Model Predictive Control with a Rigorous Model of a Solid Oxide Fuel Cell

Dr. Benjamin Spivey

ExxonMobil

Lee Jacobsen

ExxonMobil

Dr. John Hedengren

Brigham Young University

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Outline

▸ Description of SOFC Power Generation

▸ Spivey Model of SOFC
  ◦ Ability to model:
    • Thermal stress indicators
    • Full Plant (prereformer, ejector, SOFC stack)

▸ Constrained Nonlinear 1st Principles Model Predictive Control
  ◦ Uses full Spivey model
  ◦ Sufficiently fast solution times to be used for control
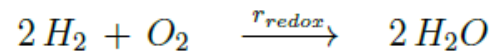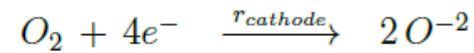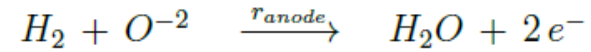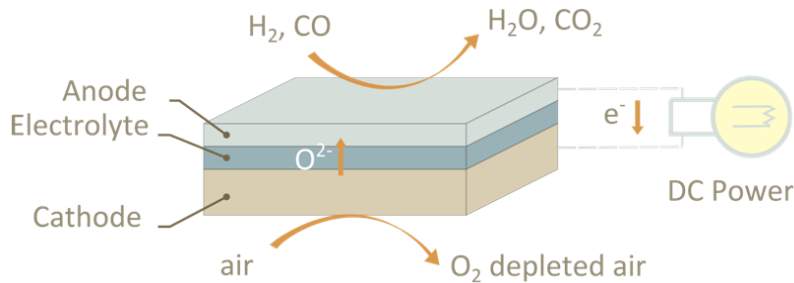
▸ Conclusion

Objective

Perform load-following with tubular solid oxide fuel cells while operating within thermal stress indicator constraints using the full nonlinear model.

- The rigorous fuel cell model accounts for the dynamic effects of load following /start ups/ shut downs on fuel cell reliability.

- Model predictive control based on this model is used to control operating conditions within the key thermal stress indicator limits

- Successful constraint of thermal stress indicator would reduce or eliminate microcracking in the EEA, improving reliability

Description of SOFC Technology

Tubular SOFC Operation

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

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

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

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

VIEW FROM TOP
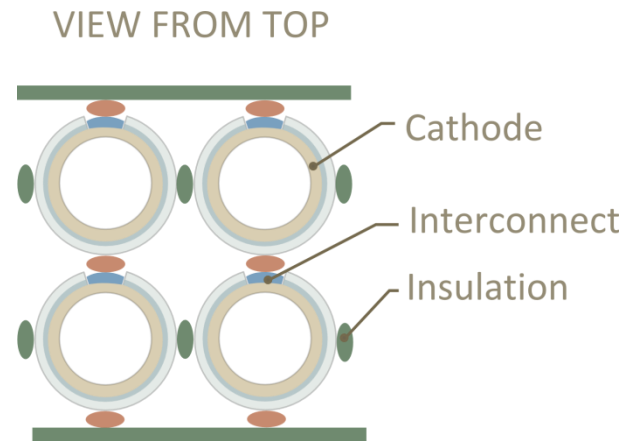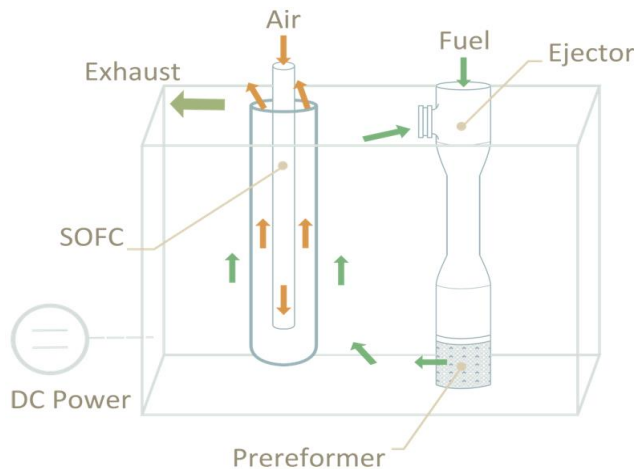
Tubular cells are arranged in bundles and connected in series.

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

SOFC MODEL

SOFC Model

- Based on Spivey's Model
  - Spivey's model was based on Campanari's model
    - Improvements over Campanari
      - Radial gradient calculation of the EEA versus lumped temperature
      - Entire plant - prereformer, ejector, and SOFC stack
  - **This research uses the entire model for real time nonlinear model predictive control**
    - APMonitor Software
    - Solved simultaneously and dynamically
    - Fast solution times

SOFC Performance and Operation 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 Fuel Starvation	Fuel Utilization (%)

SOFC Discretization- 2D Axial and Radial
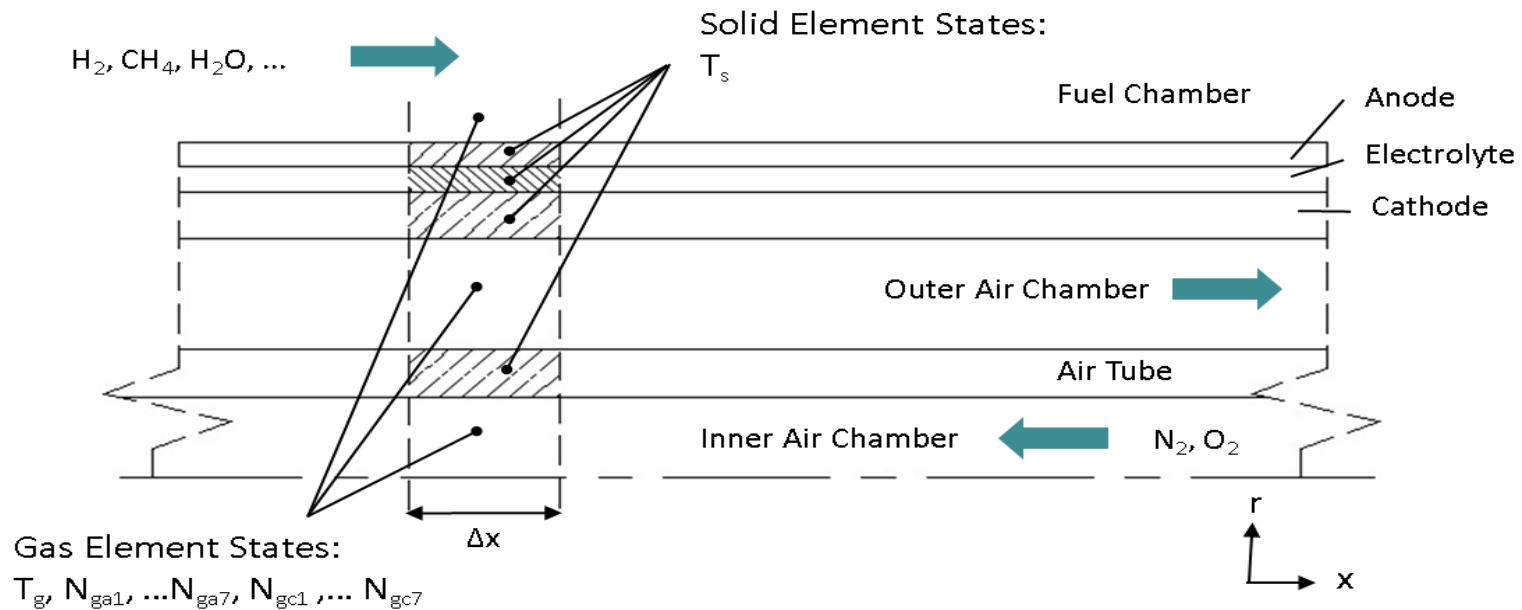
Temperatures, Molar Flows, Current, and Intermediate Variables calculated for each radial element for both dynamic and steady state operation.

SOFC 1ST Principles Equations

Electrochemical Model

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

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

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

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

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

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

Model solved simultaneously and dynamically using APMonitor software
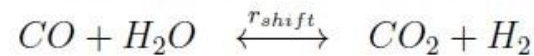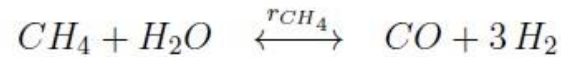
Energy Conservation Model

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

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

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

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

Steam Methane Reforming Model

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

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

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

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

$$K_{eq} = \exp \left(-0.2935 \, \zeta^3 + 0.635 \, \zeta^2 + 4.1788 \, \zeta + 0.3169 \right)$$
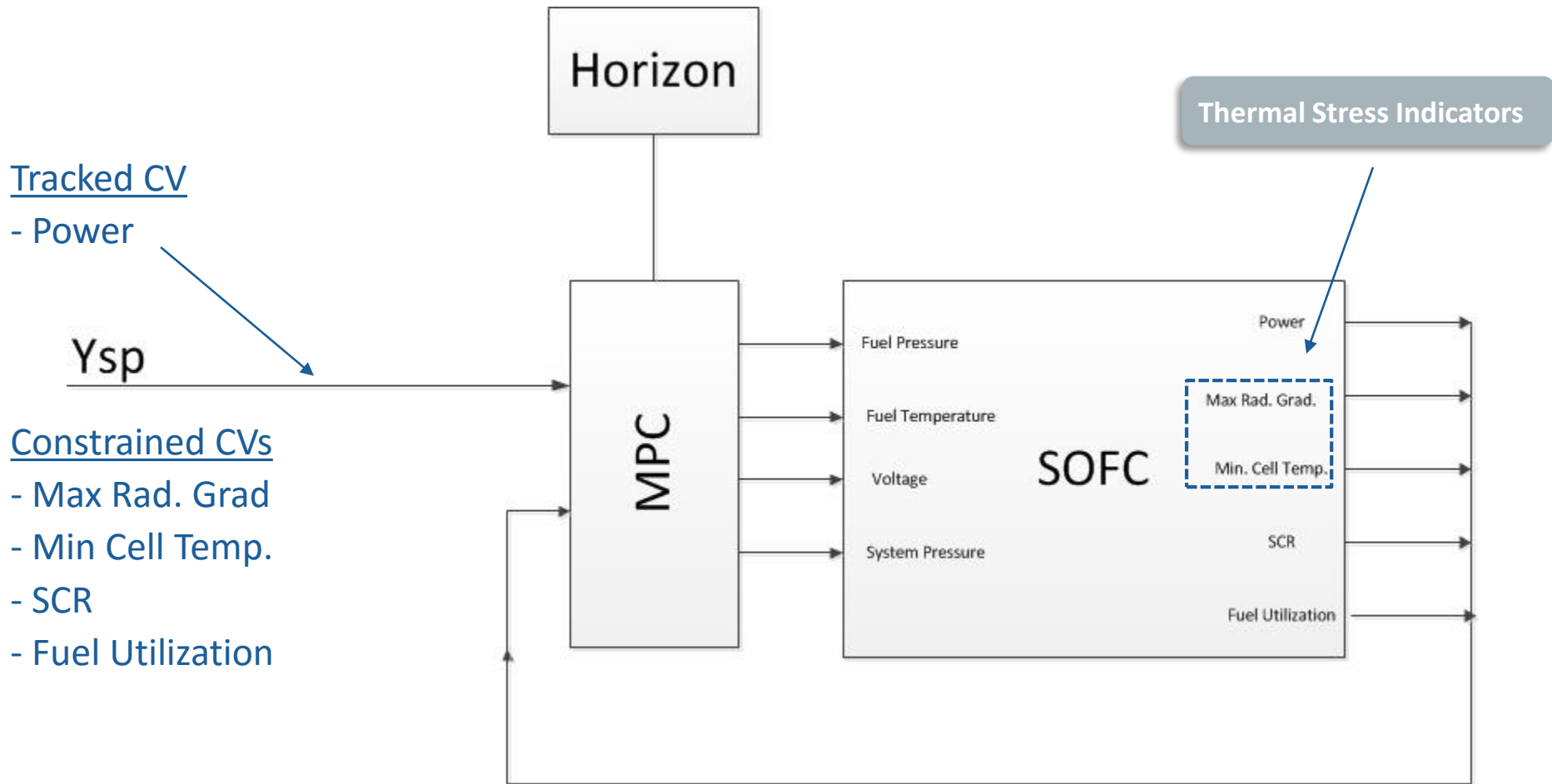
$$\zeta = \frac{1000}{T} - 1$$

Nonlinear Model Predictive Control with Full Spivey Model

Model Predictive Control

- Solution Method
  - APMonitor
  - Solved Simultaneously and Dynamically (vs sequentially)
    - Orthogonal collocation on finite elements technique converts partial differential equations to algebraic equations
    - Model is not only discretized axially and radially, **but also by time**
      - 4 Manipulated Variables (fuel temperature & pressure, voltage, and system pressure)
      - 349 State Variables
    - Study used a 10 time step predictive horizon (500 second horizon)
      - 3490 state variables
      - 40 DOF
    - This method solves much more efficiently bringing solution times for each cycle to less than 1 minute, typically 30 seconds or less
      - Dynamic open loop simulations required 2.5 days of CPU time in a MATLAB simulink environment vs. less than 2 minutes of CPU time for the same simulation solved simultaneously in APMonitor
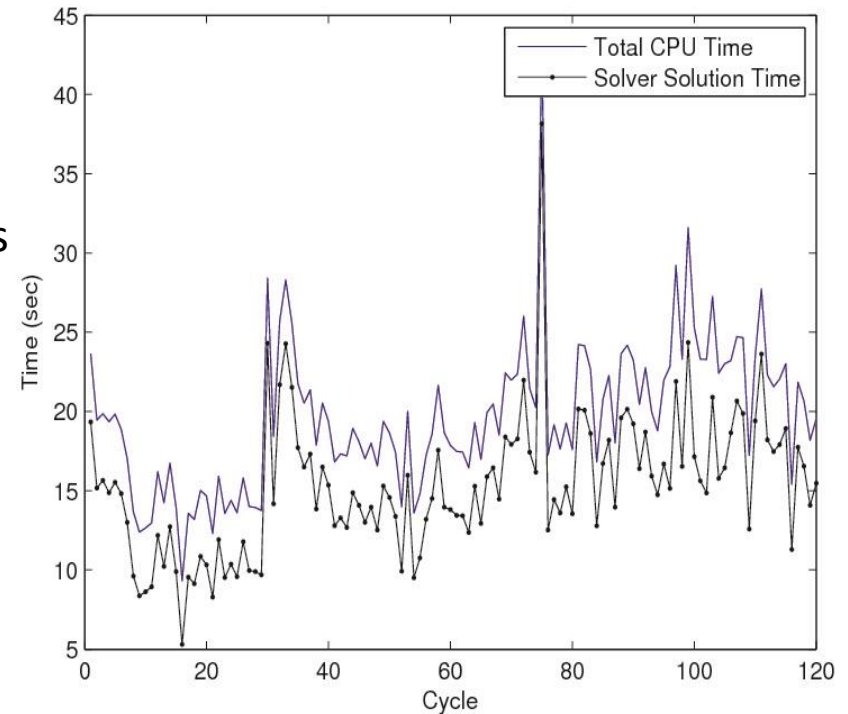
Model Predictive Control Structure

Horizon

Thermal Stress Indicators

Tracked CV
- Power

Ysp

Constrained CVs
- Max Rad. Grad
- Min Cell Temp.
- SCR
- Fuel Utilization

MPC

SOFC

Fuel Pressure
Fuel Temperature
Voltage
System Pressure

Power
Max Rad. Grad.
Min. Cell Temp.
SCR
Fuel Utilization

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

Practical Implementation

- Using a rigorous 1st principles model to control an SOFC has been unrealistic previously due computing limitations. Solution times for a complex model was too long for useful real time model predictive control.

- This research has been able to reach solutions to the rigorous model in times sufficient for real time control.

- Because a rigorous model is used, thermal stress indicators can be predicted much more accurately and quickly to allow control steps to be taken to ensure operation below the thermal stress limits of the SOFC equipment.

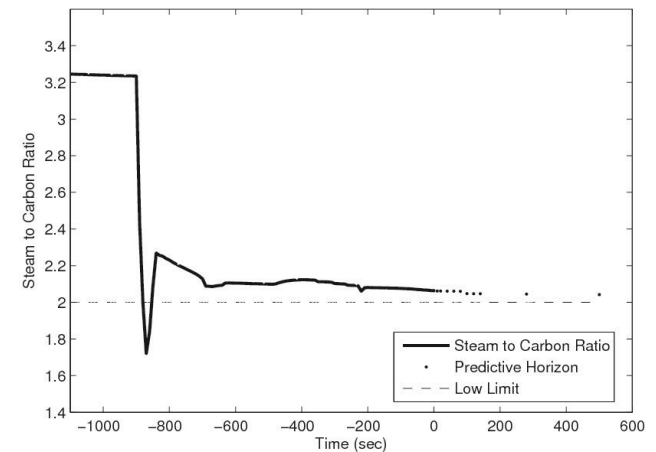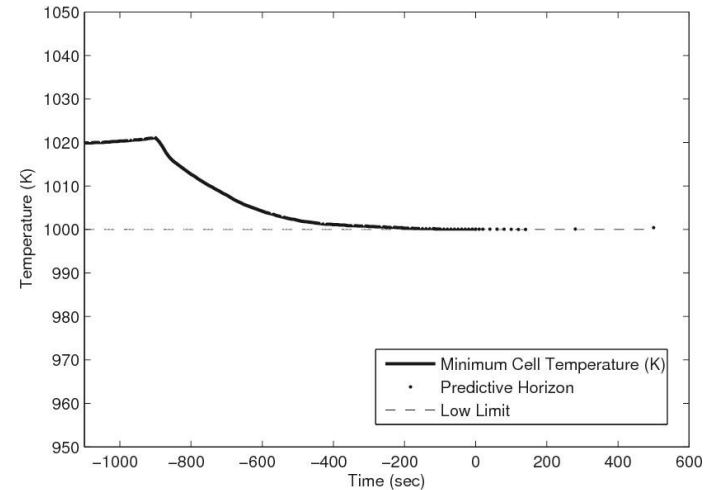# Full Rigorous Model Predictive Control Load Following Study

- Power set point tracking during load change
  - Load change from 260 kW to 273 kW high setpoint dead band
  - 500s horizon shows settling on the low setpoint of dead band

- Constrained control of Max Radial Gradient below 3000 K/m
  - Operation does occur briefly above 3000 K/m for a few seconds, but then settles out below the constraint, protecting the SOFC
  - Radial gradient temperatures only possible with rigorous model
  - Further tuning would prevent deviation
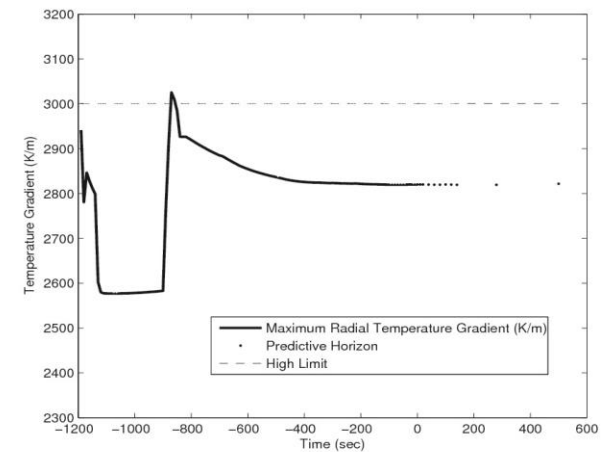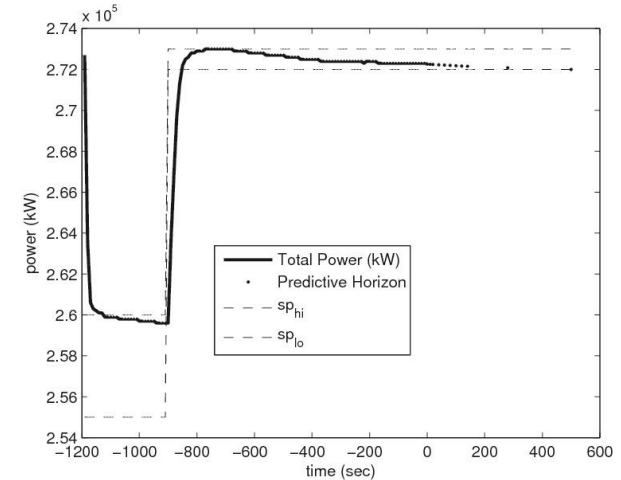
# Full Rigorous Model Predictive Control Load Following Study

- Constrained control of minimum cell temperature
- Fresh fuel is what is driving the minimum cell temperature (temperature at inlet) lower
- Figure shows successful constraint at 1000 K

- Constrained control of steam to carbon ratio
- Literature shows that a minimum of 2:1 steam to carbon is necessary to prevent carbon deposition
- During the load change, the ratio drops slightly below 2 for 1-2 solution cycles but then successfully constrains the ratio above 2

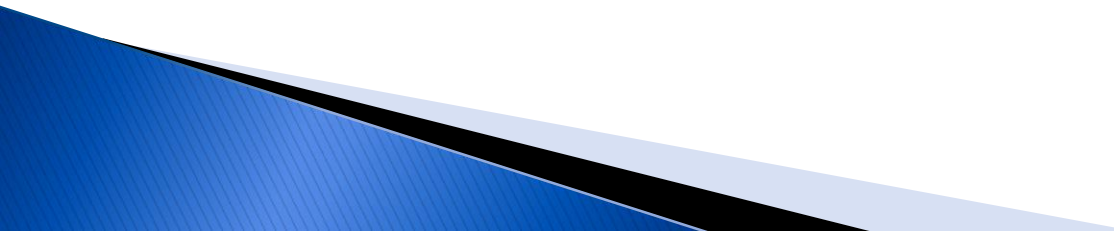# Full Rigorous Model Predictive Control Load Following Study

- Constrained control of fuel utilization
- Successfully maintained above 0.8
- Relates to minimum cell temperature as it pertains to the amount of fuel at the inlet
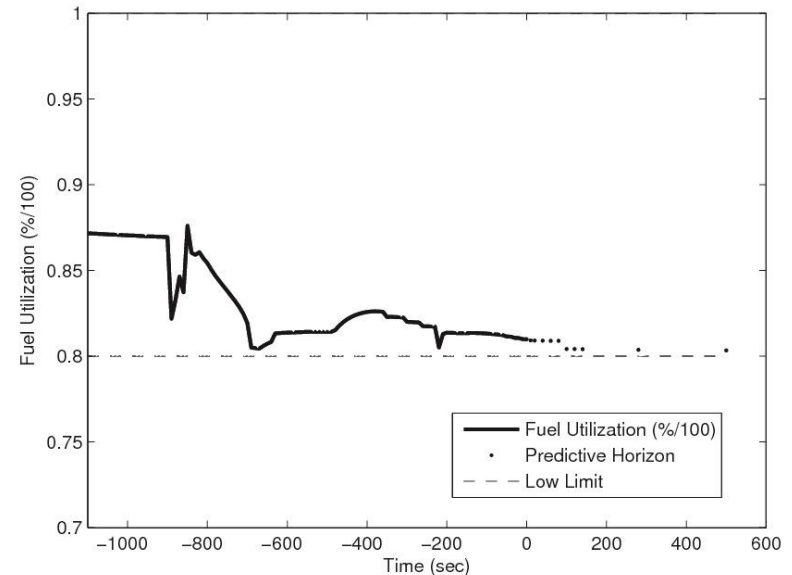
Conclusion

- ◦ Real time model predictive control can improve the reliability of SOFCs
- ◦ Operators can understand the impact of a setpoint changes long into the future on thermal stress indicators and take proactive action
- ◦ The full nonlinear model is more accurate at predicting the dynamic effects of a setpoint change on thermal stress indicators, such as during a start up or a shut down
- ◦ Efficient solution times of the full nonlinear model can enable realistic training situations for new operators
- ◦ Optimization can now take place where operation at constraint can now occur without sacrificing reliability
- ◦ Future Work: Application to an in service SOFC and improved tuning of the controller.
    - • This approach to efficient solutions to complex models for MPC can also be applied to other fields

Acknowledgements

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Questions?

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