Solid Oxide Fuel Cell Model Predictive Control Using APMonitor

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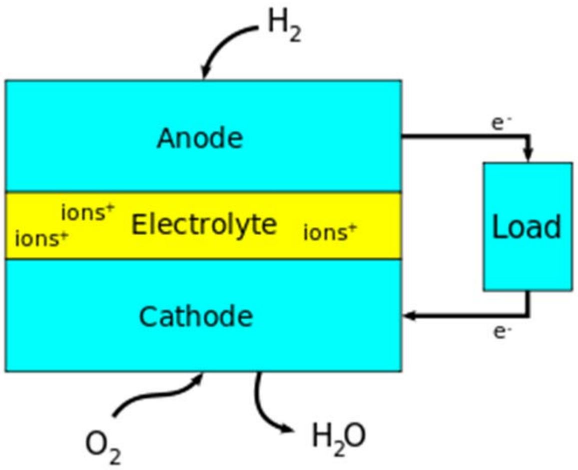
Outline

- Overview of Solid Oxide Fuel Cells (SOFCs)
- Current problems with SOFCs- Objective: Control thermal reliability parameters
- Dr. Spivey's comprehensive SOFC model
- Open-loop testing & simplified model for model predictive control
- Preliminary results in APMonitor MPC environment
- Conclusions
- Future work

Overview of Fuel Cells

- Converts chemical energy to electrical energy
- Not a battery: continuous inputs = continuous supply of electricity
- Typically one cell produces very little voltage or current so they are stacked in series and parallel
- Many types of fuel cells; they are classified by their electrolyte:
  - Proton Exchange Membrane (PEM)
  - Alkaline (AFC)
  - Direct Methanol (DMFC)
  - Phosphoric Acid (PAFC)
  - Molten Carbonate (MCFC)
  - Solid Oxide (SOFC)



The Solid Oxide Fuel Cell (SOFC)

Characteristics

- Electrolyte: ceramic Yttria-stabilized-zirconia (YSZ) about 40 µm
- O^{2-} is the mobile ion
- High operating temp: 600-1000 deg C
- Anode: Porous combination of metallic nickel and YSZ
- Cathode: Usually porous strontium doped lanthanum-manganite

Pros

- Uses relatively inexpensive Ni-YSZ catalyst at anode
- Fuel is internally reformed within the fuel cell
- Simple
- Can achieve efficiencies up to 60%

Cons

- Requires fuel pre-heaters
- Expensive to fabricate
- Reliability

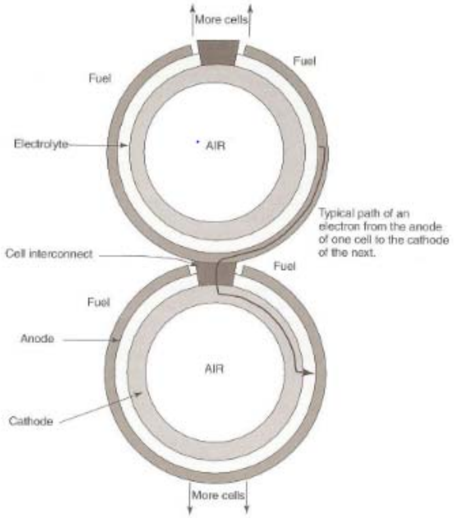


Figure 7.25 End view of tubular type solid oxide fuel cell produced by Siemens Westinghouse. The electrolyte and the anode are built onto the air cathode.

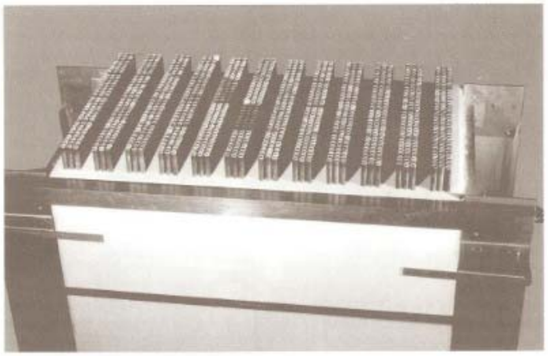


Figure 7.28 Larger stack made from bundles of 24 SOFC tubes. There are 1152 cells, and this stack has a power of about 200 kW. (Photograph reproduced by permission of Siemens Westinghouse.)

Problems- Objective: Control Thermal Reliability Parameters

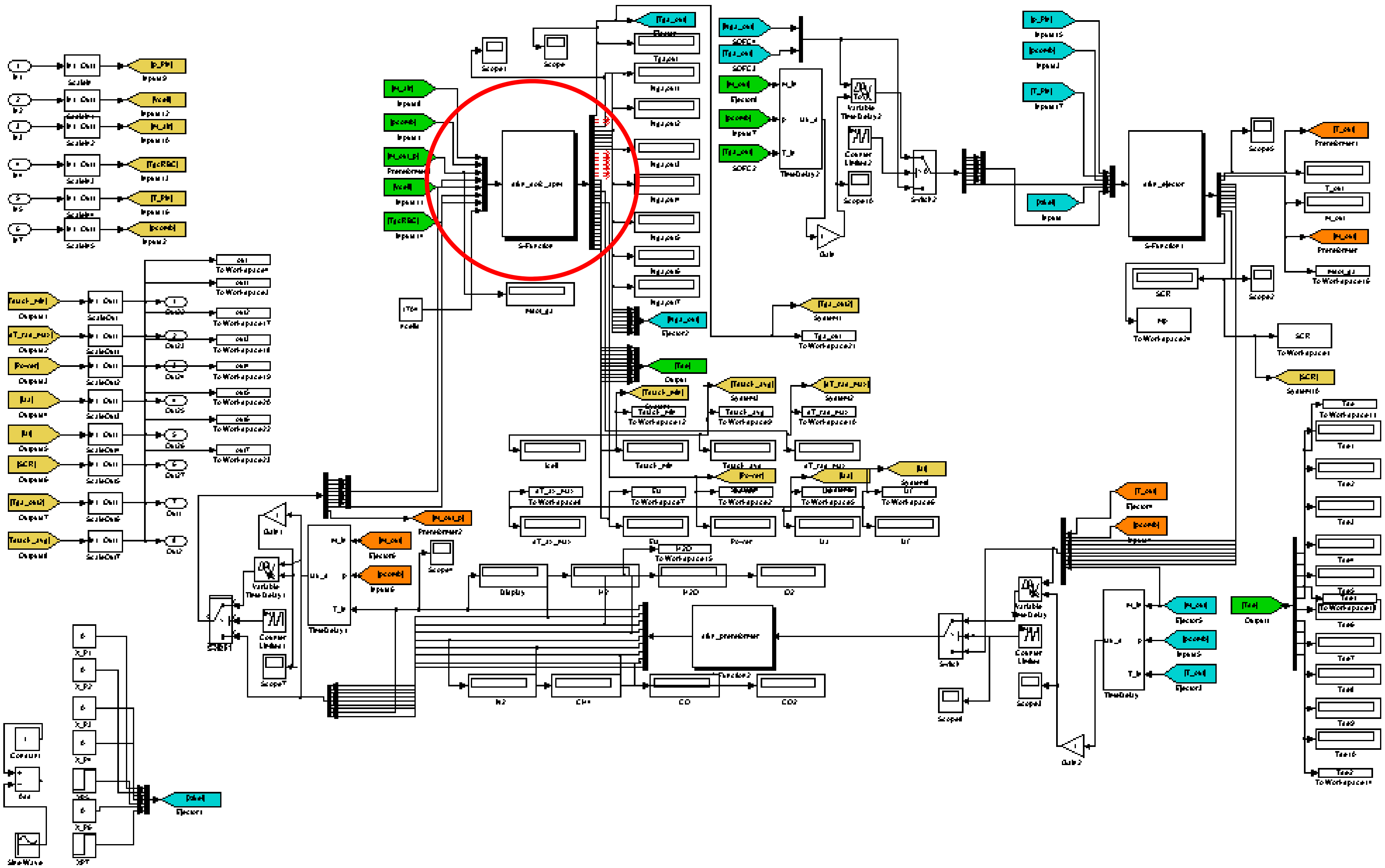
In the past SOFC technology generated a lot of interest and subsequent funding. This technology was expected to achieve widespread use thanks to SOFC's flexible fuel capability and high efficiency, but interest has waned.

- Reliability problems decrease the life of the fuel cell, requiring frequent replacement and driving up the cost of electricity produced with this technology
- Failure modes
  - Thermal cracking of electrolyte
  - Corrosion
  - Redox material degradation
  - Catalyst poisoning

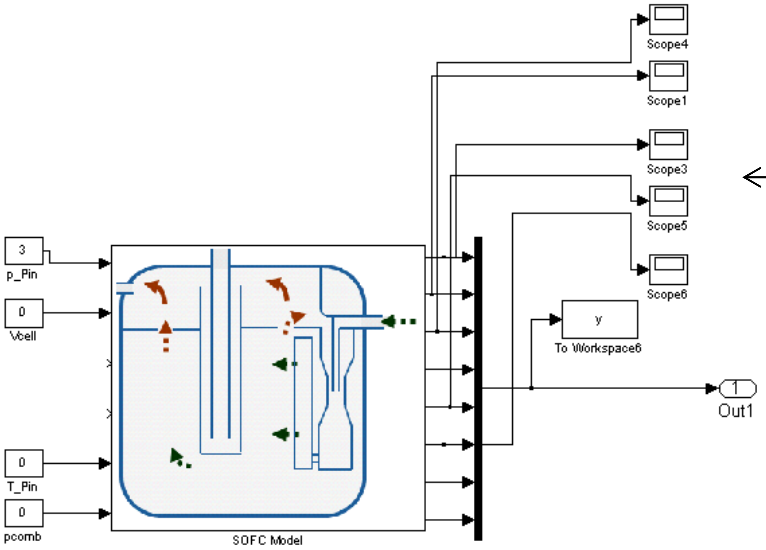
Use of advanced control for thermal management

- Fuel cell life is extended by choosing CV's that increase cell life time
- The minimum stack temperature and max radial gradient have been identified as key reliability parameters to manage thermal cracking
- Need for advanced control to allow fuel cell to operate up to parameter constraints and maximize power output during load following

Comprehensive Model- *Dr. Spivey*

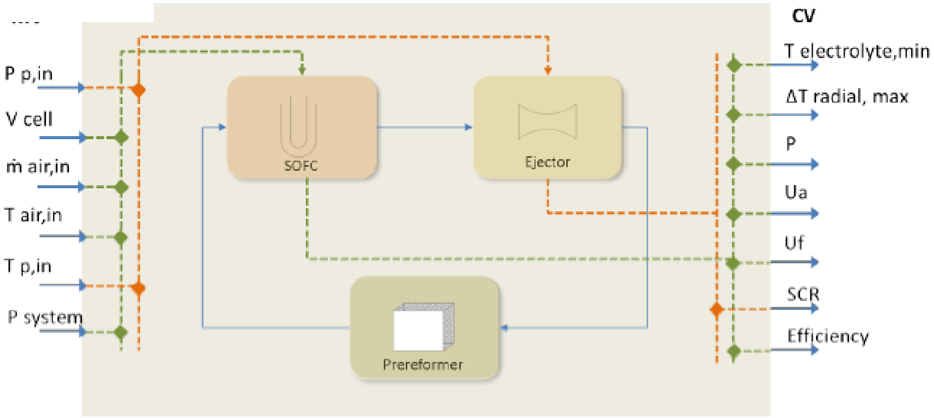


Comprehensive Model- *Dr. Spivey*



Fuel Cell Module

Simplified diagram showing inputs and outputs

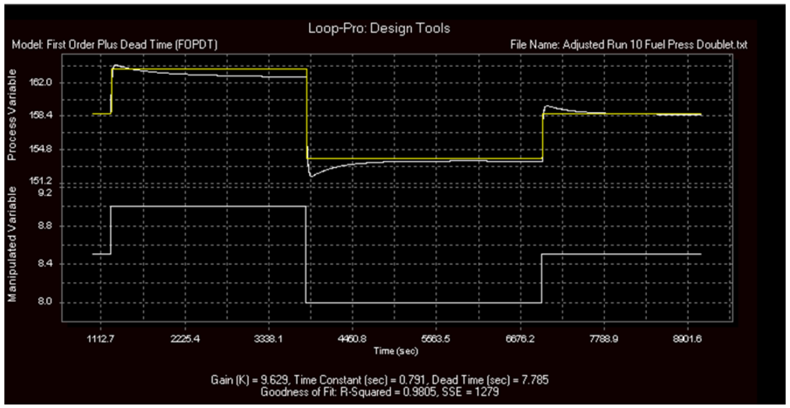


Open-Loop test data from model

Open-Loop testing to obtain gains and time constants for linear model controller

- For preliminary controller, fuel pressure and fuel temperature were used as inputs
- Power, minimum-stack temperature, and max radial gradient as outputs
- Loop-pro software was used to get a FOPDT fit

Power ➔



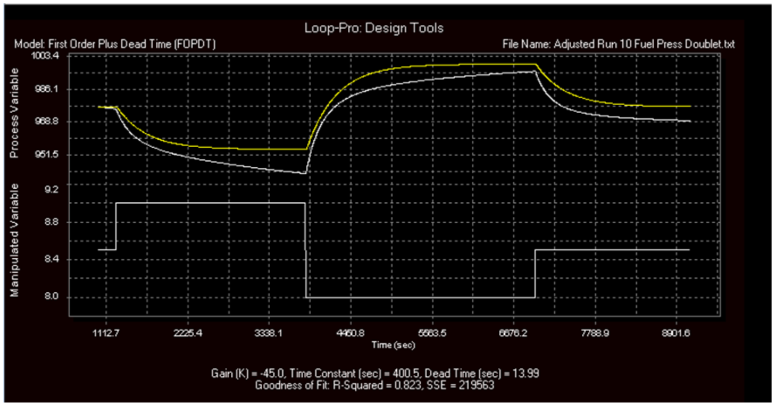
Loop-Pro: Design Tools

Model: First Order Plus Dead Time (FOPDT)

File Name: Adjusted Run 10 Fuel Press Doublet.txt

Gain (K) = 9.629, Time Constant (sec) = 0.791, Dead Time (sec) = 7.785
Goodness of Fit: R-Squared = 0.9805, SSE = 1279

Tstack-Min ➔



Loop-Pro: Design Tools

Model: First Order Plus Dead Time (FOPDT)

File Name: Adjusted Run 10 Fuel Press Doublet.txt

Gain (K) = -45.0, Time Constant (sec) = 400.5, Dead Time (sec) = 13.99
Goodness of Fit: R-Squared = 0.823, SSE = 219563

	Control Parameters					
Outputs	Kp w/ Fuel Temperature	Kp w/ Fuel Pressure	τ w/ Fuel Temperature	τ w/ Fuel Pressure	ϴ w/ Fuel Temperature	ϴ w/ Fuel Pressure
Power	-0.0818	9.63	5.12	0.791	3.8	7.79
Tstack minimum	0.208	-45	239	401	12	14
Max Radial Gradient	-2.29	328	0.487	136	5	3.08

Simplified Model- Model Predictive Control

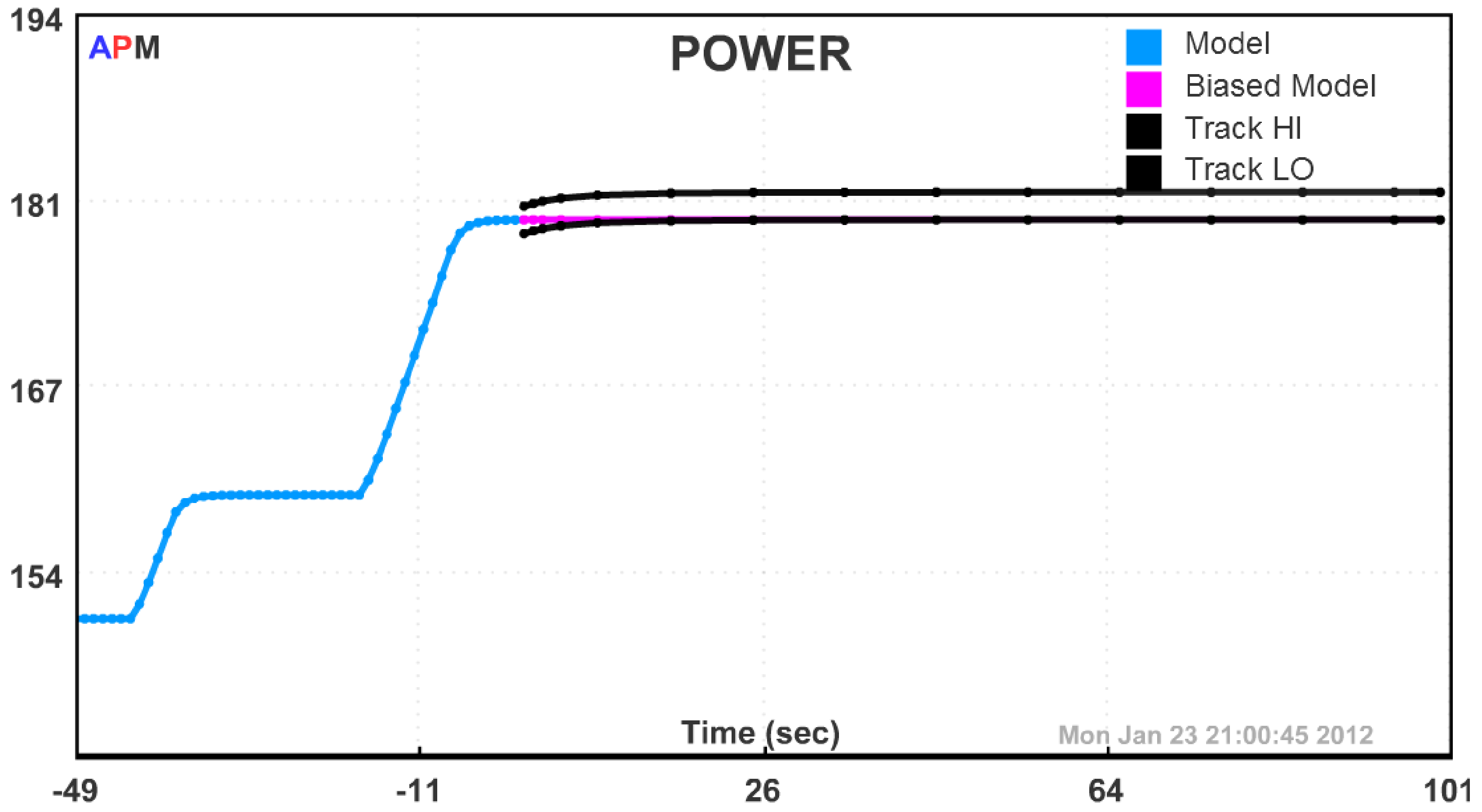
APMonitor software used for model predictive control

- Programmed using Python scripting language
- First order model equations used for linear controller:
  - **taupp * $Power = -(Power-Power_0) + kpp*(fuel_pressure-fuel_pressure_0)+ kpt*(fuel_temp-fuel_temp_0)**
  - **tauprg * $Rad_gradient = -(Rad_gradient-Rad_gradient_0) + kprg*(fuel_pressure-fuel_pressure_0)+ krgt*(fuel_temp-fuel_temp_0)**
  - **tautsmp*$Tstack_min=-(Tstack_min-Tstack_min_0)+ktsmp*(fuel_pressure-fuel_pressure_0)+ ktsmt*(fuel_temp-fuel_temp_0)**
- Dollar signs represent derivative sign

Results in APMonitor

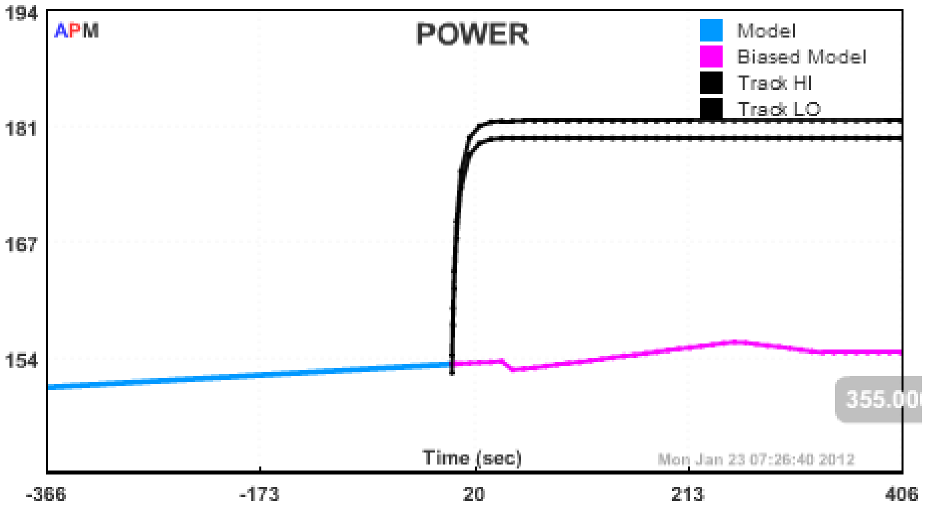
APMonitor software used for model predictive control

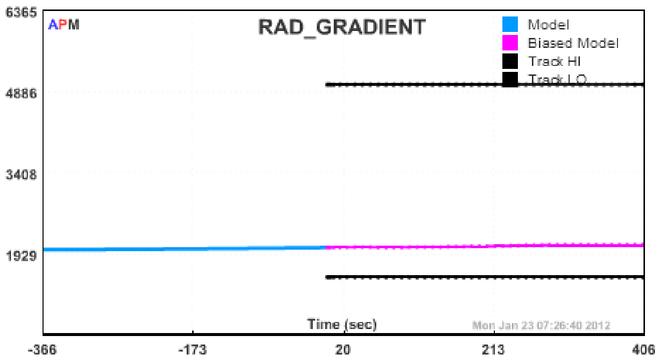
Minimum cell temperature constraint at 950 deg C

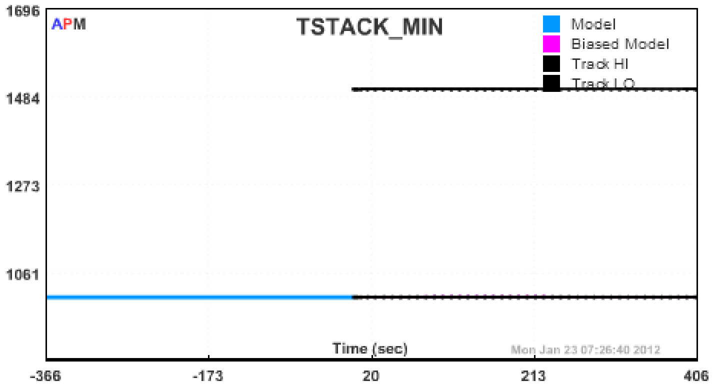


Results in APMonitor

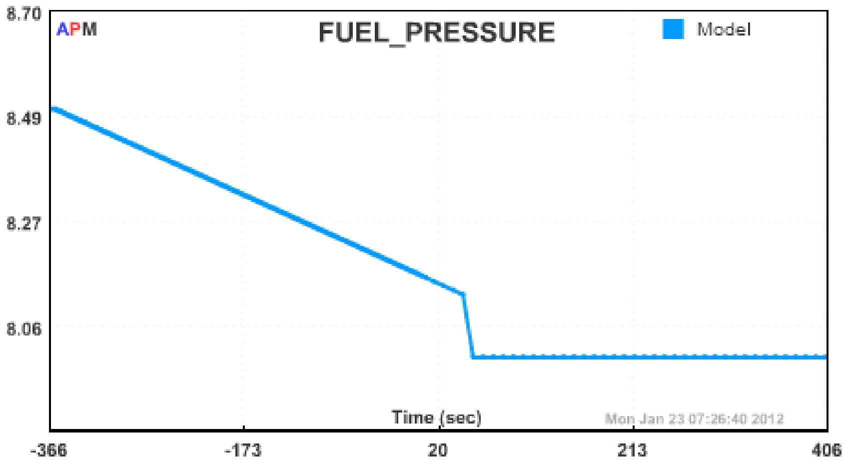
Using a minimum cell temperature constraint of 1000 deg C

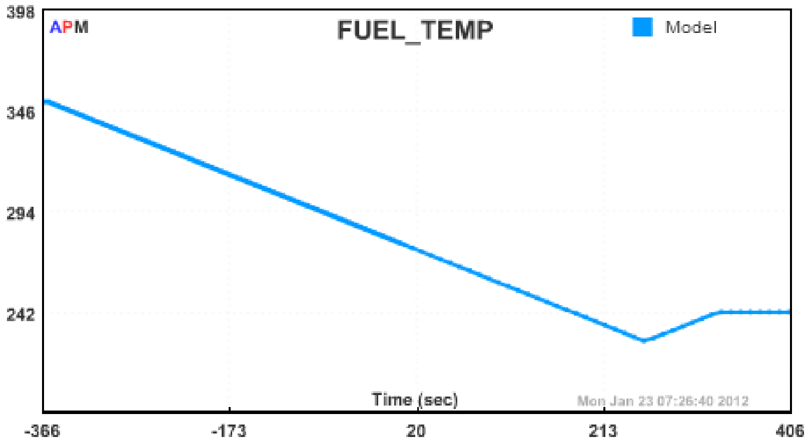






Results in APMonitor





Conclusions

- There is potential to extend fuel cell lifetime by using advanced control to maximize power output and operate up to reliability constraints
- Dr. Spivey's model has provided a very useful non-linear first principles model from which to obtain open-loop response data
- APMonitor control environment provides a very user-friendly platform to simulate SOFC conditions
  - Very simple to change constraints, set-points, and view responses
  - Changes could be in the code or in APMonitor web interface

Future Work

- Continue refine linear model to better match what Dr. Spivey’s comprehensive model would predict
- Use Dr. Spivey’s entire model for non-linear model predictive control in APMonitor

Questions?

Works Cited:

1. Benjamin J. Spivey, John D. Hendengren, Thomas F. Edgar. "Constrained Control and Optimization of Tubular Solid Oxide Fuel Cells for Extending Cell Lifetime." 2011: 6

2. Spivey, Benjamin James. *Dynamic Modeling, Model-Based Control, and Optimization of Solid Oxide Fuel Cells.* 2011.

3. James Larminie, Andrew Dicks. *Fuel Cell Systems Explained.* 2nd. West Sussex: John Wiley & Sons Ltd., 2003

Appendix

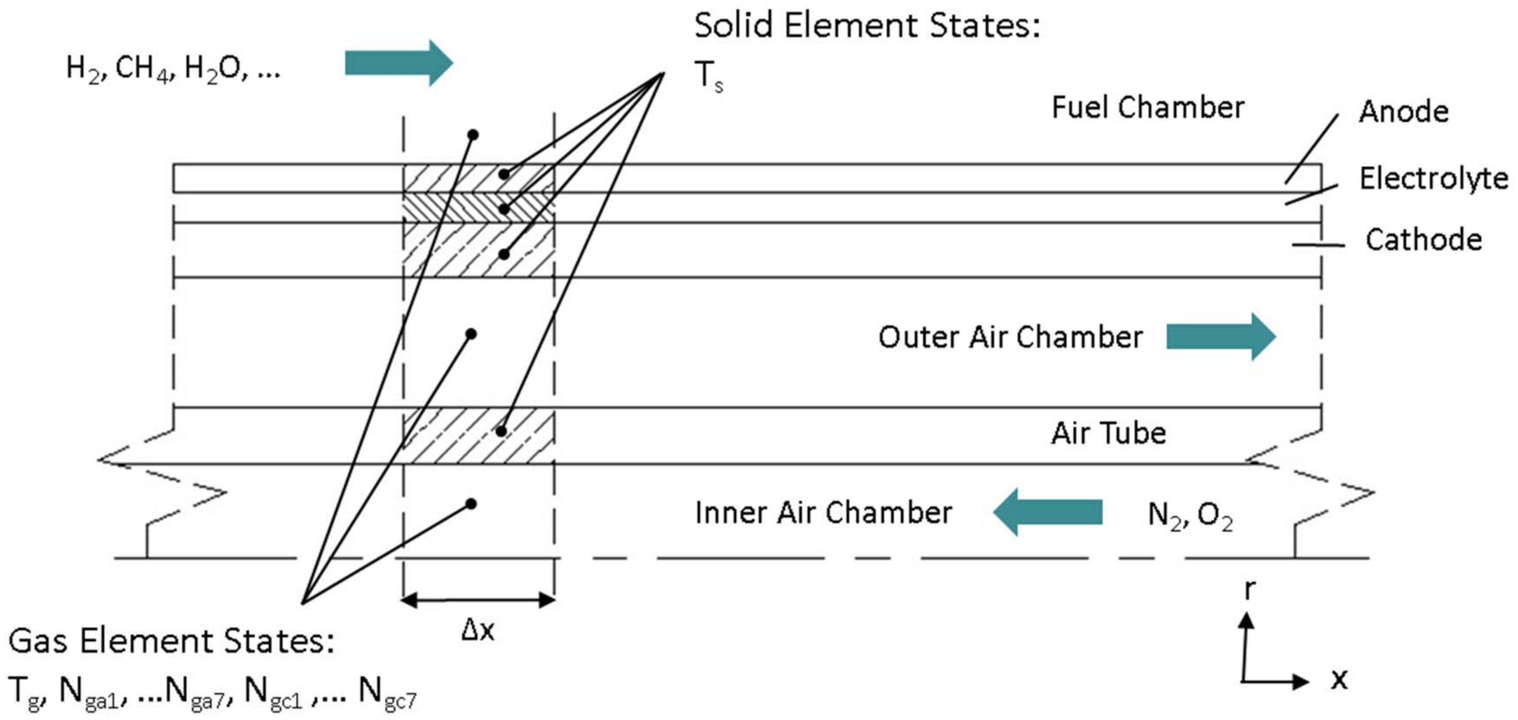
SOFC System Modeling Decisions

Feature	Description
7 Molar Gas Species	7 species (H2, H2O, N2, O2, CH4, CO, CO2) are needed to accommodate methane fuel and air oxidant. Some models may use 3 (H2, H2O, O2).
Reformation Reactions	Steam-methane reformation, water-gas shift. Introduce nonlinearities and implicit equations – increased convergence difficulty. Unnecessary with H2 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 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

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

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

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

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

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

Steam Methane Reforming Model

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

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

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

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

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

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

Some authors resort to iterating b/t electrochemical and energy models for steady-state solutions **– here it is solved simultaneously and dynamically.**

This model is unique and references multiple articles and books.

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).