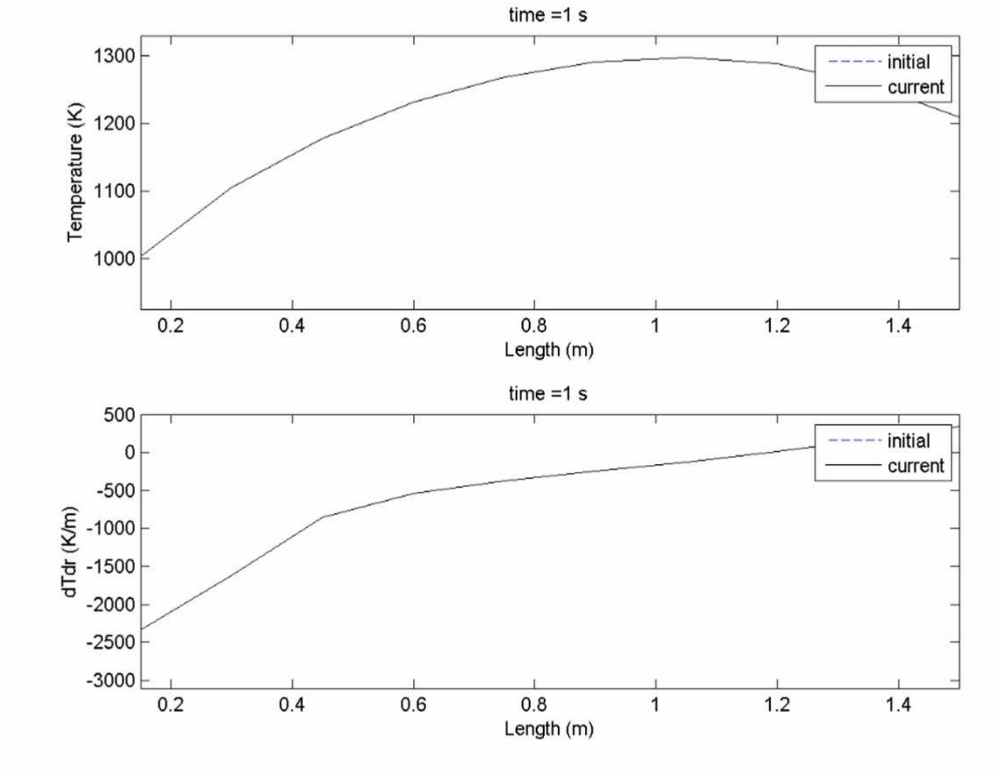


- Numerator dynamics response is real and due to quickly changing anode chamber gas conditions.
- Discontinuous curves can result between step changes when location of max gradient changes.
- The maximum radial thermal gradient does not change quickly due to varying cathode-side conditions.

Dynamic Evolution of the Temperature Profile



Electrolyte Temperature and Radial Gradients



Open-Loop Fuel Pressure Step Increase → Power Increase

→ -Lower Min Cell Temp.
-Higher Max dTdr → Increased Thermal Stresses

Minimum temperature and radial gradients undergo unique dynamics

Conclusions

- Modeling:

  Distributed parameter modeling for SOFC is critical to accurately capture overall performance as well as local gradients and minimum temperatures – key reliability criteria.

- Simulation
  - Radial thermal gradients may increase quickly in response to changing input conditions. Control algorithms should account for dynamics of minimum cell temperature and maximum radial gradients.
  - Most properties have an initial rise time < 1 min in response to 1 s input steps despite final settling times of hours. Control input intervals should be several times less than the rise time.

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