Resolving the Interactions between the Balance of Plant, SOFC, Power-Conditioning, and Application Loads

Project Investigators

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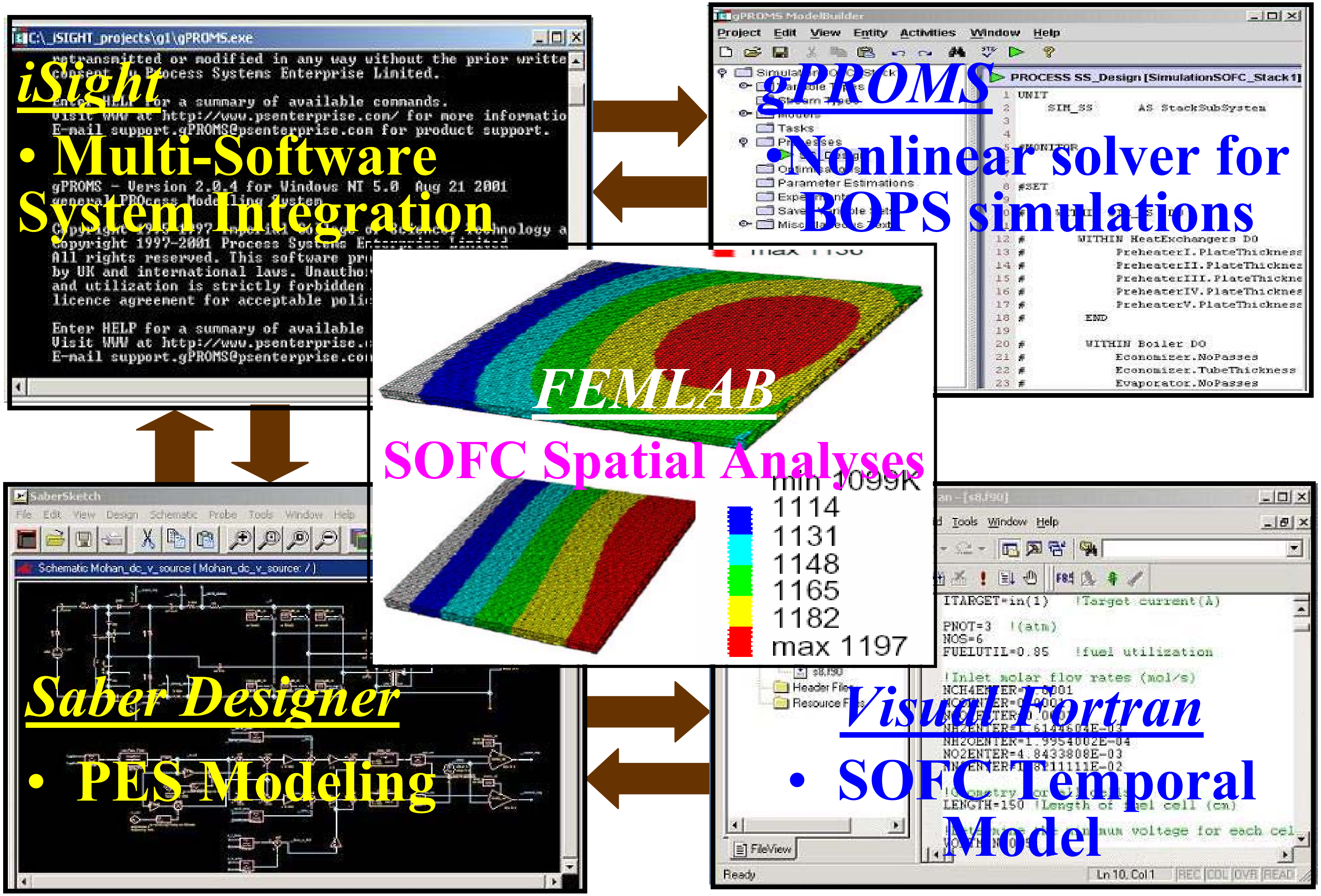
SECA Core Technology Program Review Meeting

May 12, 2004
Boston, Massachusetts

PES Modeling &
System Integration and Analysis

Phase-I Comprehensive SOFC-PS Modeling



iSight

- **Multi-Software System Integration**

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```

gPROMS

- **Nonlinear solver for BOPS simulations**

```
UNIT
    SIM_SS        AS  StackSubSystem


#MONITOR


#SET

#           WITHIN HeatExchangers DO
#                 PreheaterI.PlateThickness
#                 PreheaterII.PlateThicknes
#                 PreheaterIII.PlateThickne
#                 PreheaterIV.PlateThicknes
#                 PreheaterV.PlateThickness
#            END

#            WITHIN Boiler DO
#                 Economizer.NoPasses
#                 Economizer.TubeThickness
#                 Evaporator.NoPasses
```

FEMLAB

SOFC Spatial Analyses

Saber Designer

- **PES Modeling**

```
ITARGET=in(1)    !Target current(A)

PNOT=3   !(atm)
NOS=6
FUELUTIL=0.85    !fuel utilization

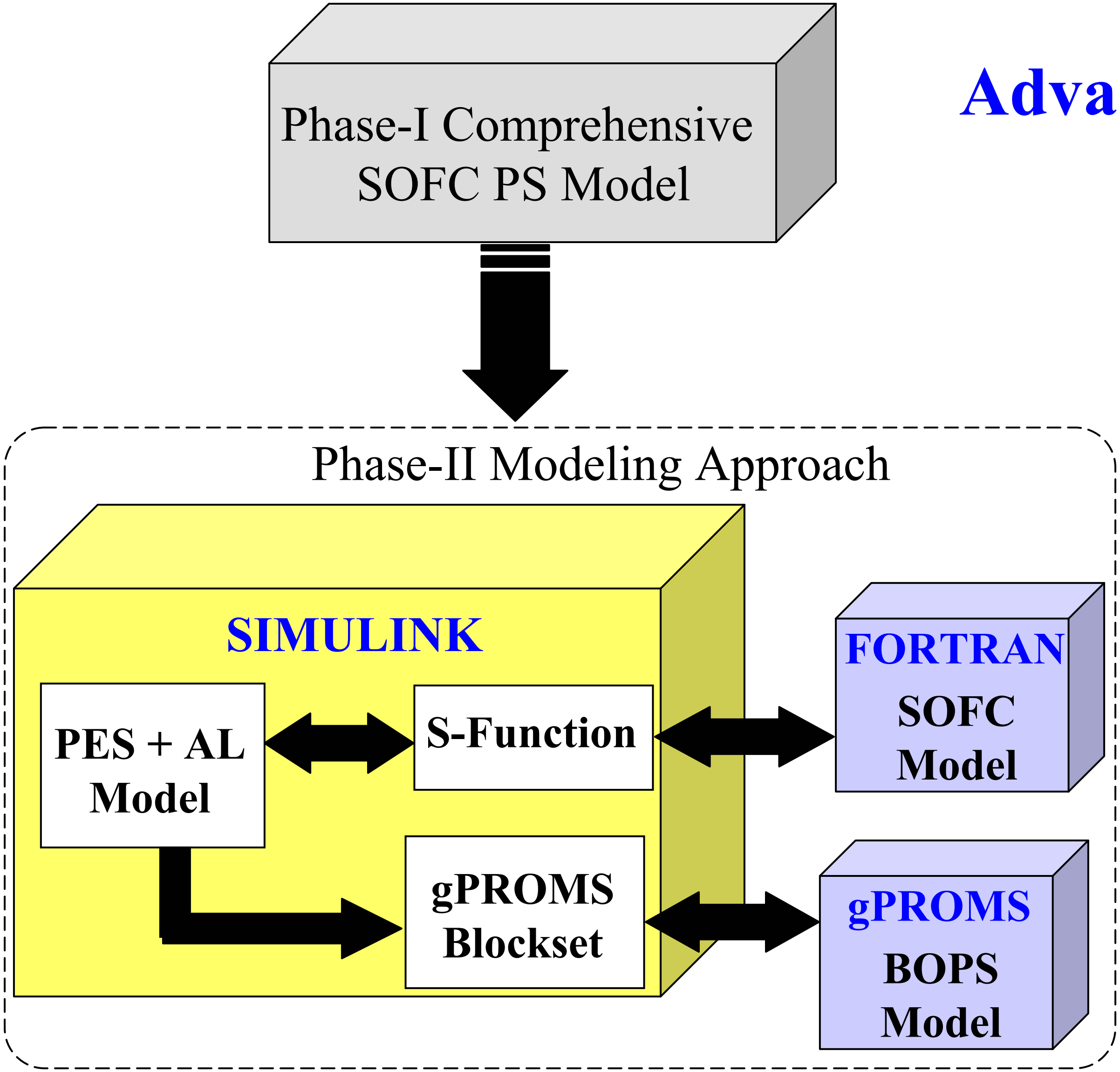
!Inlet molar flow rates (mol/s)
NH2ENTER=1.6144604E-03
NH2OENTER=1.9954002E-04
NO2ENTER=4.8433808E-03

LENGTH=150  !Length of fuel cell (cm)
```

Visual Fortran

- **SOFC Temporal Model**

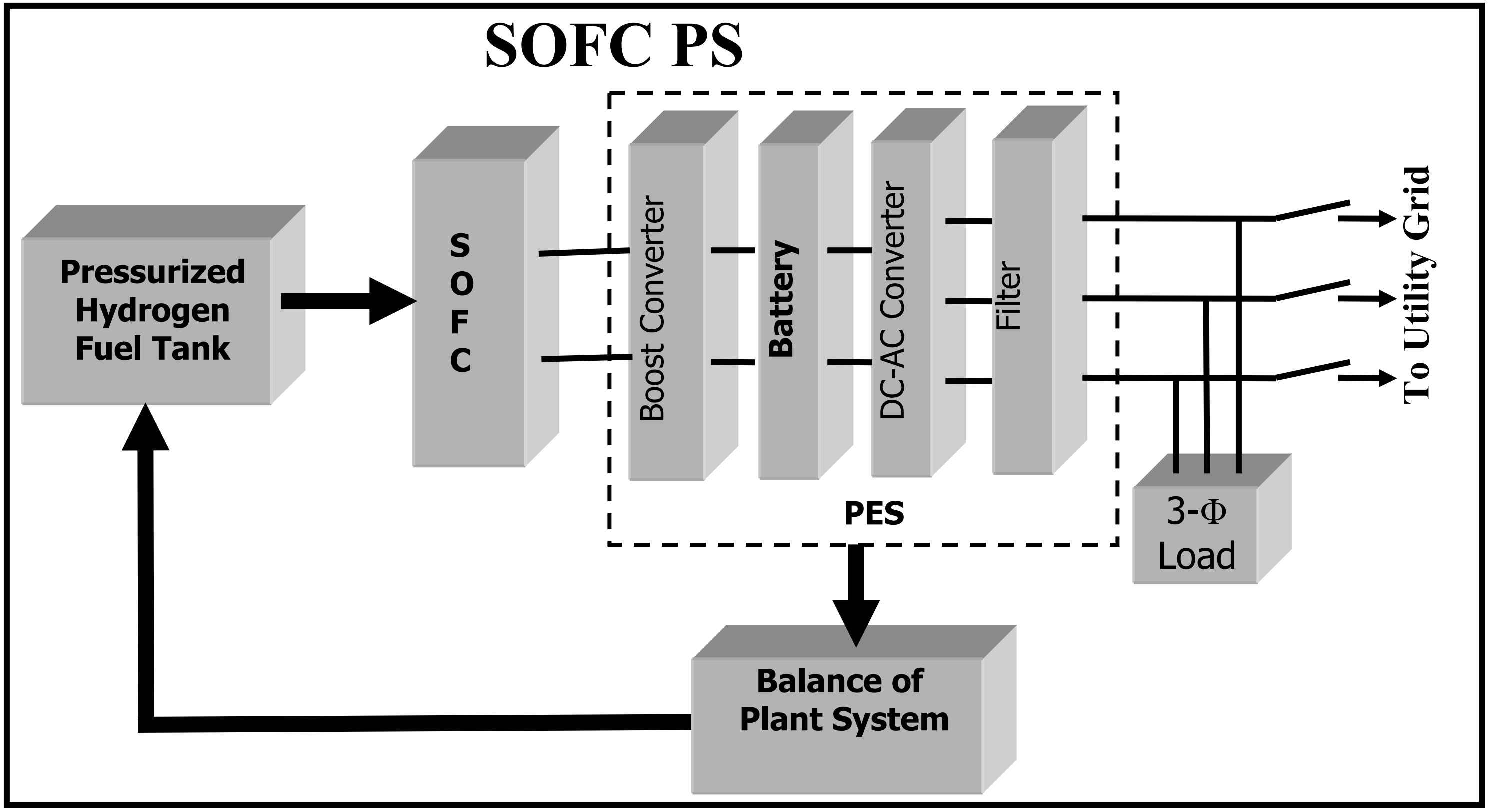
Modeling Approach for Phase-II



Advantages of SIMULINK

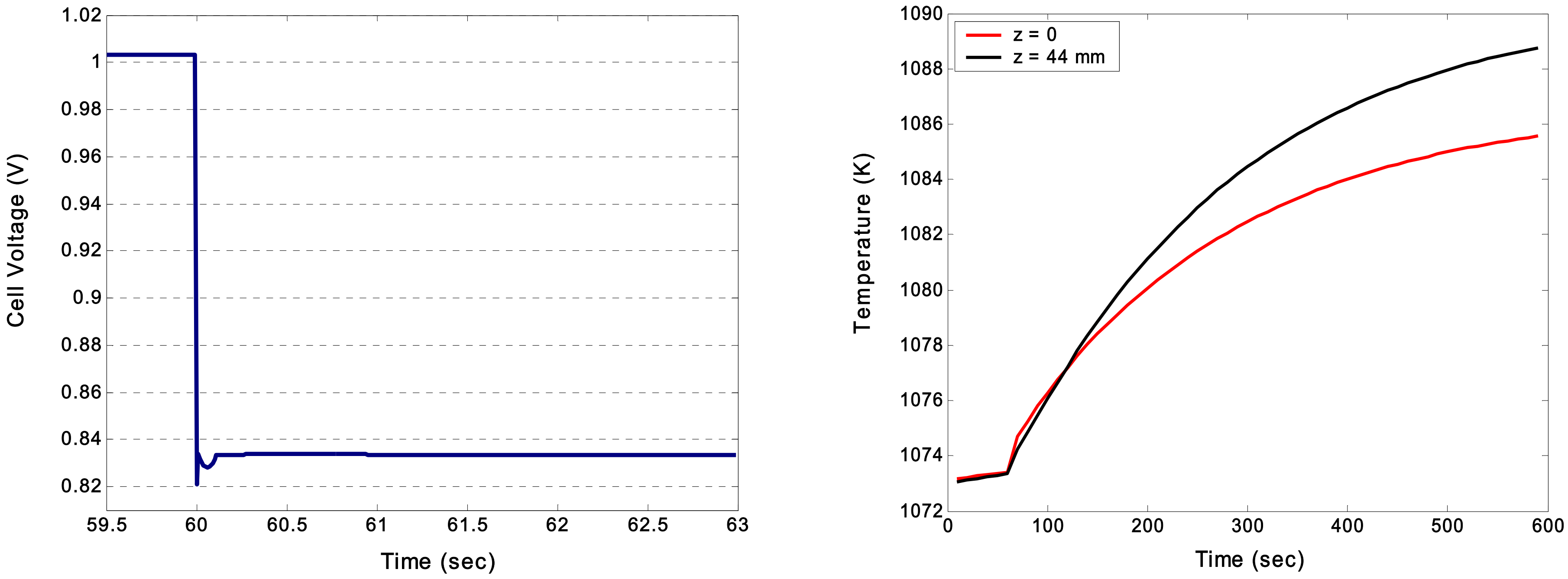
- Cost effective
- Easily accessible to members of SECA industrial group
- Can seamlessly integrate with FORTRAN and gPROMS; hence existing SOFC and BOPS models can be used for offline simulation

Load Transient Mitigation
Energy-Storage Devices



- Energy storage devices to mitigate the effects of load-transients on SOFC
  - Batteries
  - Pressurized-hydrogen storage tanks

SOFC Response to Load Transients



- ❖ Increase in load results in the increases of the current density, which increases the polarization drop in cell, and hence a drop in the cell voltage.

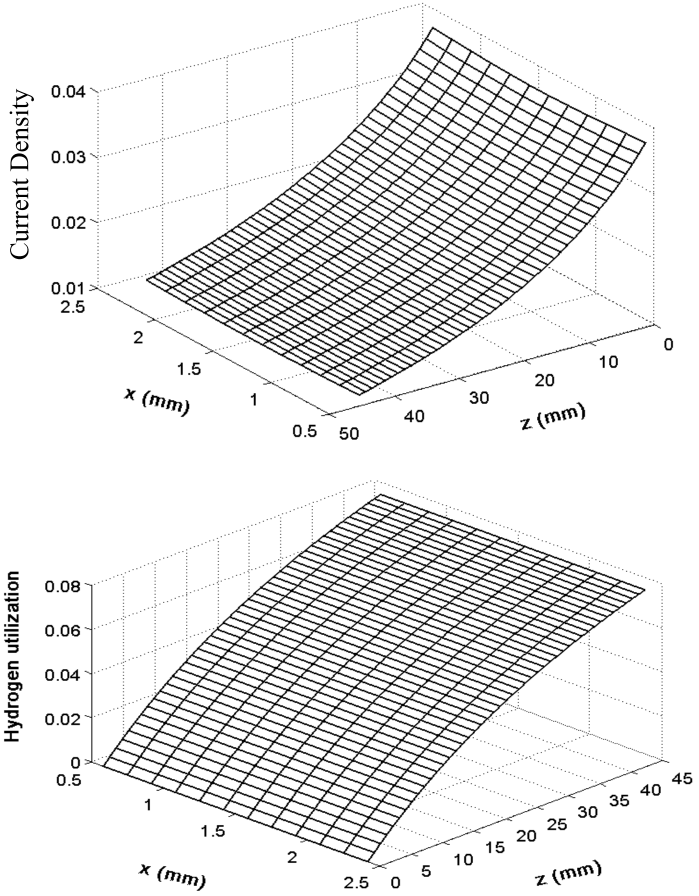
- ❖ Increase in the temperature due to higher thermal energy release resulting from more electro-chemical reactions, i.e.

$$T_{n+1} = \frac{\Delta t}{\rho \cdot Cv \cdot (\Delta V)} q_{total} + T_n$$

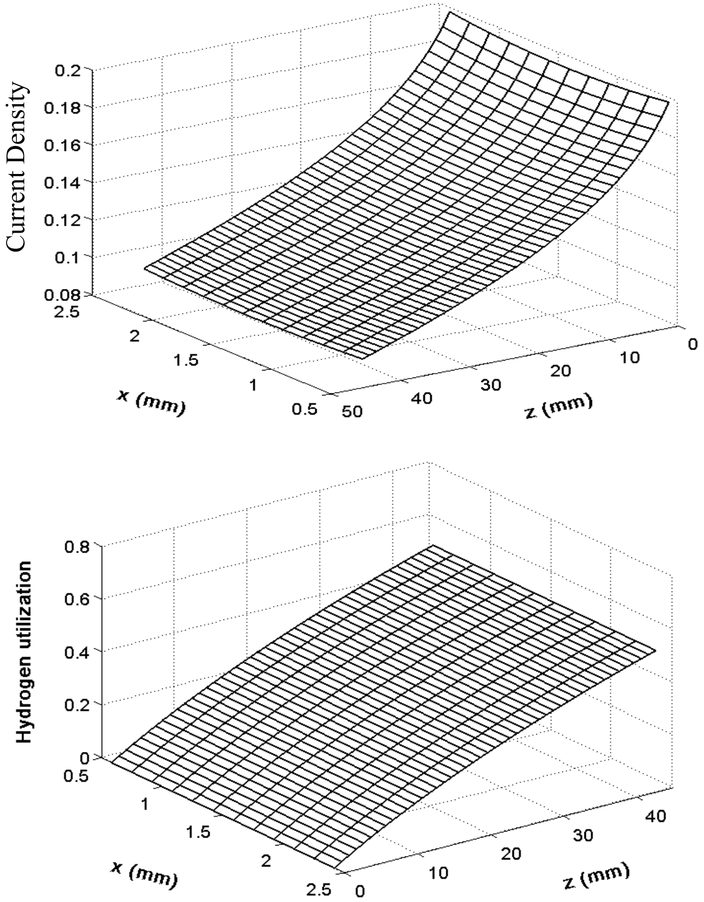
SOFC Response to Load Transient

Current Density and Fuel Utilization

Before Load Transient



After Load Transient

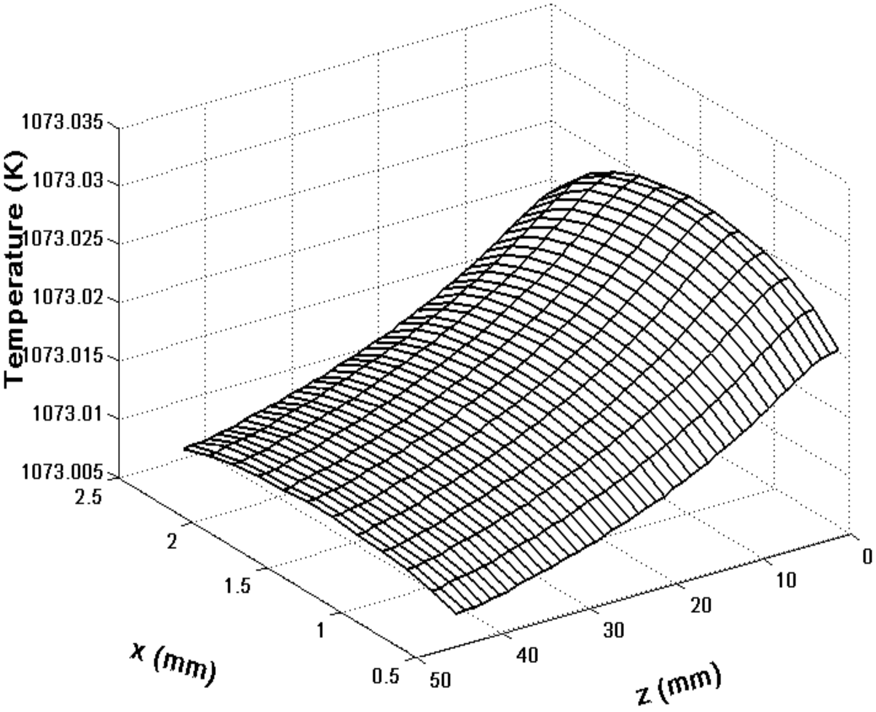


- ❖ A sudden increase in the current density just after the load transient
- ❖ Higher current density increases the fuel utilization drastically just after the load transient

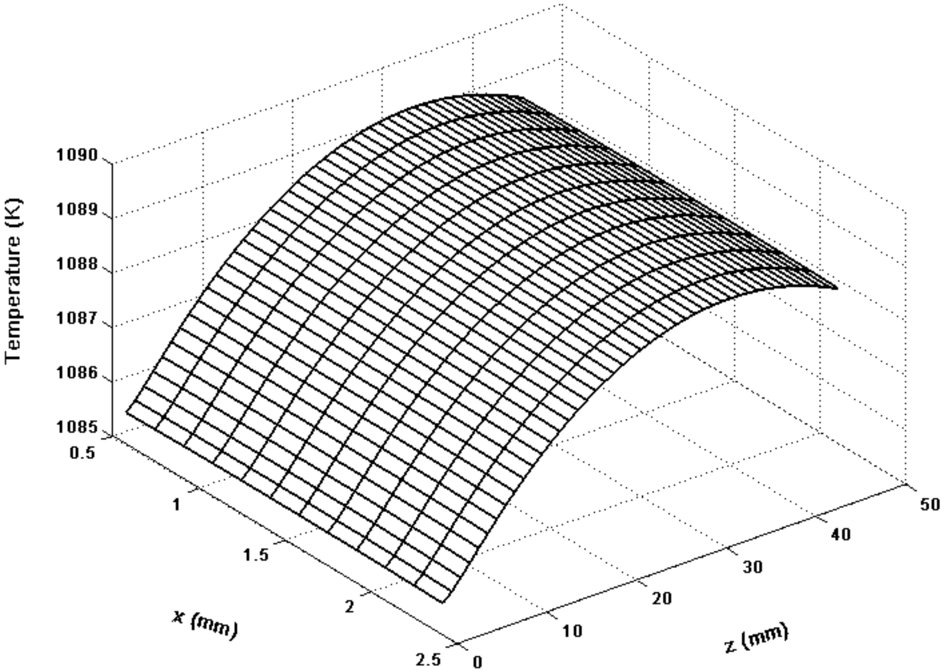
SOFC Response to Load Transient

Spatial Temperature Distribution

Before Load Transient



After Load Transient

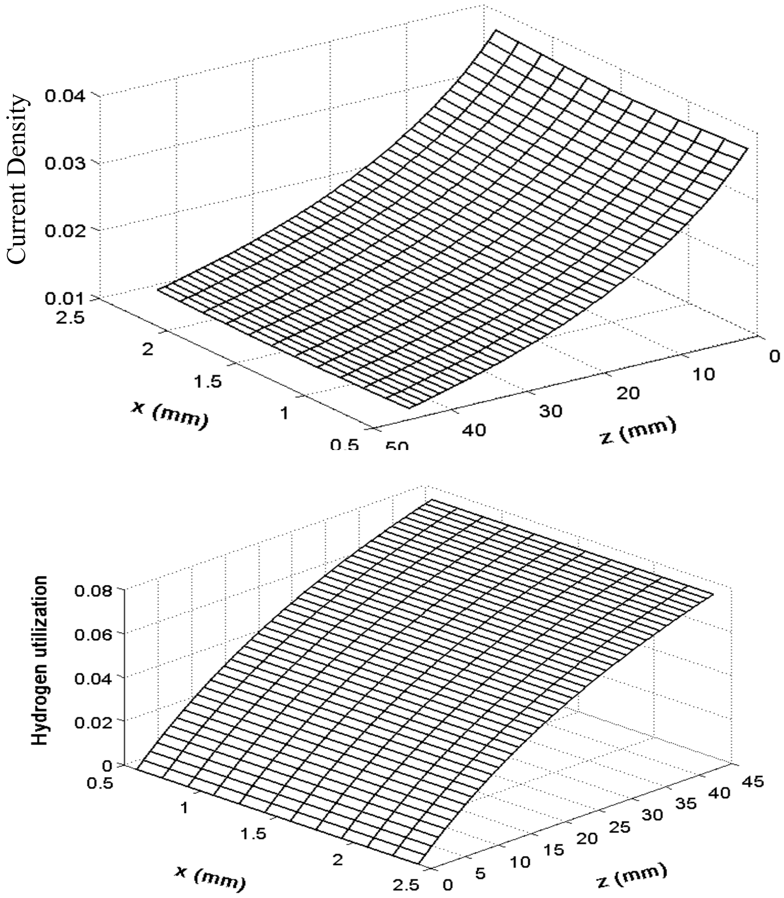


- **Issues**
  - ❖ Cathode may be subjected to significant stresses (thermal expansion mismatch)
  - ❖ Increase in the cleavage strength (comparable to the grain boundary strength)
  - ❖ May result in the appearance of inter-granular fracture

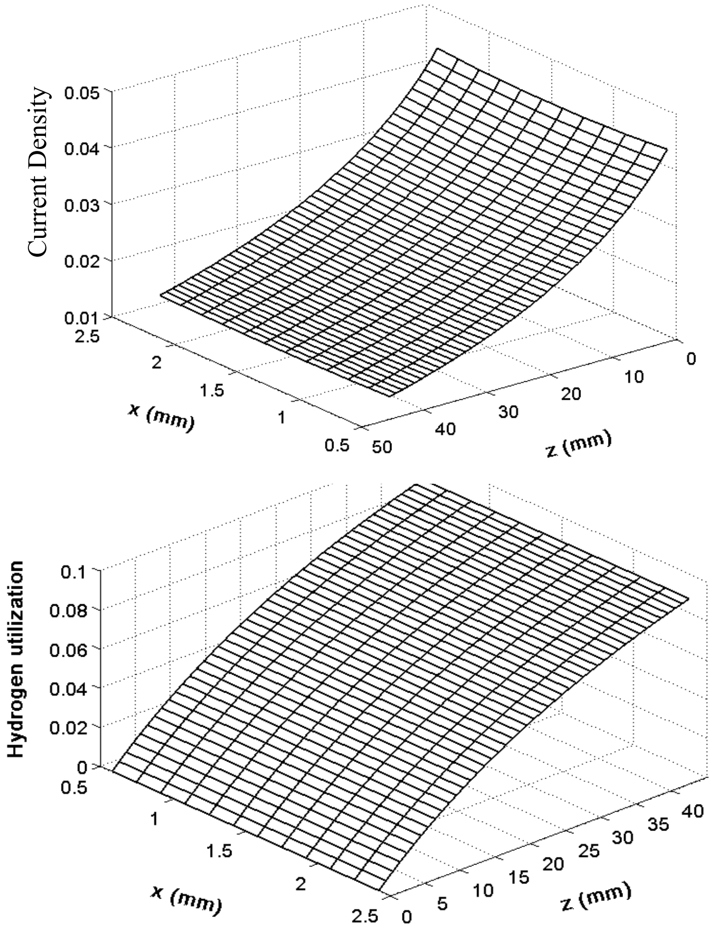
Load-Transient Mitigation

Effects of Energy-Buffering Devices

Before Load Transient



After Load Transient

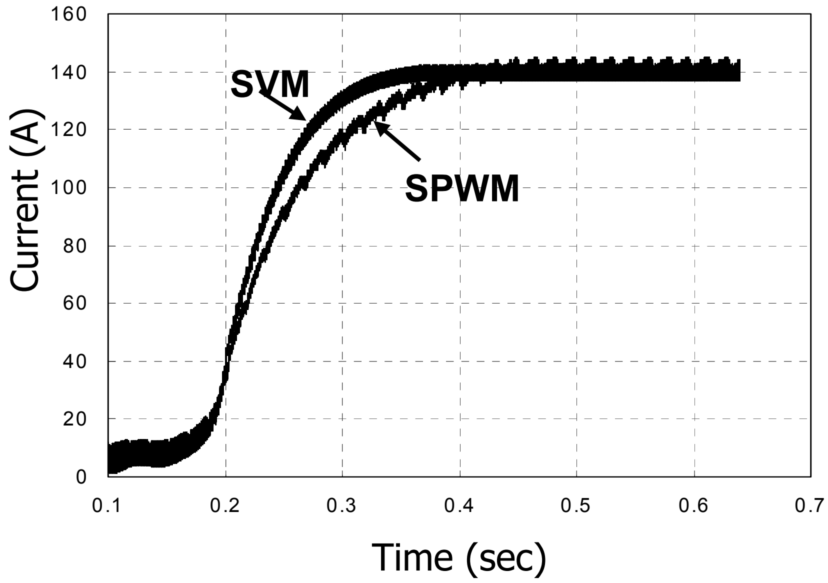


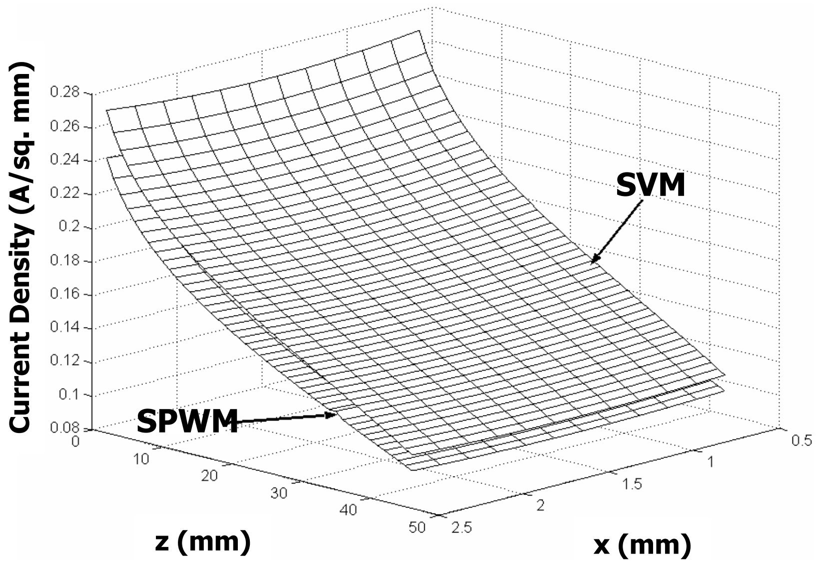
- Battery provides the required load current during the transient
- Minimal increase in the current density and in turn minimal increase in the fuel utilization

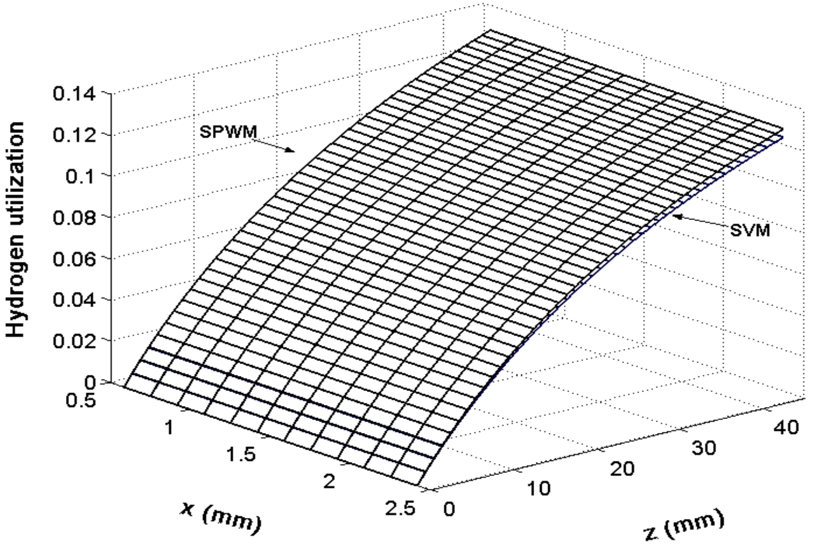
Load-Transient Mitigation

Effect of Advanced Inverter Modulation Techniques

- Space-vector modulation used for the inverter
- Slow boost converter response to prevent immediate change in SOFC energy demands







Georgia Tech/Ceramatec

SOFC
Modeling and Analysis

SOFC Transient Response Time Scales

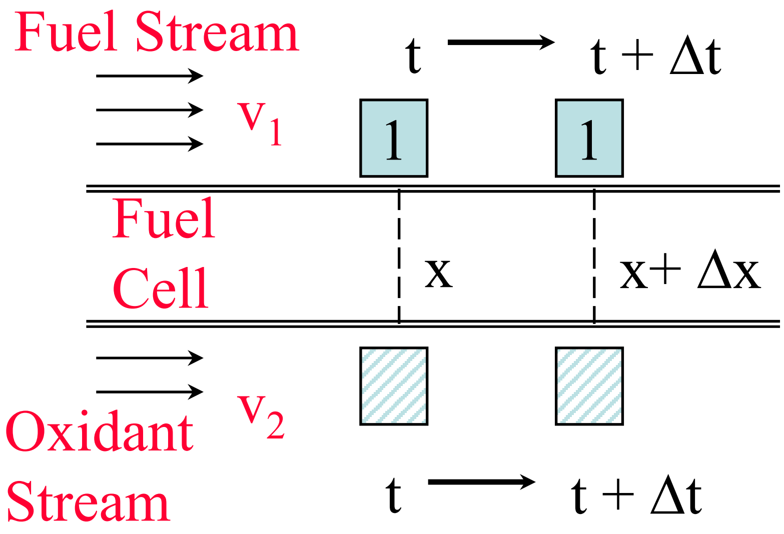
- Electrochemical (µsec)
  - Gas phase phenomena
  - Diffusion/surface absorption relaxation

- Hydraulic (msec) - Time Scale in Simulink Model
  - Reactant depletion/accumulation effects within electrode
  - Gas flow transit time

- Thermal (ksec)
  - Too slow to notice power electronics transients
    - Startup
    - Load change

- Aging (years)
  - Lifetime degradation
    - Solid state cation interdiffusion/reaction
    - Microstructural coarsening

Operational Reactant Feed/ Load Variation



Fuel Stream

t → t + Δt

v_1

1

1

Fuel Cell

x

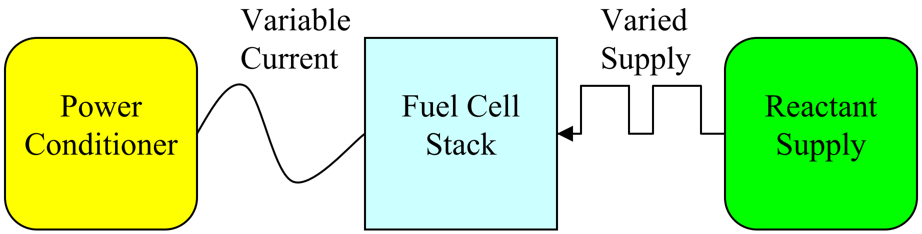
x+ Δx

v_2

Oxidant Stream

t → t + Δt

$$\eta_{element}(t+\Delta t) = \eta_{field}(x+\Delta x, t+\Delta t)$$



Power Conditioner

Variable Current

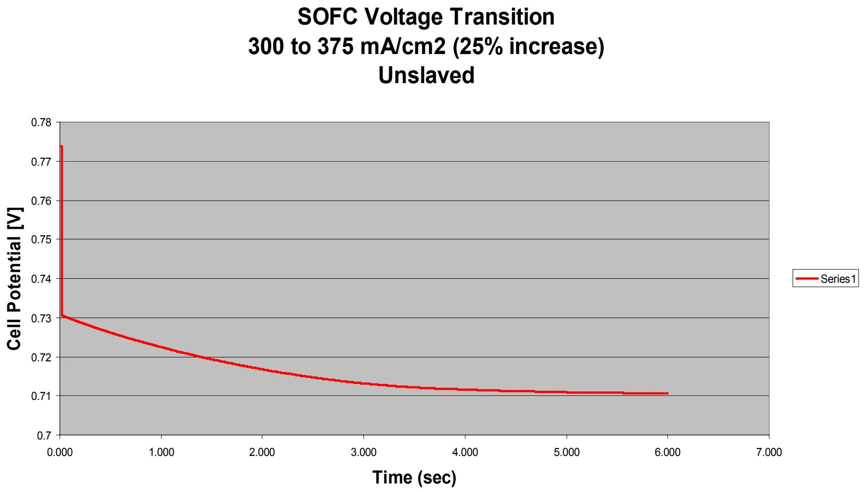
Fuel Cell Stack

Varied Supply

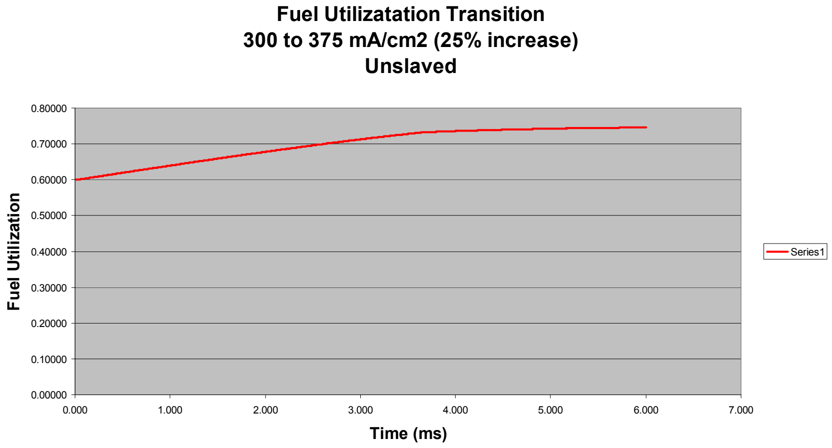
Reactant Supply

- *Variable cell discretization based upon changing reactants flow rates to maintain msec synchronization*
- *Serial "packets" of time wherein quasi-steady flow supplies are predicated*

Preliminary Results



SOFC Voltage Transition
300 to 375 mA/cm2 (25% increase)
Unslaved



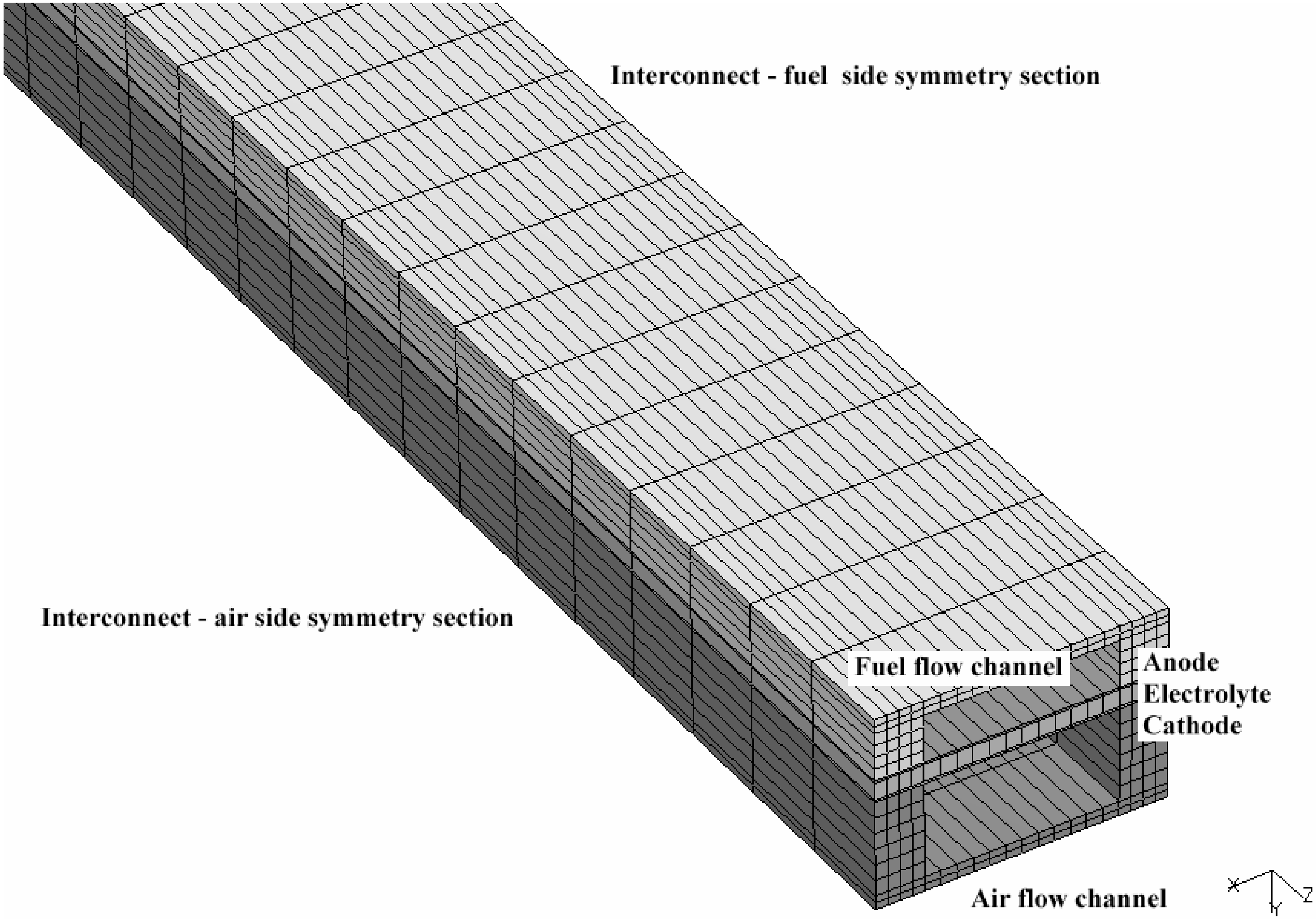
Fuel Utilizatation Transition
300 to 375 mA/cm2 (25% increase)
Unslaved

- **Plausible transient transition path shown from validated steady state end points**

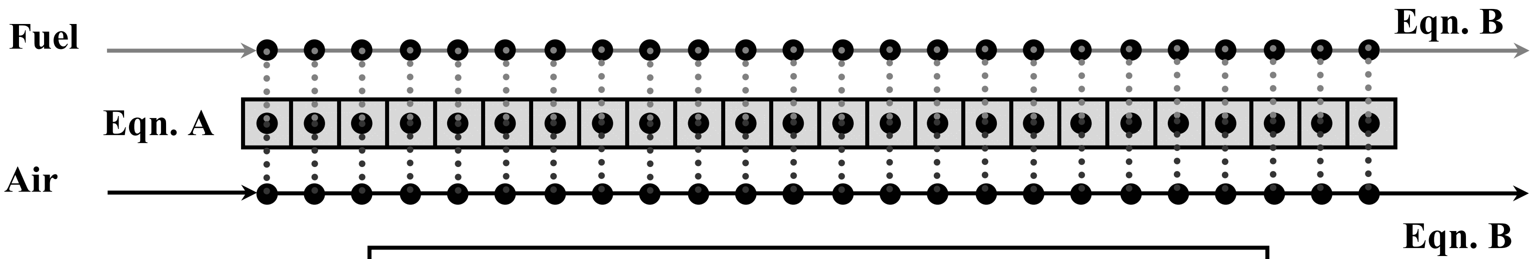
- **Greater attention will be added to the electrode mass transfer transients for higher fidelity modeling (e.g., capturing "undershoot" associated with increases in load current)**

- **Matlab/Simulink and FORTRAN developmental environments simultaneously are being accommodated**

Spatial Effects Resolving Co-flow SOFC Model



Temporal Effects Resolving Homogenized Spatial Model



Equation A. Heat equation in solid

$$\rho C_p(T)V_f(x)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[kV_f(x)\frac{\partial T}{\partial x}\right] + \frac{q'''(x)}{A_c}$$

Equation B. Energy transport in gas streams

- Neglecting axial conduction and viscous dissipation

$$\rho C_p \frac{DT}{Dt} = \sum_{i=1}^{nsp} \overline{H}_i \frac{r_i}{m_i} + q(x)$$

$\overline{H} = 3.5RT$, For an ideal diatomic gas

$\frac{DT}{Dt} = \frac{\partial T}{\partial t} + v\frac{\partial T}{\partial x}$, For a 1-D scalar

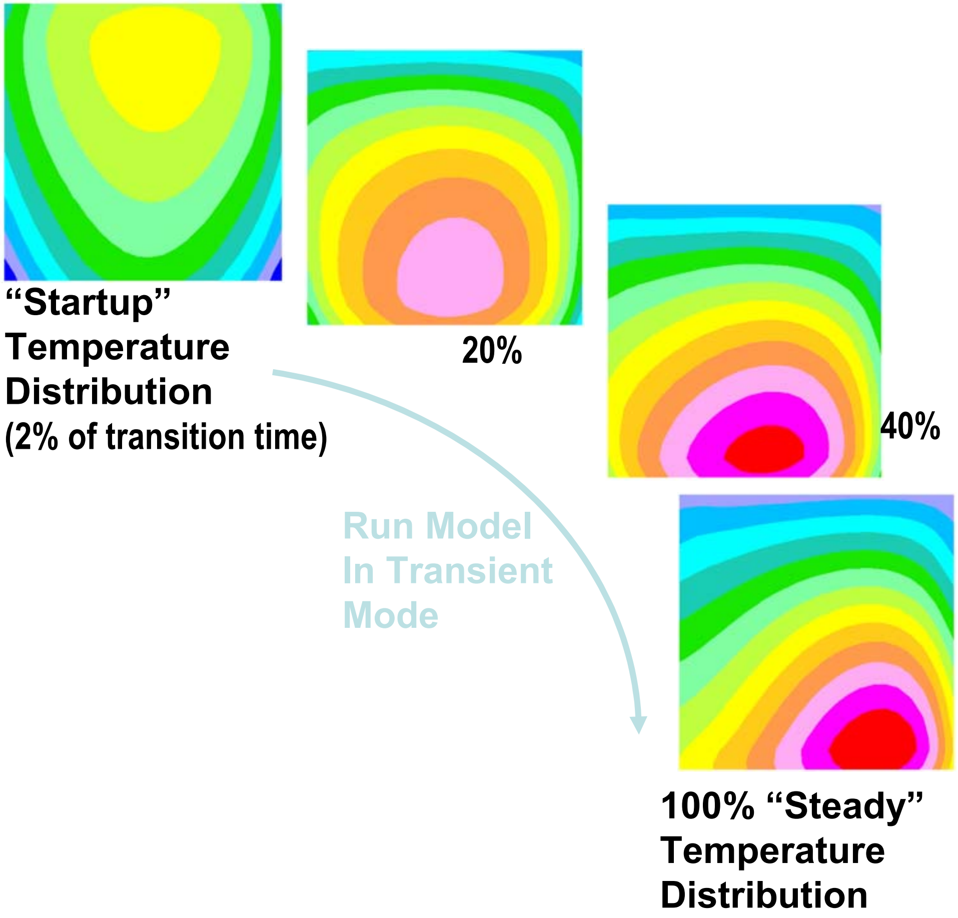
$dq_g(x) = h_c P(T_s(x) - T_g(x))dx$

Thermal-Electrochemical Coupling

- Electrochemical
  - Temperature dependence
    - Cell ASR, k_e, E_{rev}
- Thermal
  - Heat generation/absorption
    - I^2R in current paths
    - Electrochemical heat of reaction ($T\Delta S$)
    - Fuel reactions endotherm/exotherm

Transient Heating: Augment SECA Efforts with Electrochemical "Light-off" Considerations

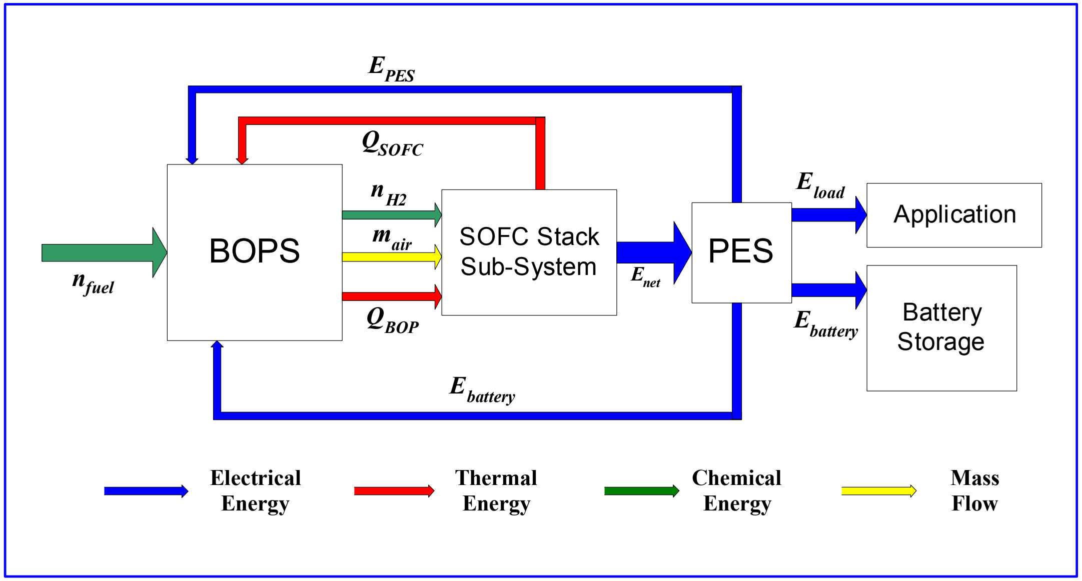
- Electrochemical light-off is the "kinetic acceleration" occurring during transitional heat-up
- May have significant impact upon cell reliability as a part of thermal cycles and ramp rate
- Electrochemical operating conditions (e.g., load current demand, NOS) provide a unique set of "controls" for this dynamic phenomenon
- Studies to characterize and optimize this intermediate thermal management stage



Graphic courtesy of PNNL

Balance of Plant Sub-system (BOPS) Modeling and Analysis

SOFC PS: Balance of Plant Sub-system (BOPS) Phase II Summary



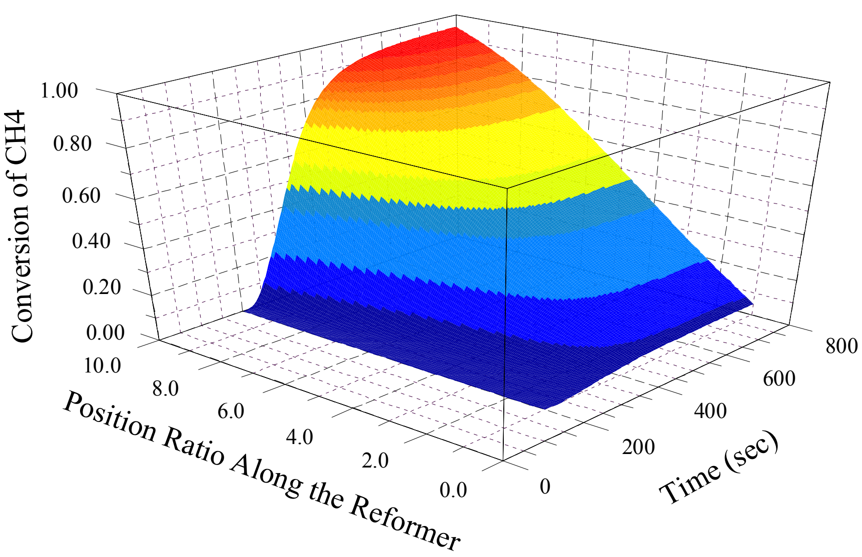
PHASE II : SYSTEM CONTROL STRATEGIES

TASKS TO BE PERFORMED

- ➢Analysis of which set of initial “best practice” control strategies to implement for start-up and shut-down
- ➢Modeling and simulation of system-level start-up and shut-down
- ➢Application of large-scale optimization using decomposition to the synthesis/design and operation of the SOFC PS
- ➢Determination of optimal control strategies for normal operation and start-up/shut-down based on their effects on system reliability, performance, and response

DETAILED MODEL STEAM METHANE REFORMER START-UP RESULTS

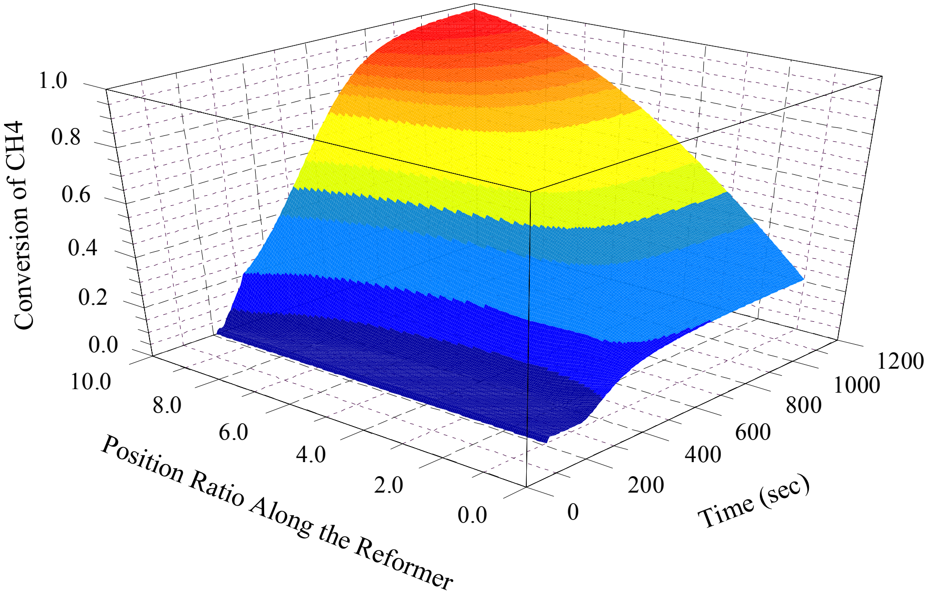
High Pre-Heating



Steam methane reformer start-up

- ➢ Slowest thermal response component of the BOPS
- ➢ Faster response. Steady state is reached in 700 sec

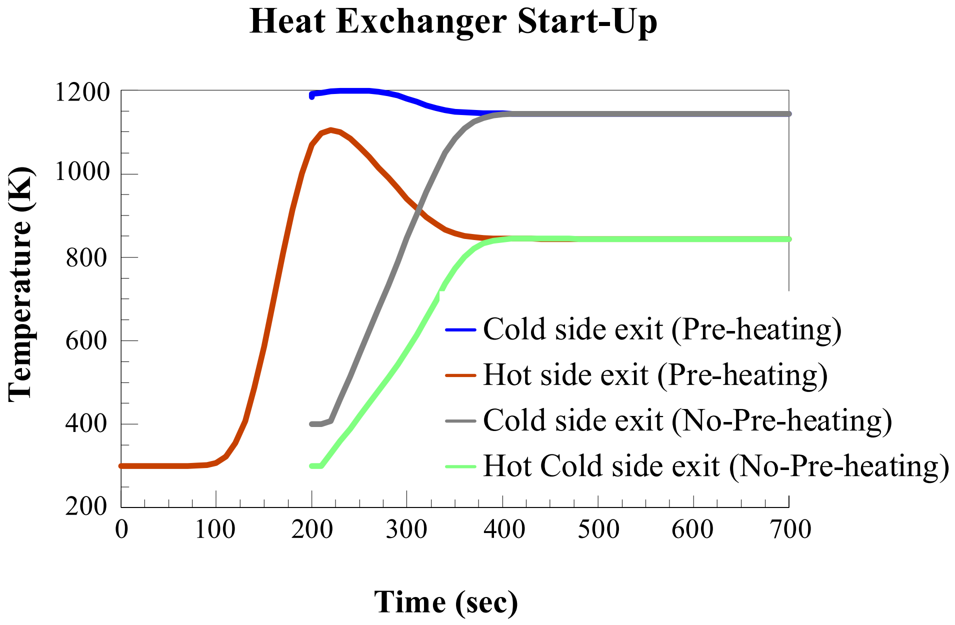
Low Pre-Heating



Steam methane reformer start-up for low pre-heating

- ➢ Slower response. Steady state is reached in 1100 sec
- ➢ The chemical response is dependent on the temperature

DETAILED MODEL HEAT EXCHANGER START-UP RESULTS

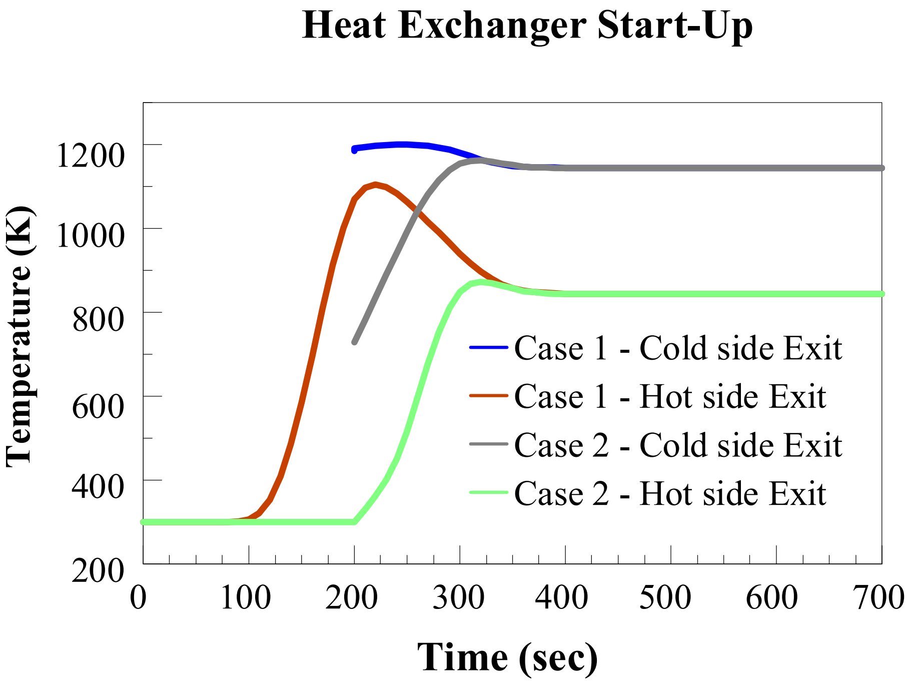


Comparison between high and no pre-heating

- ➢ Pre-heating significantly reduces the time to reach operational temperature

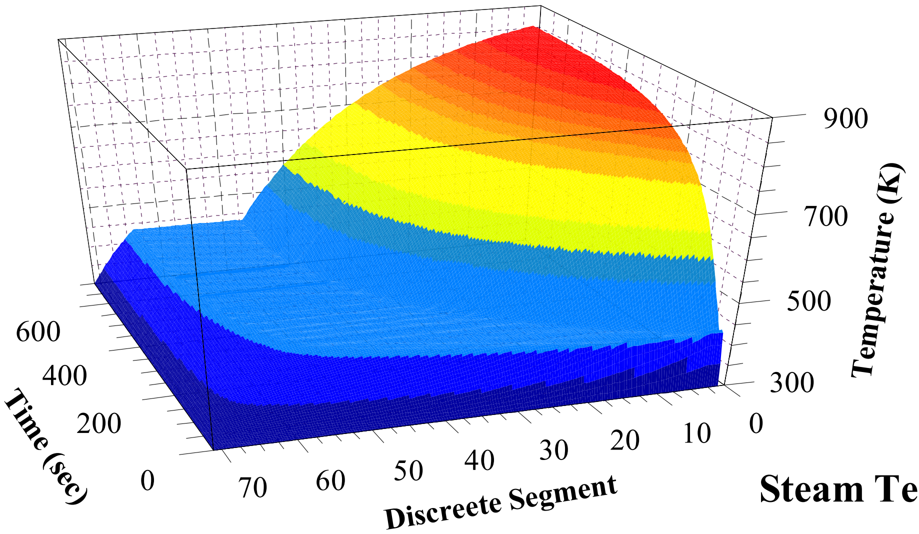
Comparison between high and low pre-heating

- ➢ The Higher the pre-heating, the sooner operational temperatures are reached
- ➢ Material temperature gradient constraints are important and should be taken into account



DETAILED MODEL STEAM GENERATOR START-UP RESULTS

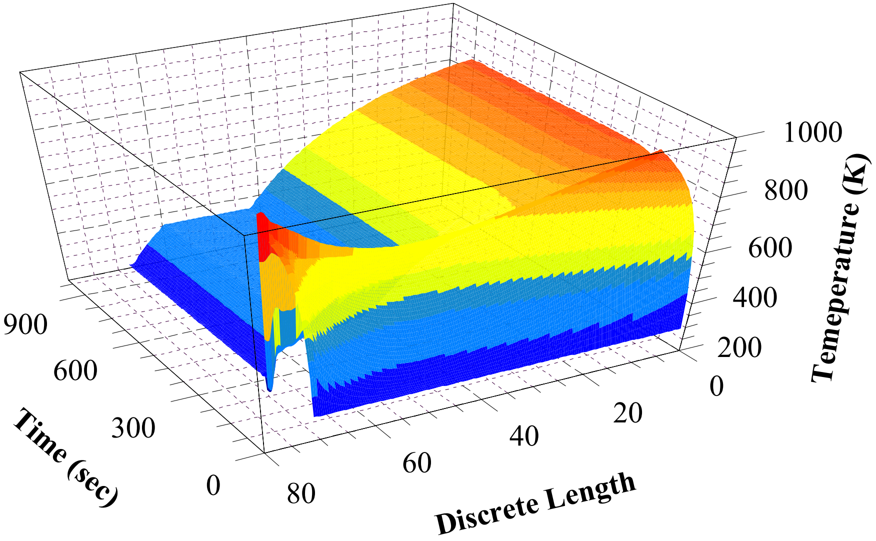
Steam Temperature (Start-Up with No Recirculation)



Steam generator start-up

- Operational (steady state) temperature (800 ºK) is reached within 600 seconds

Steam Temperature (Start-Up with Recirculation)



Steam generator start-up

- Operational (steady state) temperature (800 ºK) is reached immediately after stopping recirculation

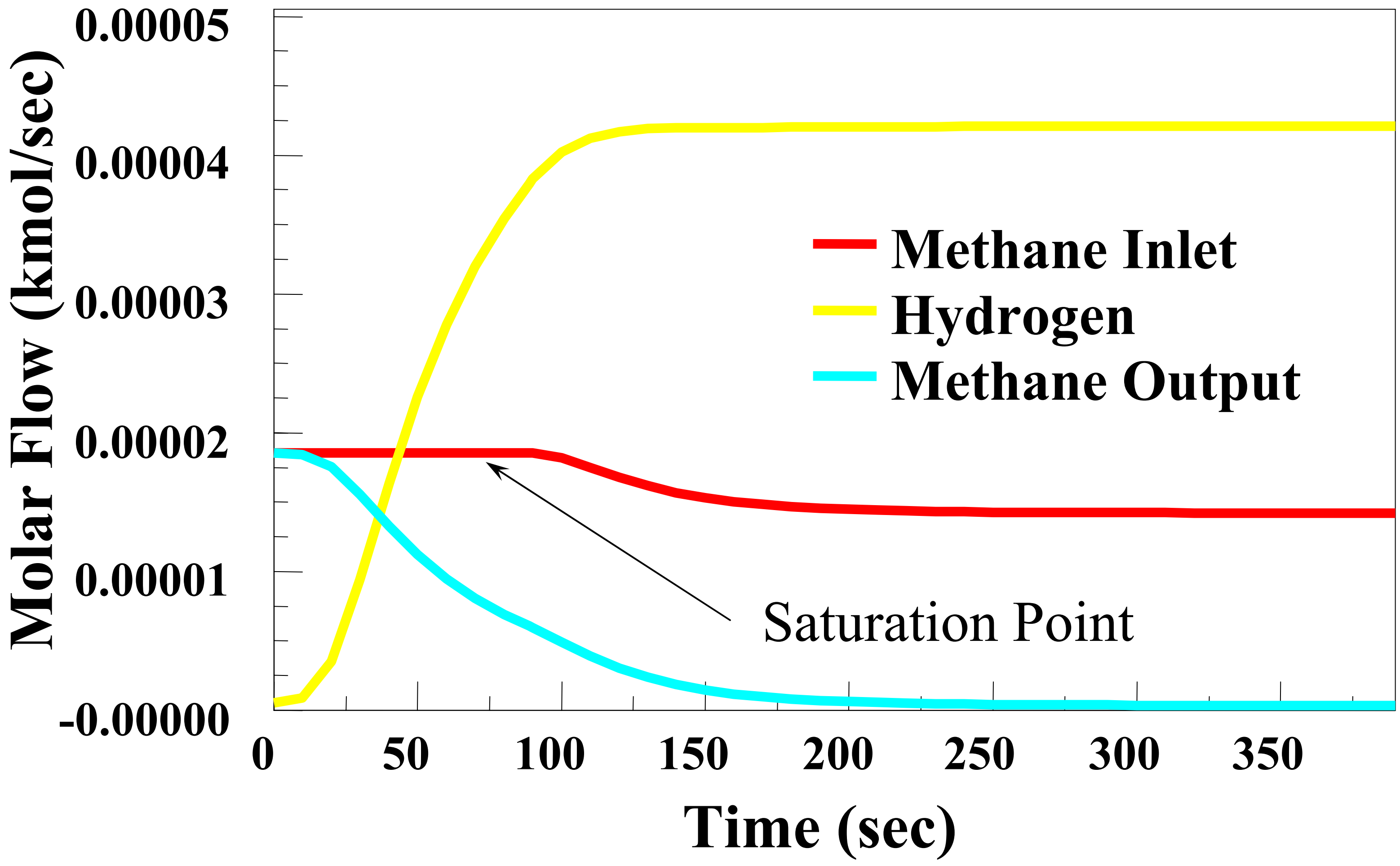
BOPS CONTROL

- Non-Linear State Space Theory:

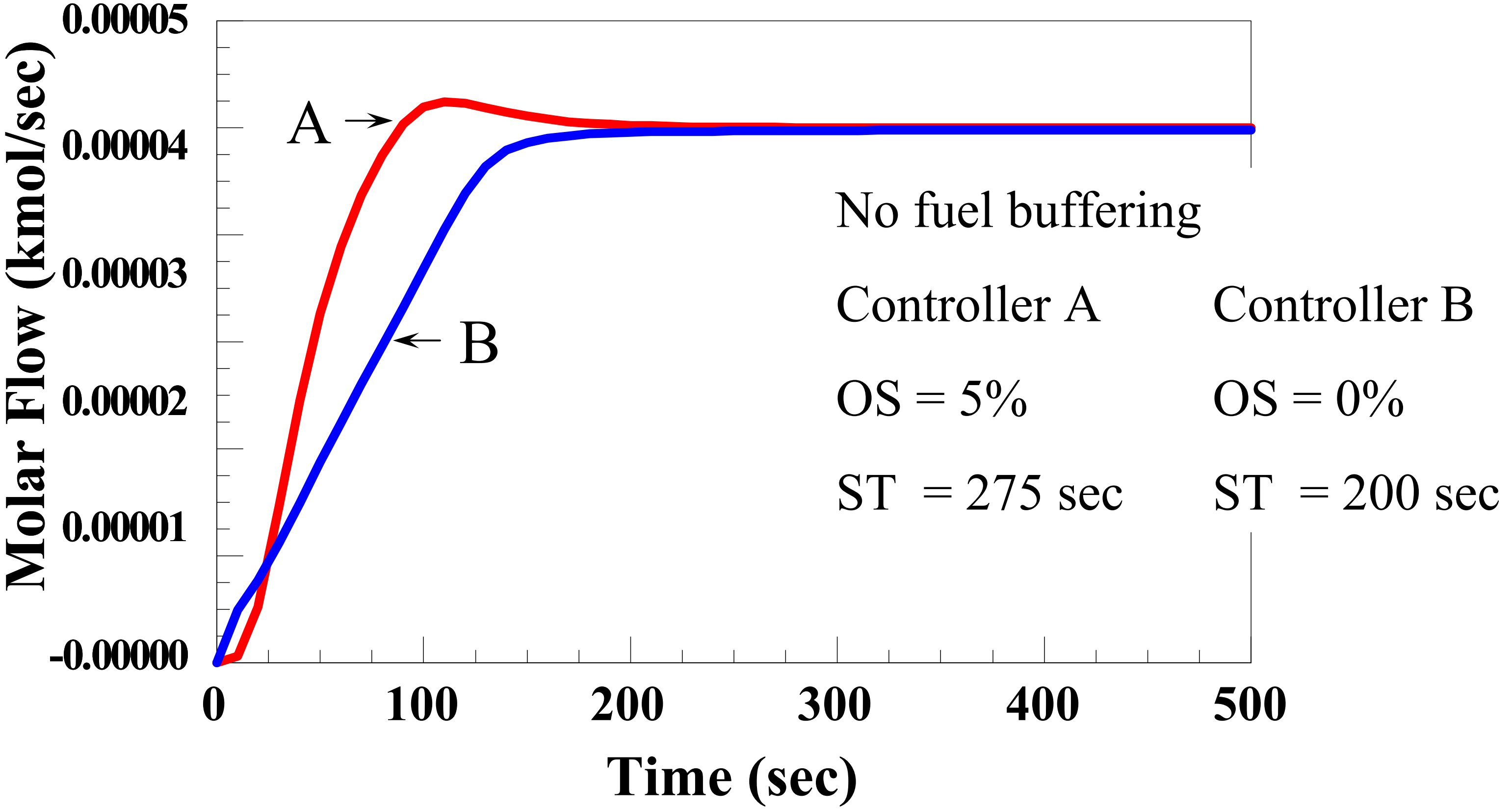
$$\underbrace{J}_{\text{Objective}} = \underbrace{C(\vec{x},\vec{z})}_{\text{Capital Cost}} + \underbrace{\underbrace{\underbrace{\int_{t_0}^{t_f} f(\dot{\vec{x}},\vec{x},\vec{u},t)\,dt}_{\text{Operational and Control Cost}}}_{\text{Lagrange Form}} + \underbrace{\underbrace{g(t_f,\vec{x}(t_f))}_{\text{Terminal Cost}}}_{\text{Meyer Form}}}_{\text{Bolza Form}}$$

- Capital and operational costs usually optimized independently of the control and terminal costs. Using ILGO, this optimization problem will be solved as a whole.
- Will develop a PID control model in order to control, e.g., hydrogen production, fuel tank level, and hydrogen flow to the fuel cell stack during start-up and load changes.
- During the optimization phase, both advanced PID and optimal control theory will be used since they are well suited for highly complex, non-linear systems with multiple components. The utility of state space control approaches is limited due to the non-linearities involved.
- Already implemented are controllers for the H_2 flow rate and temperature at the exit of the reformer.

CONTROL VARIABLE CASE B



SYSTEM CONTROL



No fuel buffering

Controller A	Controller B
OS = 5%	OS = 0%
ST = 275 sec	ST = 200 sec

u(t) = Control Variable: $\dot{m}_{CH_4 in}$

x(t) = State Variable: $Power$ or $\dot{m}_{H_2 out}$

Future Work

Real-Time Simulation

- Reduction of individual complexity of modules
  - PES model (discontinuous and hybrid nonlinear dynamics)
  - BOPS model (large response times; high order, nonlinear, dynamic)
  - SOFC model (algebraic loops and root convergence)
- Specific executables for PES, BOPS and SOFC for fast interaction
- Execution in MATLAB/ Simulink environment
- Significant decrease in simulation time for the integrated system
  - **Enabling the study of SOFC durability and reliability**
  - **Design of optimized control scheme for the system as a unit for optimized performance, reliability and durability.**

Future Work

Planar Solid Oxide Fuel Cell (Planar SOFC)

- Planar SOFC stack model (electrical, thermal and electrochemical) development, enhancement and model validation
  - Georgia Tech & Cerametec
- Implementation and validation of a comprehensive balance of plant system model (thermodynamic, kinetic, and geometric) and optimal control strategies (*bottoms-up approach*)
  - Virginia Tech & Cerametec
- Development of PES nonlinear topologies (stationary and non-stationary application loads)
  - U of I at Chicago
- System integration and interaction analyses
  - U of I at Chicago

Future Work

Development of New Control Strategies

- Optimal control strategies using a *bottoms-up approach* to improve BOPS response to load transients
- Optimal balance between overall system efficiency, cost, and SOFC stack durability at each load point
- Could lead to the control of each subsystem in such a way that the system responds optimally to any given load
- Greater fidelity as a result of the rigorous simulation of the subsystems and a sufficient consideration of system dynamics