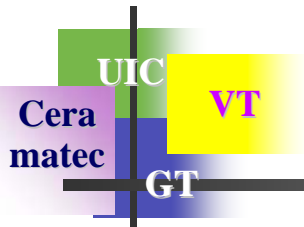


# Comprehensive Modeling and System Interactions in Planar SOFC Power-Conditioning System



**Sudip K. Mazumder (PI) and Sanjaya Pradhan**  
(University of Illinois)

**Joseph Hartvigsen, S. Elangovan and Michele Hollist**  
(Ceramatec Inc.)

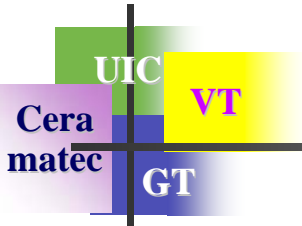
**Michael von Spakovsky, Diego Rancruel and Doug Nelson**  
(Virginia Tech)

**Comas Haynes**  
(Georgia Tech.)

**SECA Core Technology Program Review Meeting**

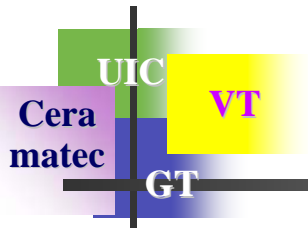
**Jan 27, 2005**

**Florida**



# Overview

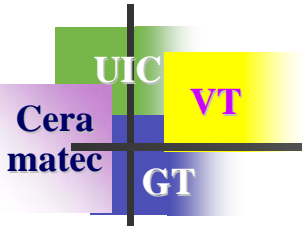
- Pre-Analysis Efforts
  - Comprehensive Planar SOFC (PSOFC) 1D and 2D Modeling
  - Model Validation
  - Power-Electronics Modeling
  - Fully-controlled BOPS Modeling
  - Comprehensive System Modeling
- Interaction Results and Analysis
  - Load Power Factor
  - Load Transients
- Conclusion
- Future Works



# Modeling

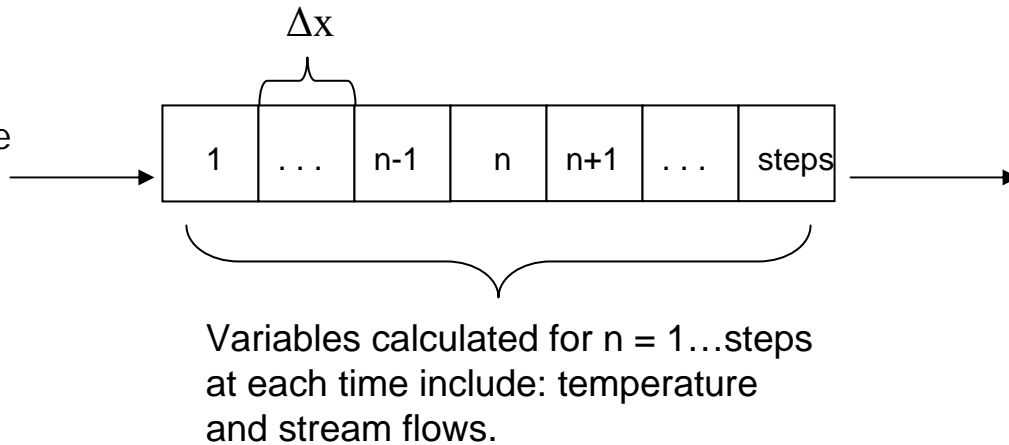
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# 1D PSOFC Model



## Inputs

- Feed temperature
- Current
- Molar flows and compositions (Fuel, air)
- Cell geometry
- Stack size



## Outputs

- Temperature
- Operating Voltage
- Molar flows and compositions (Fuel, air)
- Power Output

- Fuel cell model run in Simulink via an embedded Matlab function.
- Finite difference method used to approximate transient parameters.
- Model returns position dependent variable values as well as outflow values.

- Interfaces with BOPS model in Simulink to form complete system.
- Radiation boundary applied to exit boundary.
- Co-flow setup between fuel and air streams.

# Model Characteristics

- Inlet fuel stream is a reformed methane stream.
- Each step (control volume) along the fuel cell is treated as having homogenous properties throughout.
- Shift equilibrium is applied to each control volume along the fuel cell.

## Shift Equilibrium Calculation

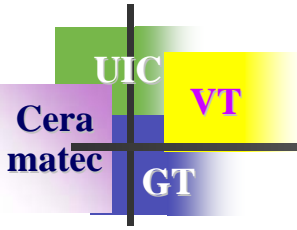
$$K_p = \frac{(p_{CO_2} + x) \cdot (p_{H_2} + x)}{(p_{CO} - x) \cdot (p_{H_2O} - x)}$$

$$K_p = e^{-dG_o/RT} \quad dG_o = f(T)$$

## Equilibrium Composition

$$p_{H_2} = p_{H_2} + x \quad p_{CO} = p_{CO} - x$$

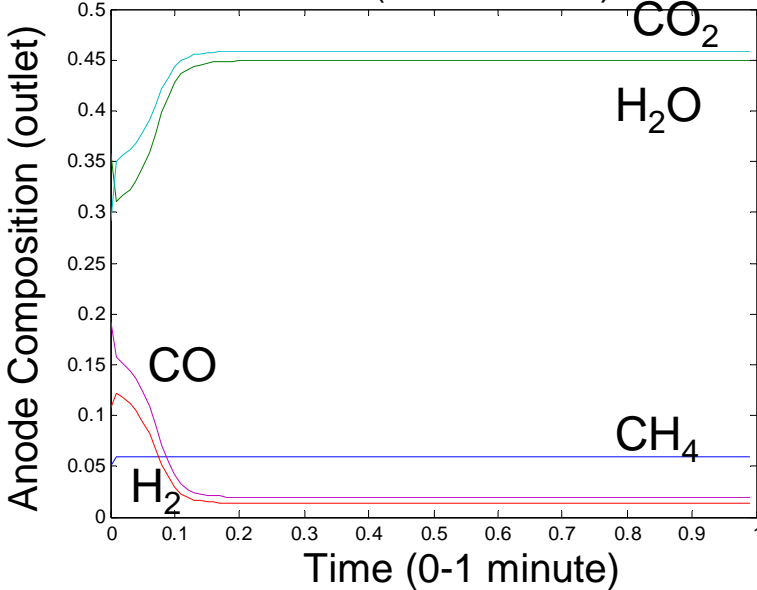
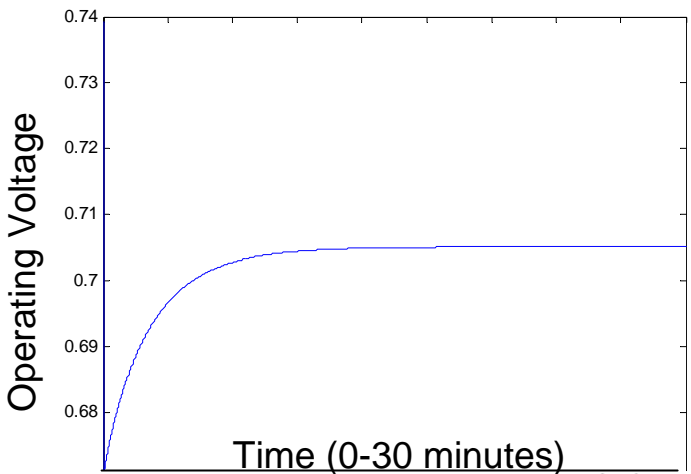
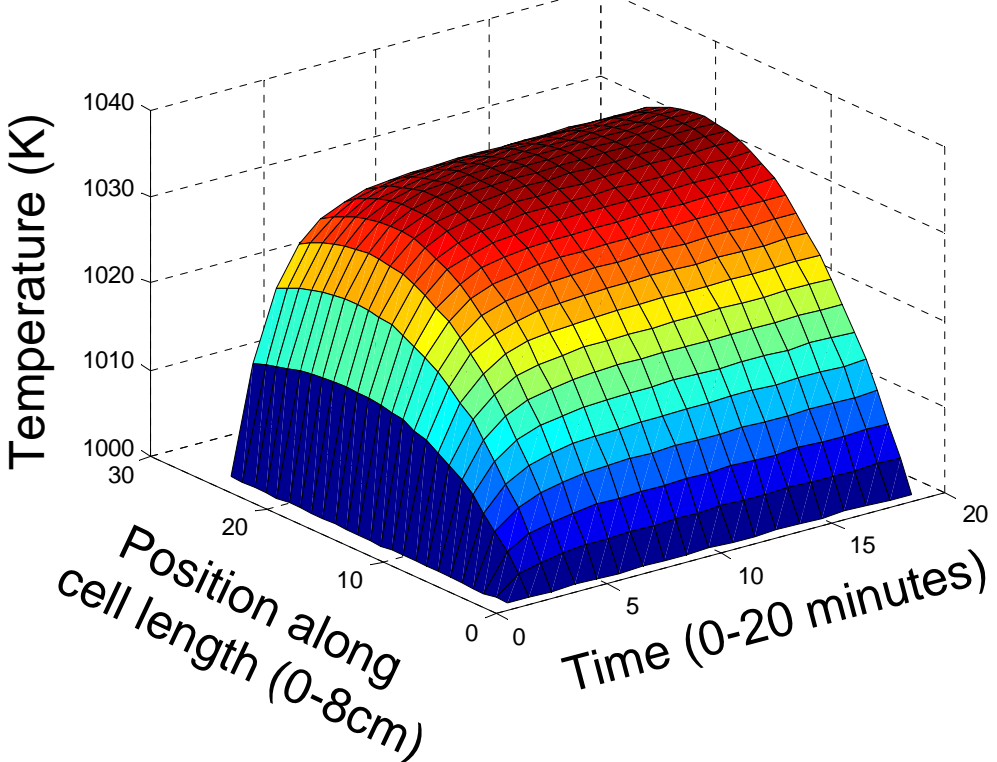
$$p_{CO_2} = p_{CO_2} + x \quad p_{H_2O} = p_{H_2O} - x$$



# 1D Model Results

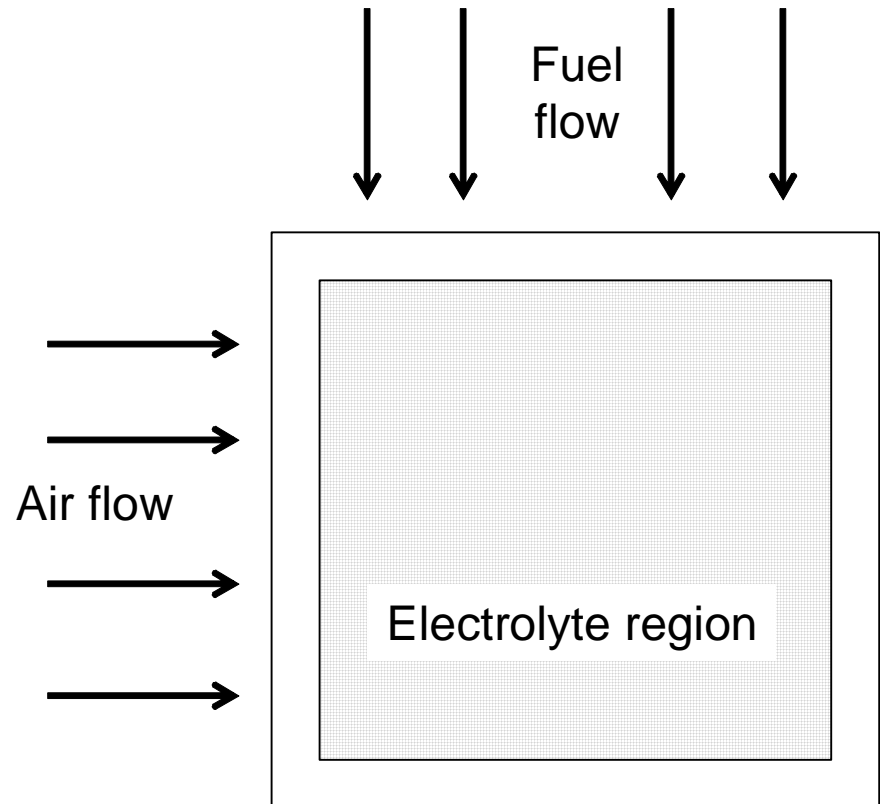
## Inlet Conditions

Air Flow (mol/s)	Fuel Flow (mol/s)	Air Comp (O <sub>2</sub> , N <sub>2</sub> )	Fuel Comp (CH <sub>4</sub> , H <sub>2</sub> O, CO, CO <sub>2</sub> , H <sub>2</sub> )	Feed temp (K)
8.87e-4	7.76e-4	(.21, .79)	(.05, .45, .2, .2, .1)	1000

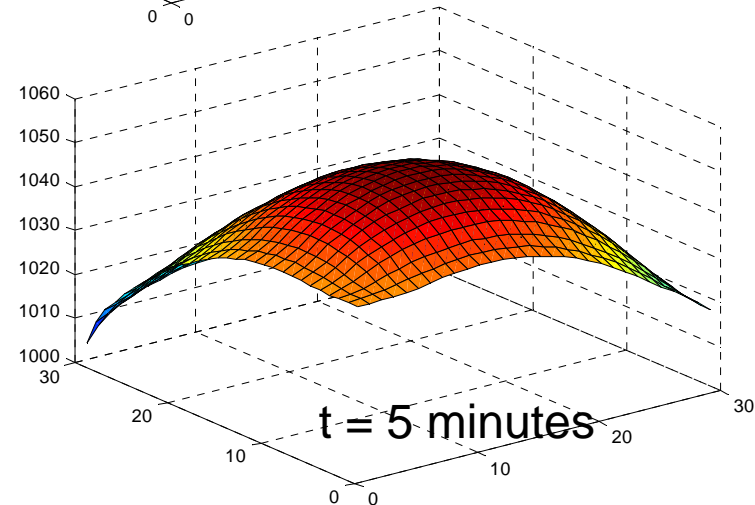
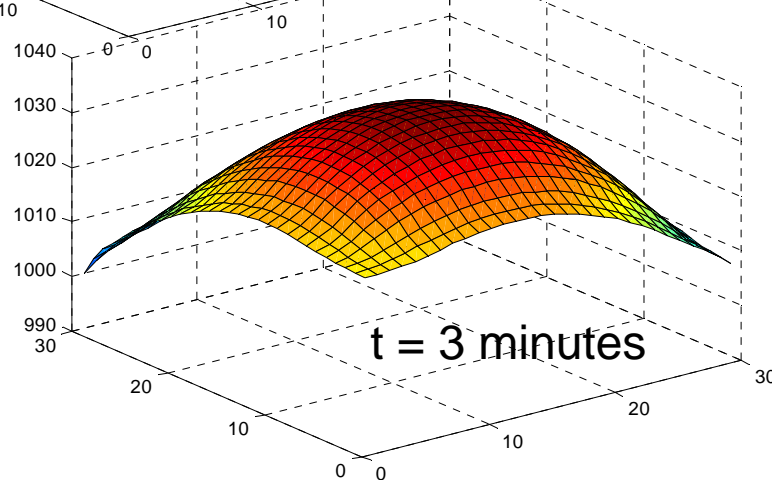
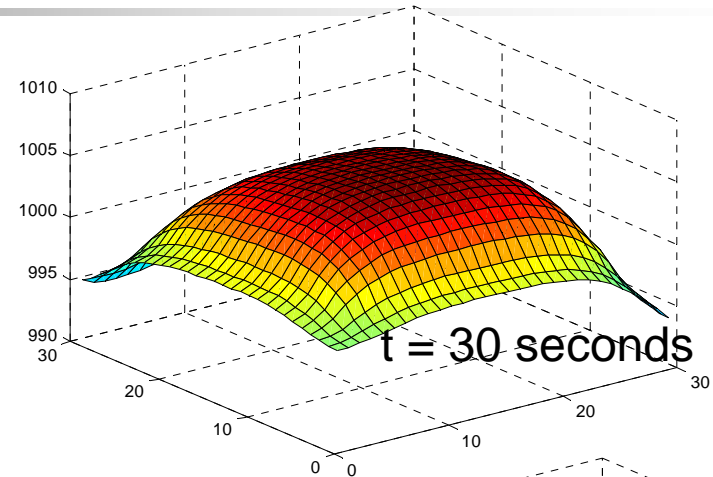
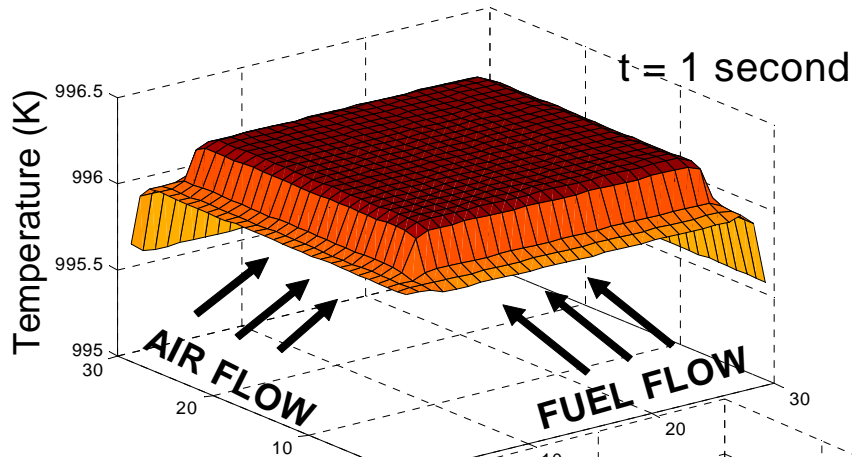
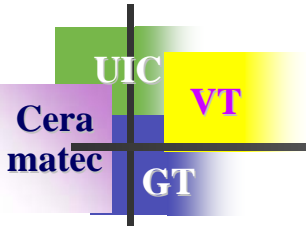


# 2D SOFC Model

- Same input and output variables as 1D model.
- Model returns variable values at outputs as well as across entire fuel cell surface.
- Radiation boundary applied to each exit stream boundary.
- Cross-flow setup between fuel and air streams.
- Includes an inactive seal area around active electrolyte region.



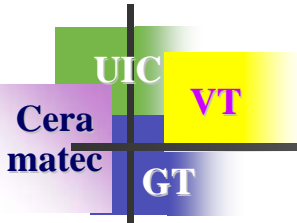
# 2D Model Results



Tracking transient temperature behavior



# 1D vs. 2D Model Comparison

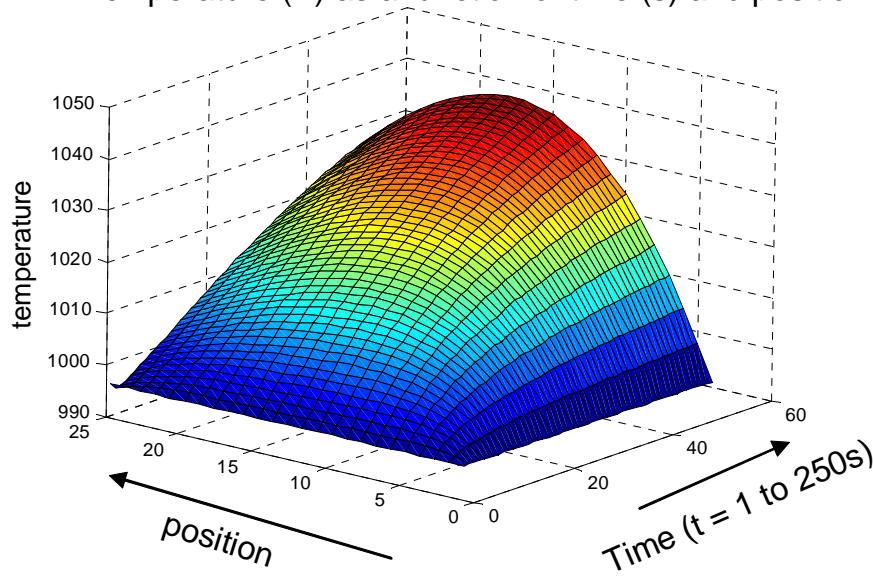


## Inlet Conditions

Air Flow per cell (mol/s)	Fuel Flow per cell (mol/s)	Air Comp (H <sub>2</sub> O, O <sub>2</sub> , N <sub>2</sub> )	Fuel Comp (CH <sub>4</sub> , H <sub>2</sub> O, CO, CO <sub>2</sub> , H <sub>2</sub> )	Current per stack (A/stack)	Feed temp (K)
3.7e-4	1.81e-4	(.069, .196, .74)	(0.006, .31, .07, .08, .54)	15	996

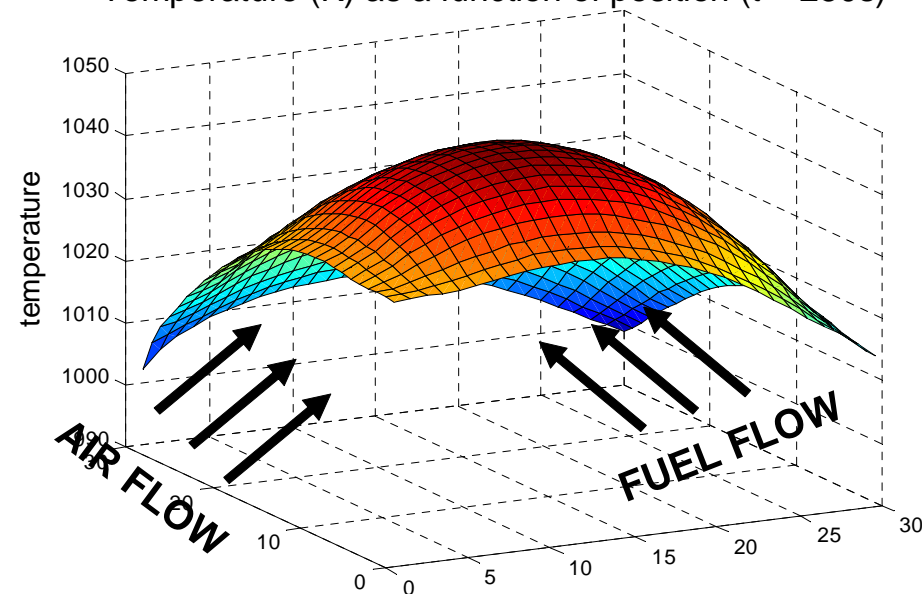
## Temperature (1D Model)

Temperature (K) as a function of time (s) and position



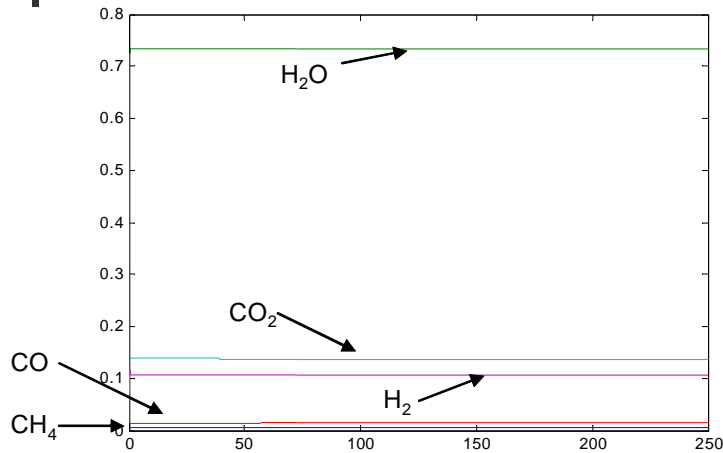
## Temperature (2D Model)

Temperature (K) as a function of position (t = 250s)

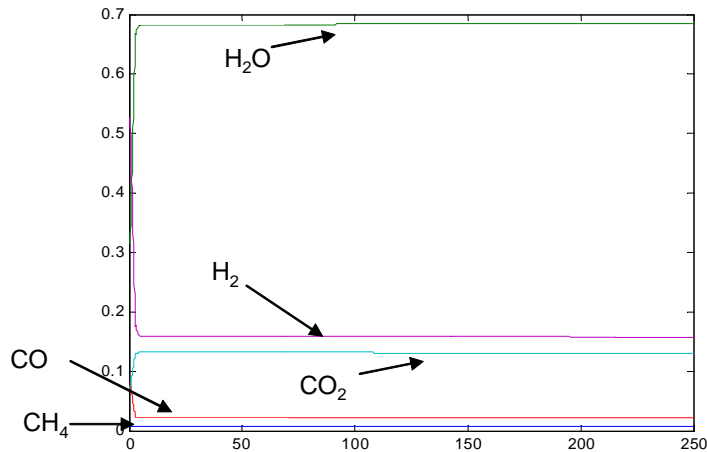


# 1D vs. 2D Model Comparison

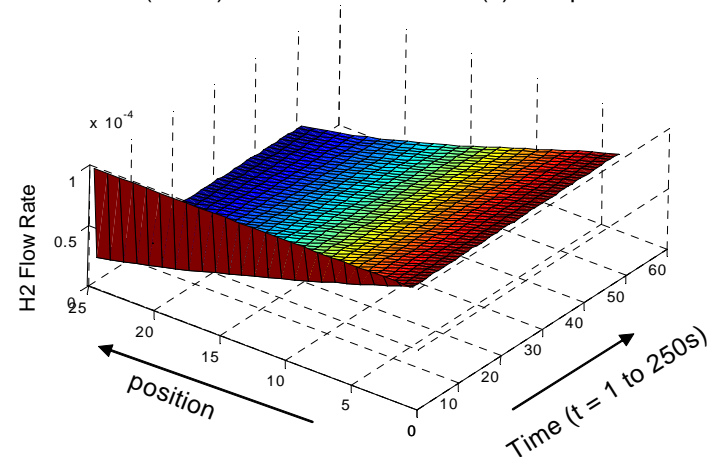
Anode Comp Out (1D Model)  
Mole fraction vs. time (s)



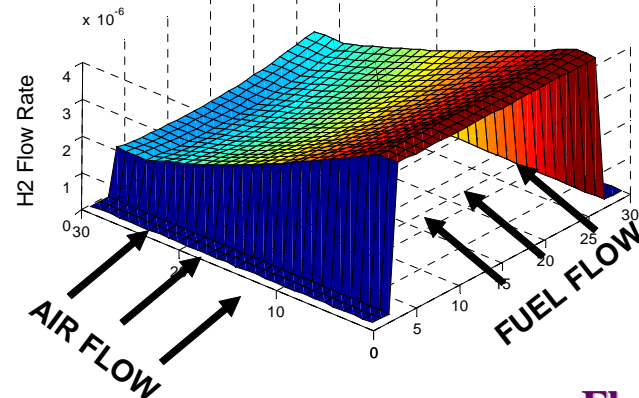
Anode Comp Out (2D Model)  
Mole fraction vs. time (s)



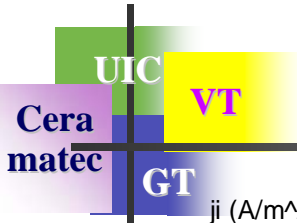
H2 flow rate (1D Model)  
Flow rate (mol/s) as a function of time (s) and position



H2 flow rate (2D Model)  
Flow rate (mol/s) as a function of position (t=250s)

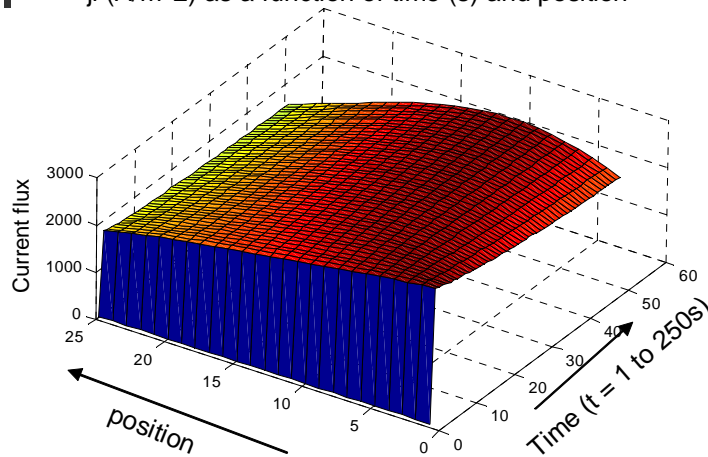


# 1D vs. 2D Model Comparison



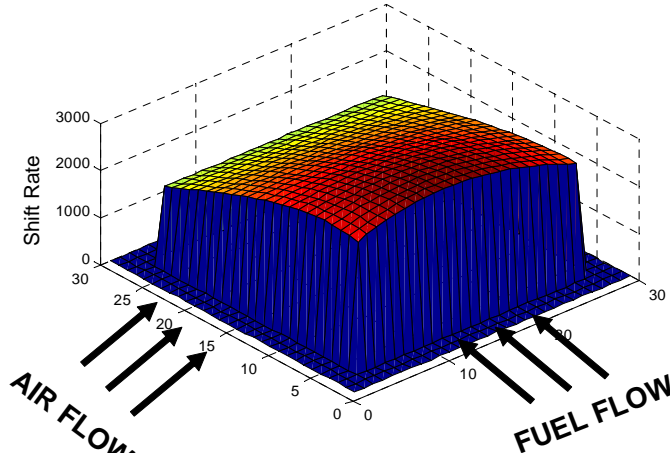
Current Flux (1D Model)

$j_i$  ( $A/m^2$ ) as a function of time (s) and position



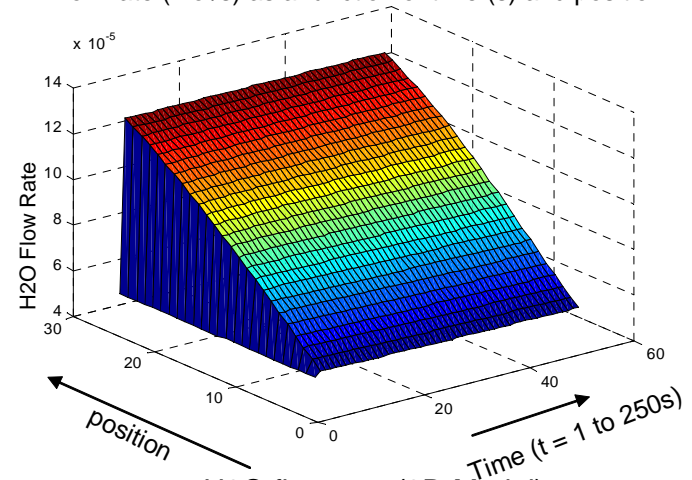
Current Flux (2D Model)

$j_i$  ( $A/m^2$ ) as a function of position ( $t=250s$ )



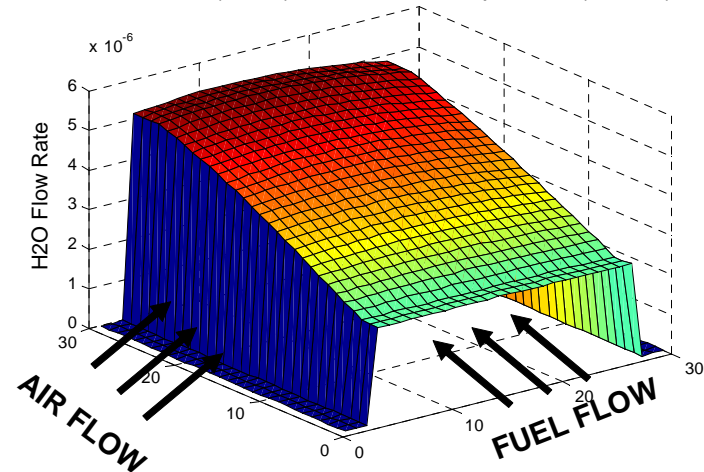
H<sub>2</sub>O flow rate (1D Model)

Flow rate (mol/s) as a function of time (s) and position

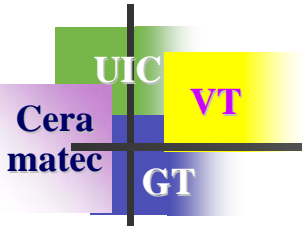


H<sub>2</sub>O flow rate (2D Model)

Flow rate (mol/s) as a function of position ( $t=250s$ )

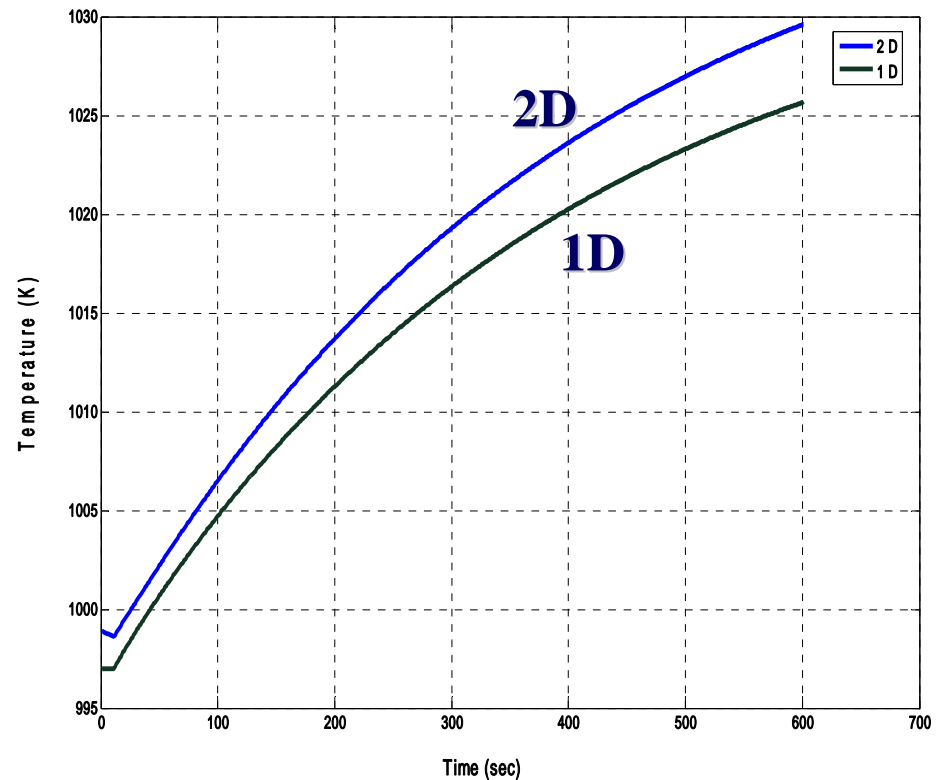


# 1D vs. 2D Model Comparison with Load-Transient



■ 600 seconds of system simulation needs

- ~ 3.5 hrs for the 2 D Model
- ~ 1.5 hrs for the 1D model



# Adjusting Model Configurations

Cera  
matec

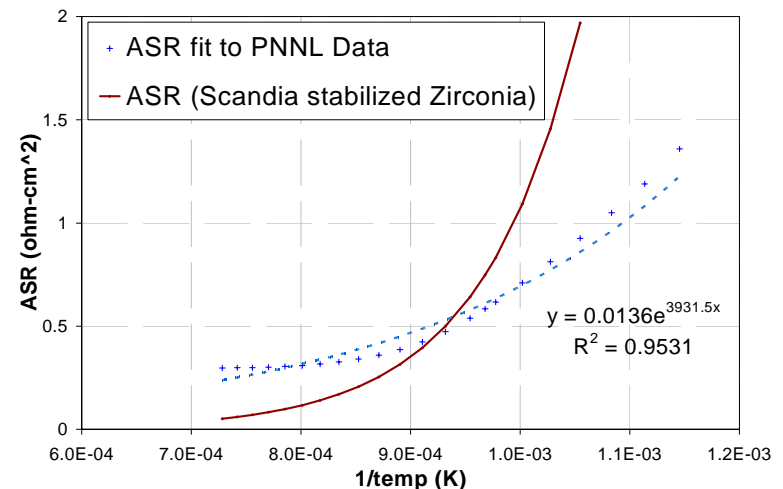
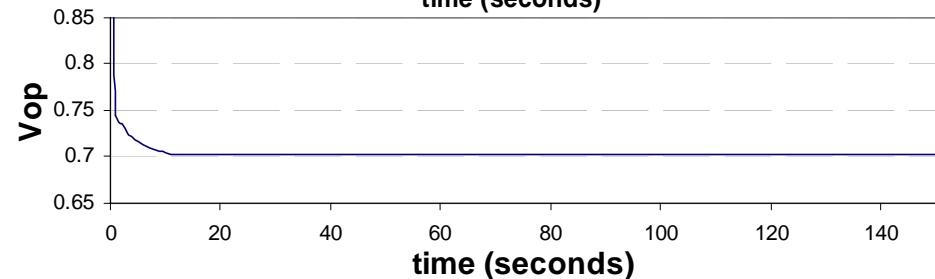
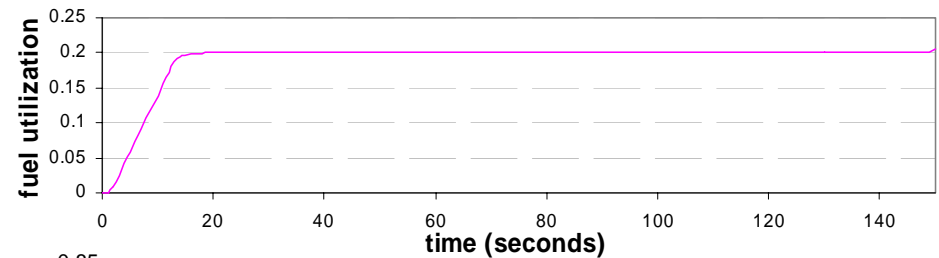
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VT

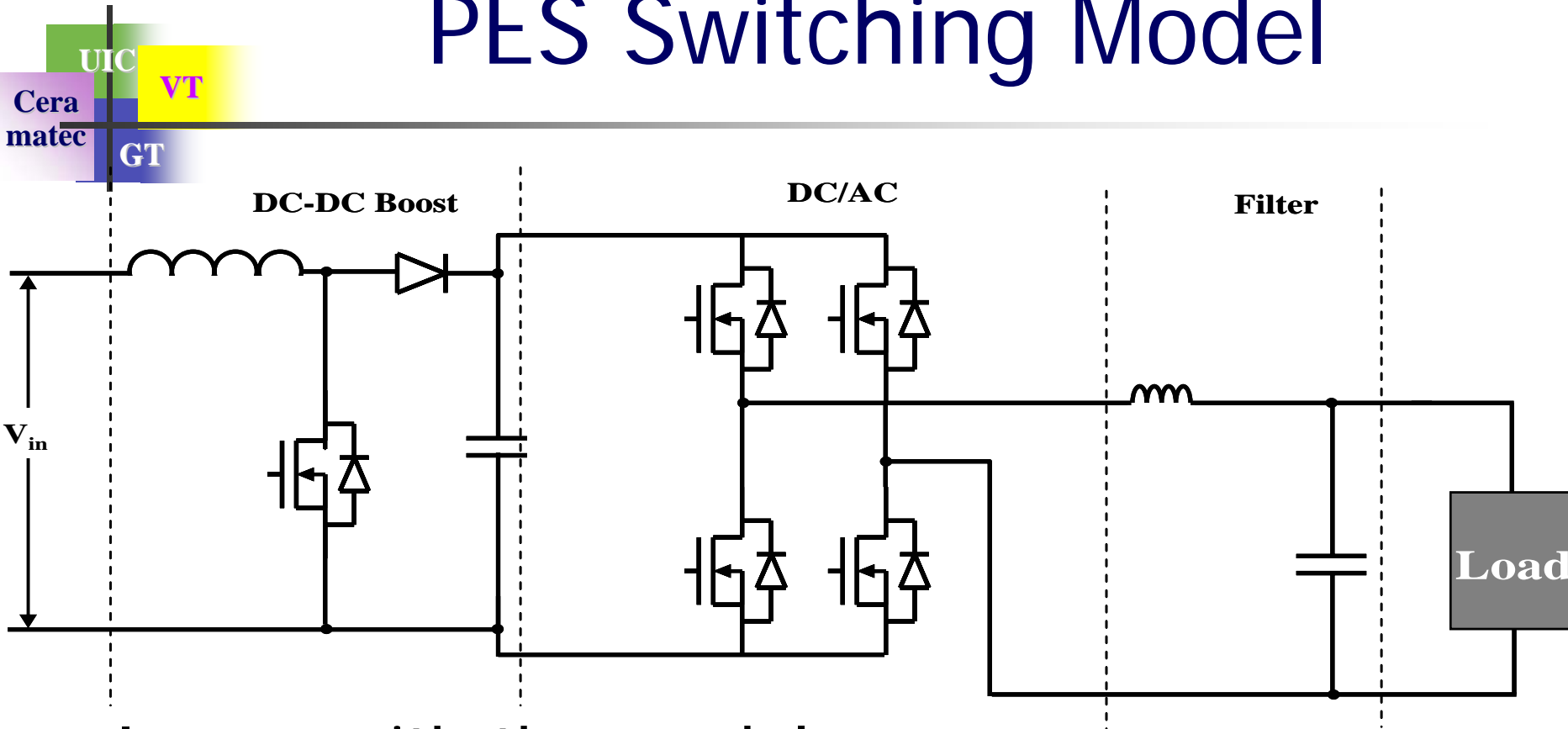
GT

Modified SOFC 2D fuel cell model for operating configurations provided by PNNL:

- Isothermal operating conditions
  - User inputs for stream flow rates, compositions, and temperatures provided
  - Single cell set-up
- 
- ASR fit to material data from PNNL model.
  - Comparable results demonstrated between PNNL model and modified SOFC model.



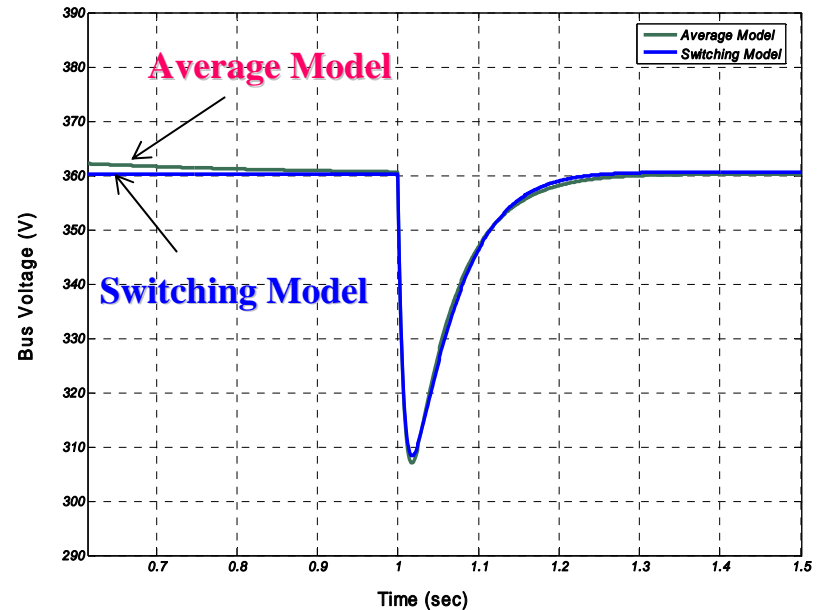
# PES Switching Model



- Issues with the model
  - Switching discontinuity
  - Stiff system with nonlinearities

# PES Average Model

- Need
  - Simpler Configuration
  - Faster Computation and guaranteed convergence with fairly larger time-steps
- Cons of the modeling approach
  - Prediction of nonlinearity and chaos
- Comparison and significance
  - 1.5 sec of system simulation using
    - **Average Model** → 5 sec
    - **Switching Model** → **540 sec**
  - Significant decrease in simulation time with appreciably high accuracy



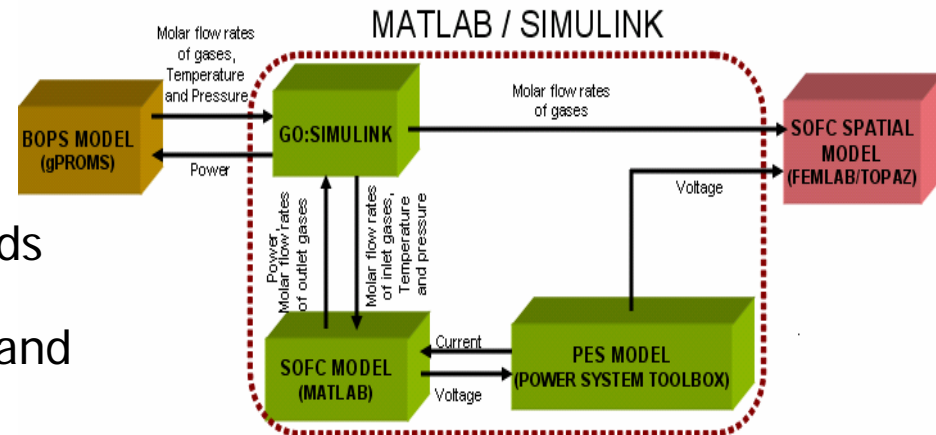
Response comparison during load transient

# Comprehensive System Model



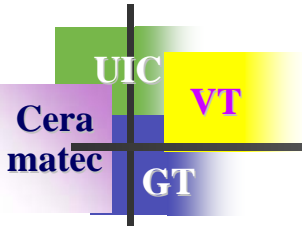
## ■ Modeling Issues

- Bulky BOPS model in gPROMS needs an gO:Simulink interface for data transfer between Matlab/Simulink and gPROMS.
- Integrity of data exchange between individual subsystems running at their individual pace on their own platforms
- Need of order reduction of models
  - PSOFC : 1D vs 2D and 2D vs 3D model
  - PES : Switching to Average model
  - BOPS : Lookup table model





# Simulation Issues

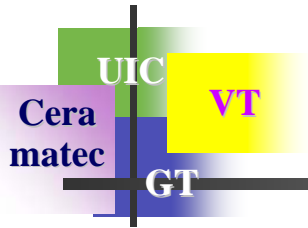


- Problems with Convergence
  - In the PSOFC model, which behaves similar to a current-controlled voltage source, the current information is unavailable at the start of the simulation ( $t = 0$ )
  - Infinite sampling time
    - The PSOFC model by default assumes a infinite sample time and hence needs to be triggered at a particular rate to proceed with the simulation
- Simulation Time
  - 1 sec of complete system simulation takes 1 million CPU (parallel processor-based Intel Xeon) seconds.



# Resolution of Simulation Issues

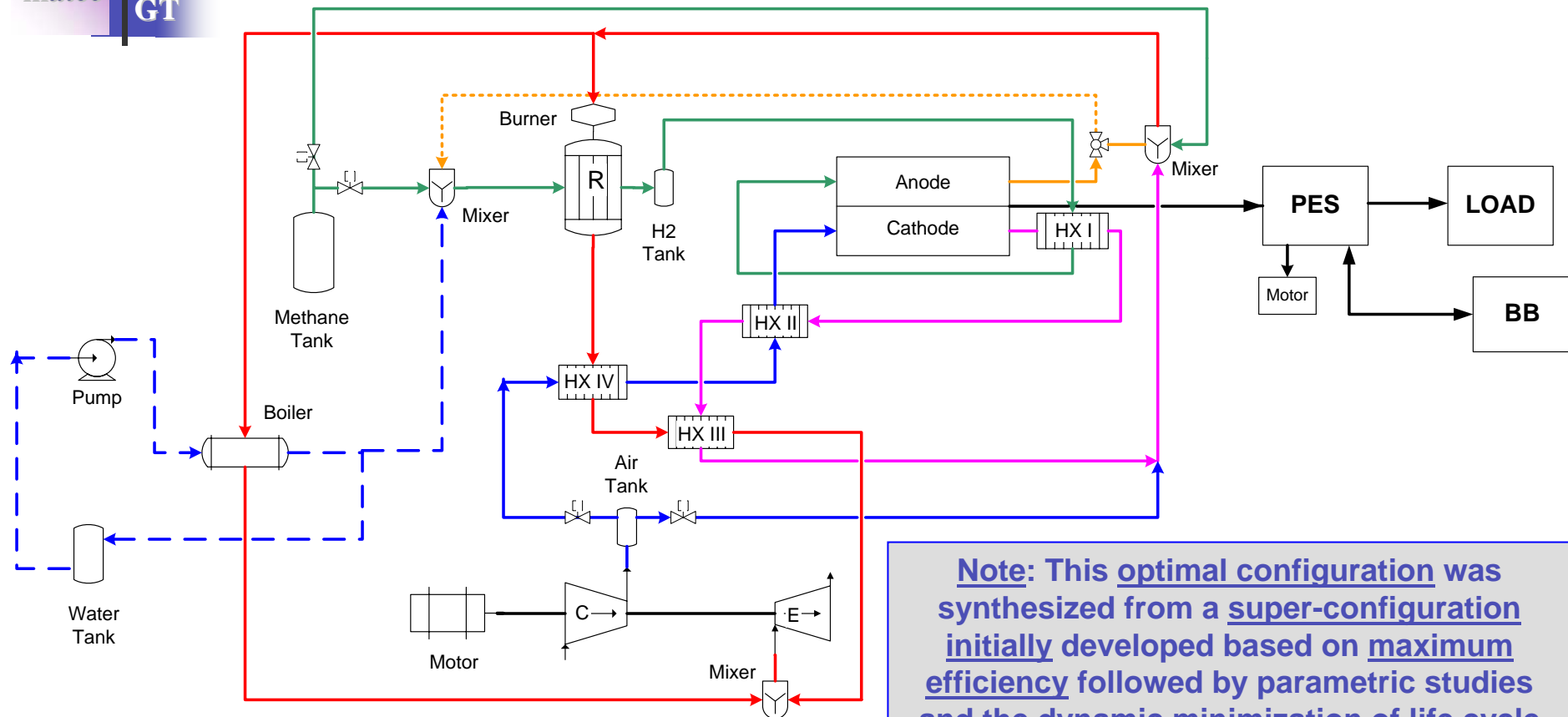
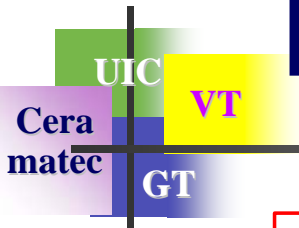
- SOFC Model Changes to resolve convergence at the PSOFC and PES interface at  $t = 0$
- Multiple sampling rates
  - For PES-BOPS interface to enhance simulation speed
- Rate transition blocks
  - Ensure data integrity at multiple sampling rates
- Solver algorithm
  - Ode23tb
    - Solving crude error tolerances to solve stiff differential equations with algebraic loops.
- BOPS reduced-order polynomial fit model
- BOPS comprehensive lookup table model (*in progress*)



# BOPS Optimization

---

# BOPS Optimum Configuration

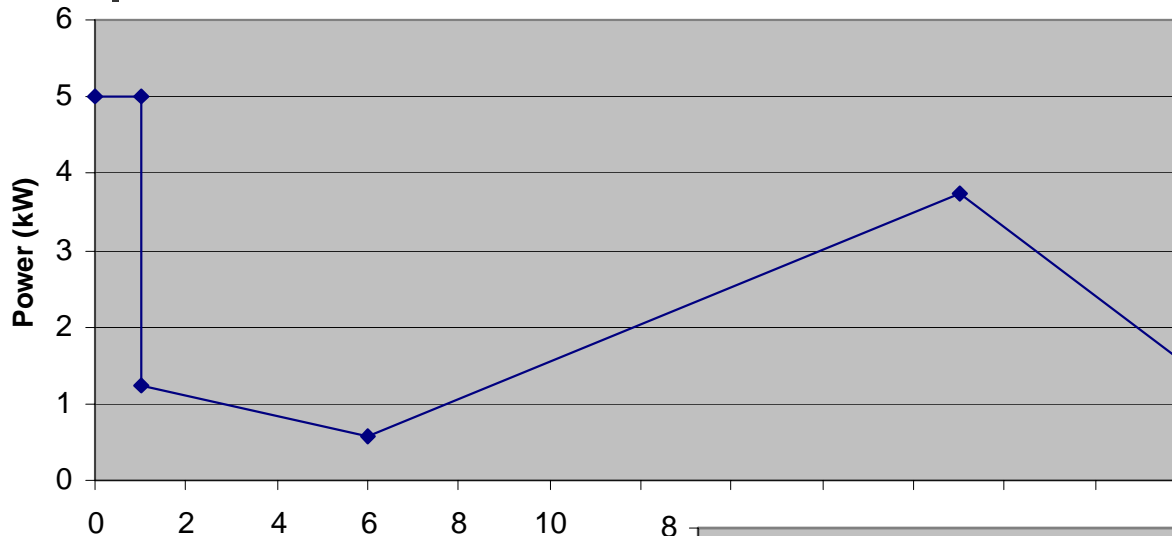
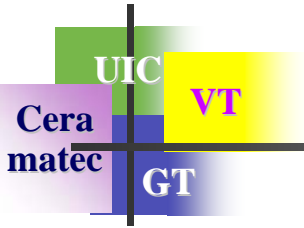


**Note:** This optimal configuration was synthesized from a super-configuration initially developed based on maximum efficiency followed by parametric studies and the dynamic minimization of life cycle costs to arrive at the subset seen in this schematic; this synthesis/design was carried out optimally taking into account the dynamic operational control of the system.

**Note:** This configuration has been optimally synthesized/ designed to respond in the shortest time possible to all transients.

Jan 27, 2005

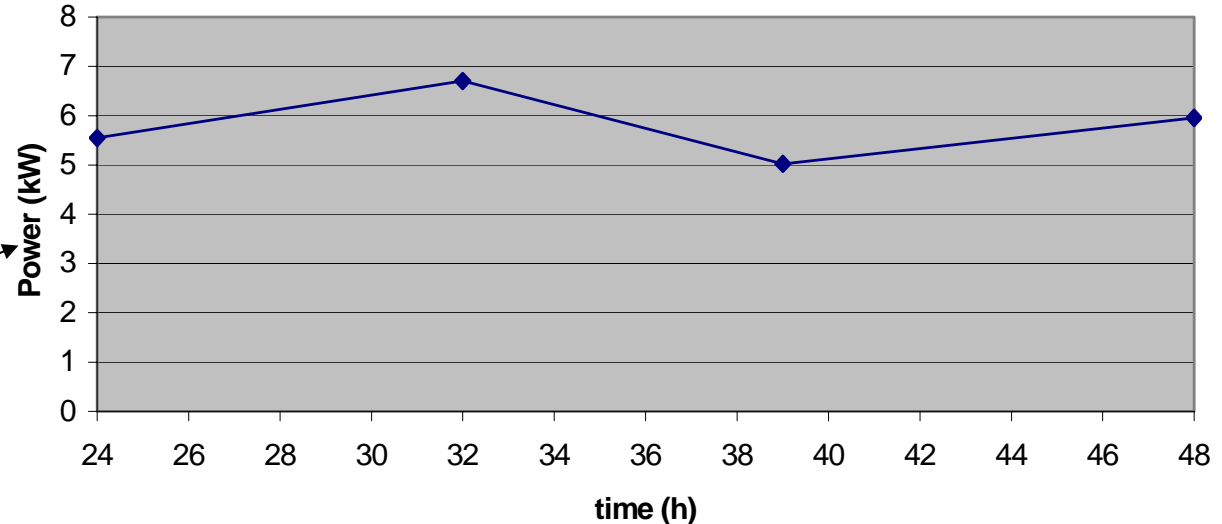
# Residential Load Profiles



**Summer Profile:**  
Approximated load profile.  
Cooling Day in Atlanta,  
Georgia Occurs on 07/11

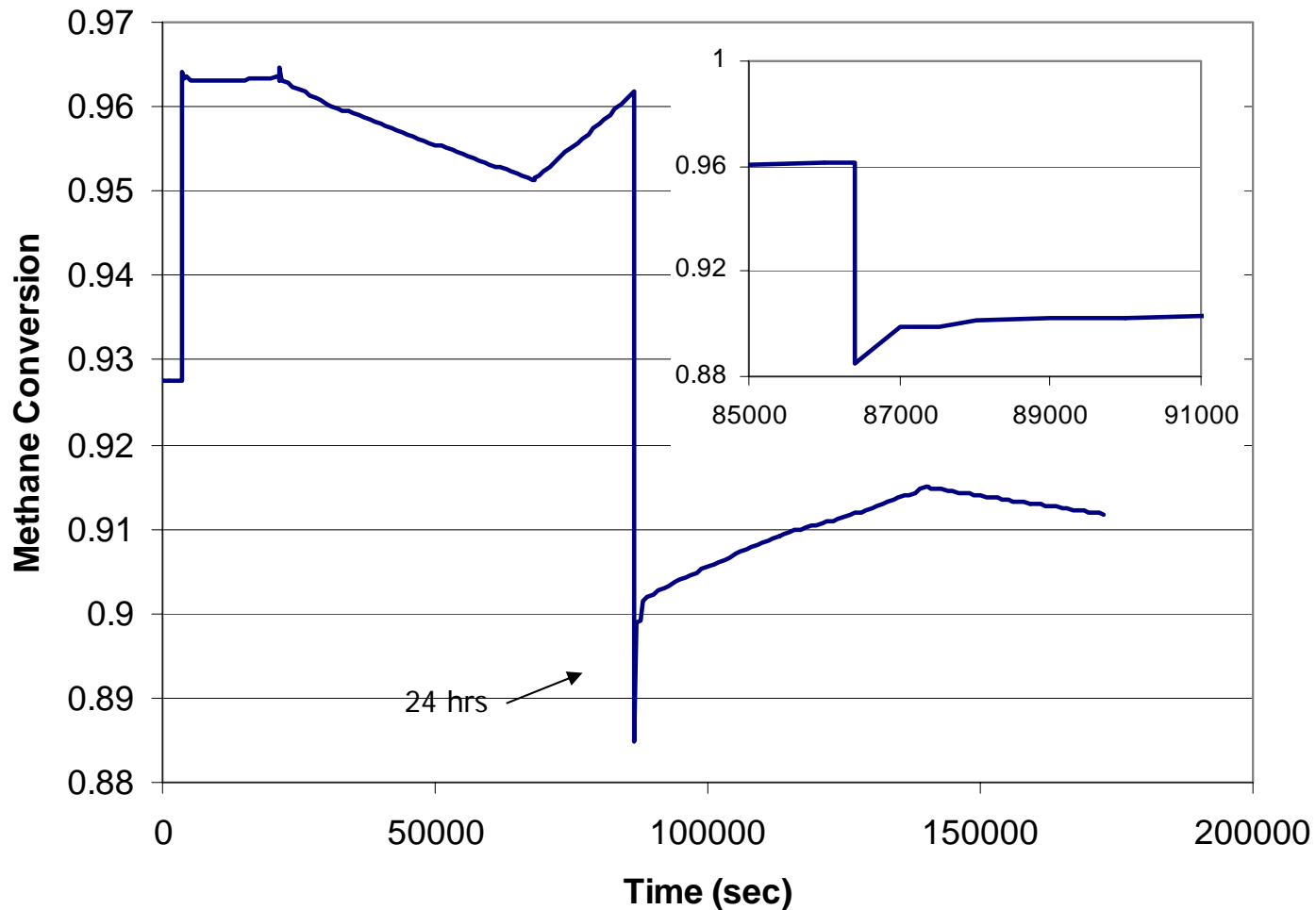
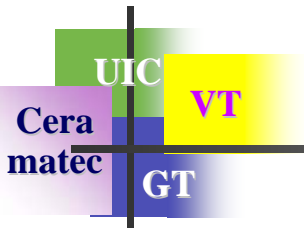
Note: The system is optimally synthesized/designed using these two profiles back to back; the synthesis/design accounts for optimal dynamic operation and control.

**Winter Profile:**  
Approximated load profile.  
Heating Day in Atlanta,  
Georgia Occurs on 01/12

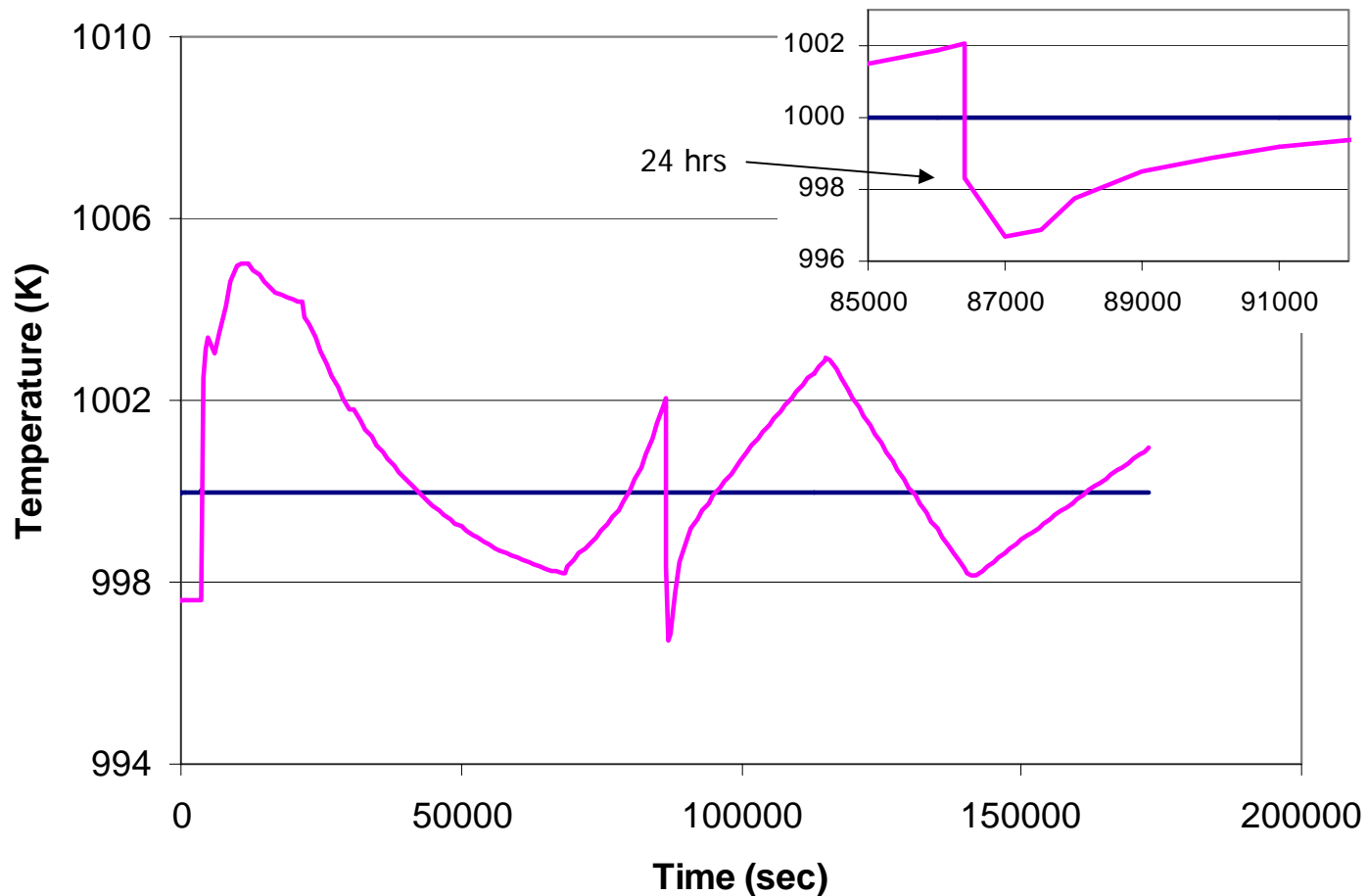
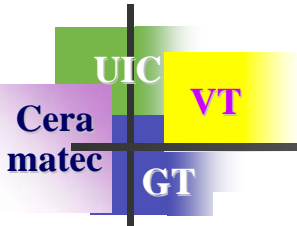


Jan 27, 2005

# Optimum Transient Response over Entire Load Profile

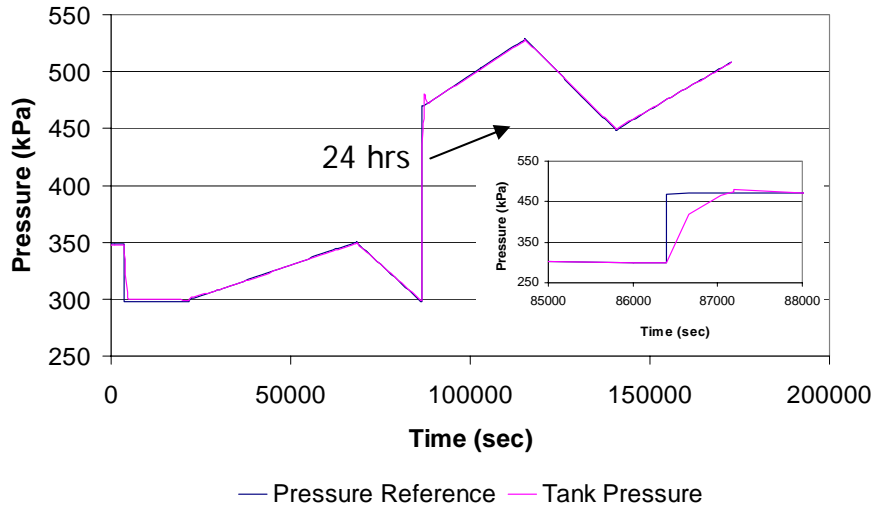
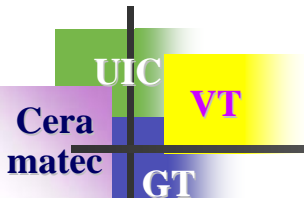


# Optimum Transient Response over Entire Load Profile



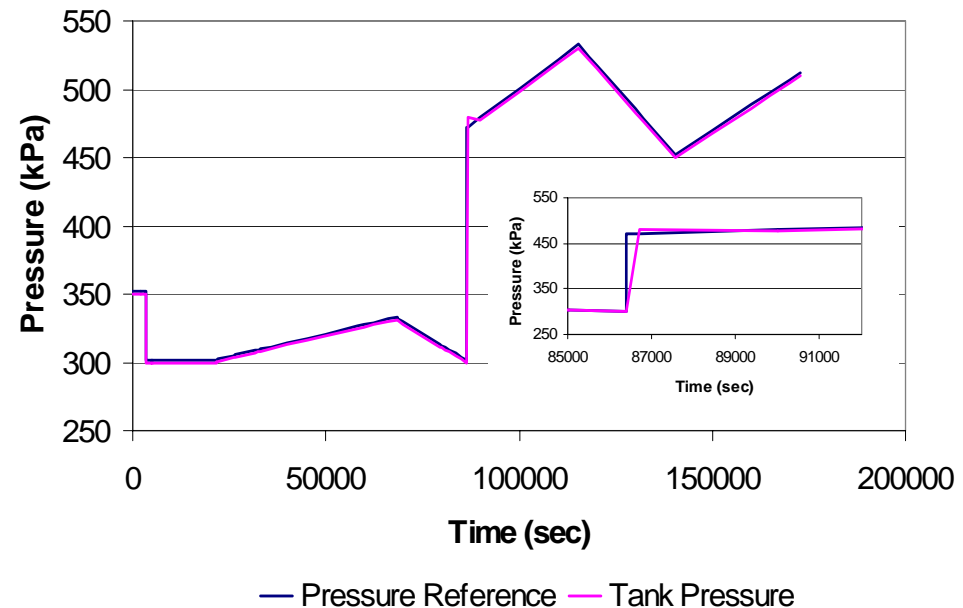
— Anode Inlet Temperature — Cathode Inlet Temperature

# Optimum Transient Response over Entire Load Profile



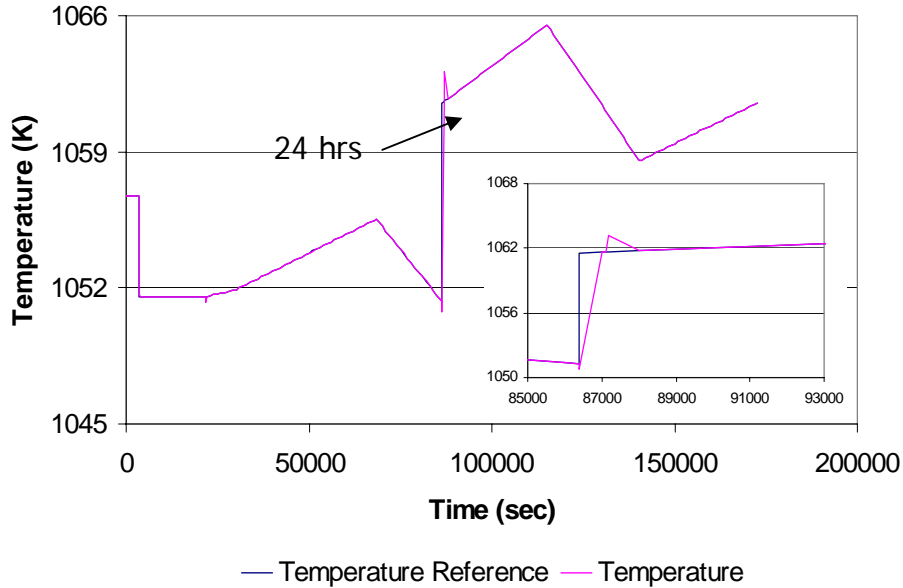
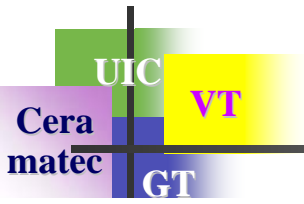
**Air tank pressure  
dynamic response.**

**Hydrogen tank pressure  
dynamic response.**



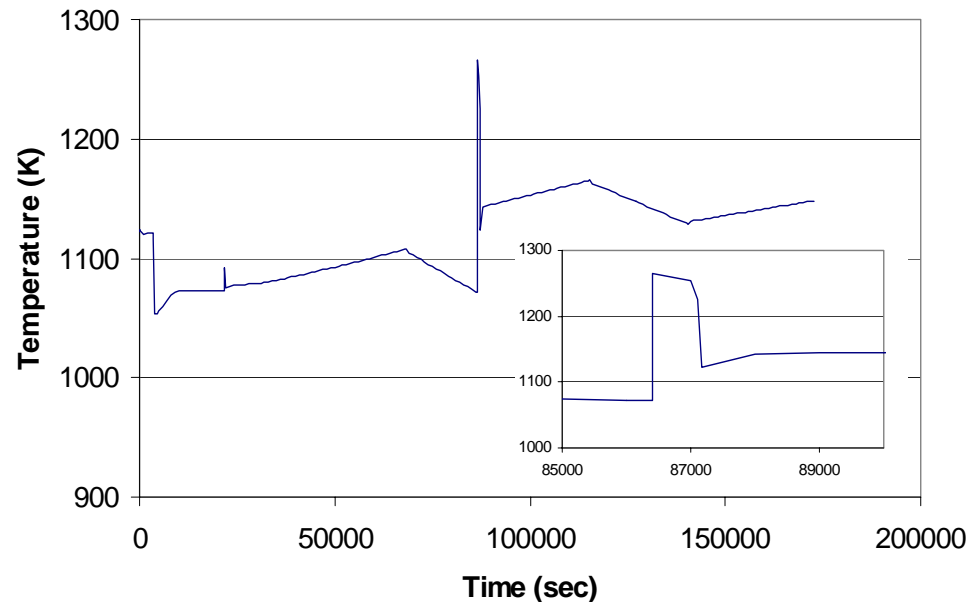


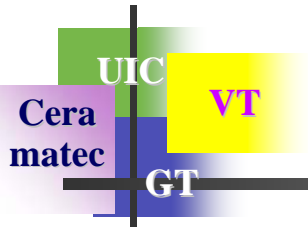
# Optimum Transient Response over Entire Load Profile



**Optimum steam-methane  
reformer hot gases inlet  
temperature (control  
variable) dynamic  
response.**

**Optimum steam-methane  
reformer reformat exit  
temperature (state variable)  
dynamic response.**

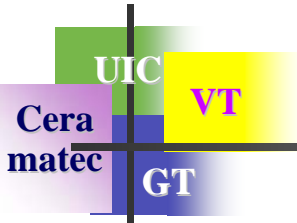




# Interaction Analysis

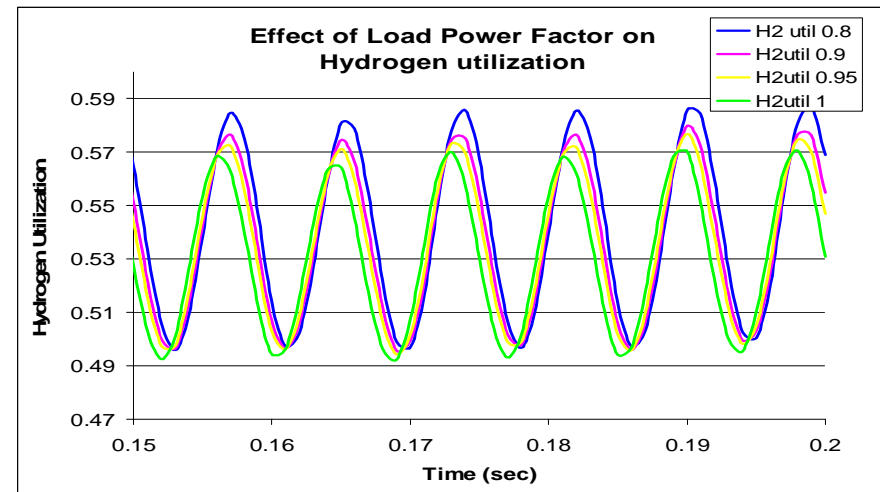
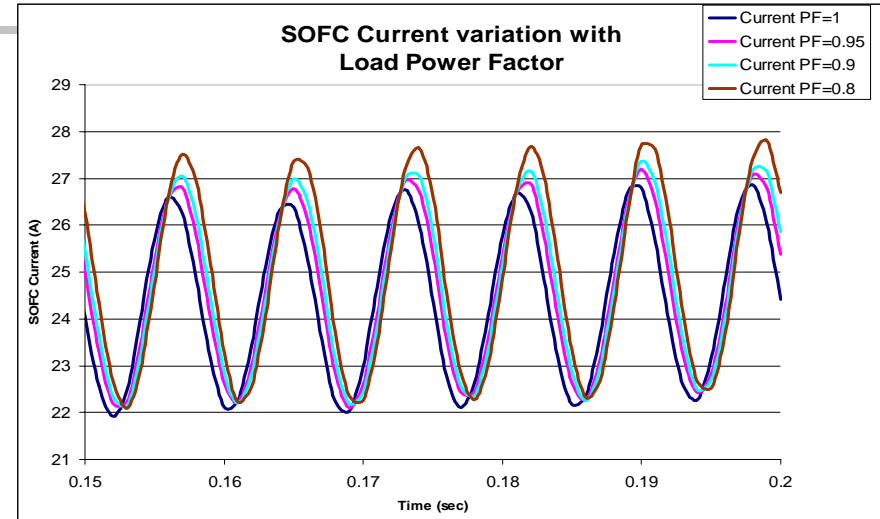
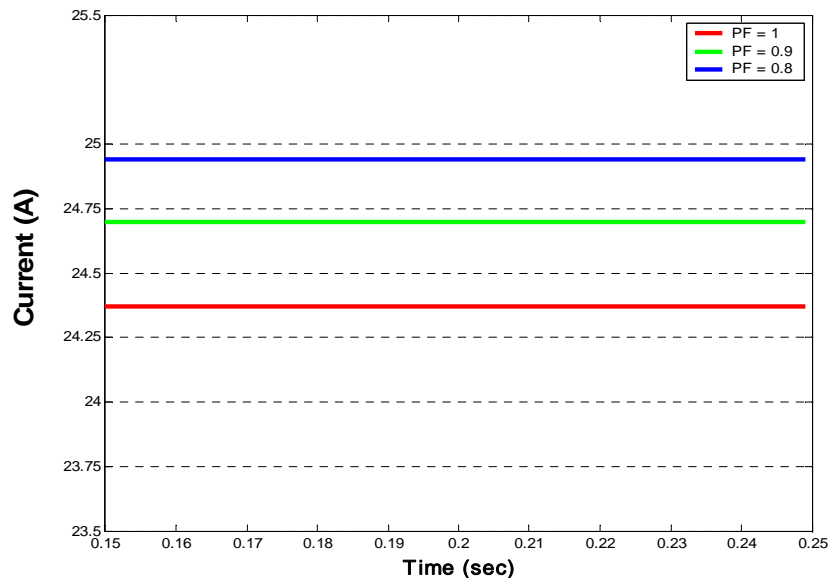
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# Effect of Load Power Factor

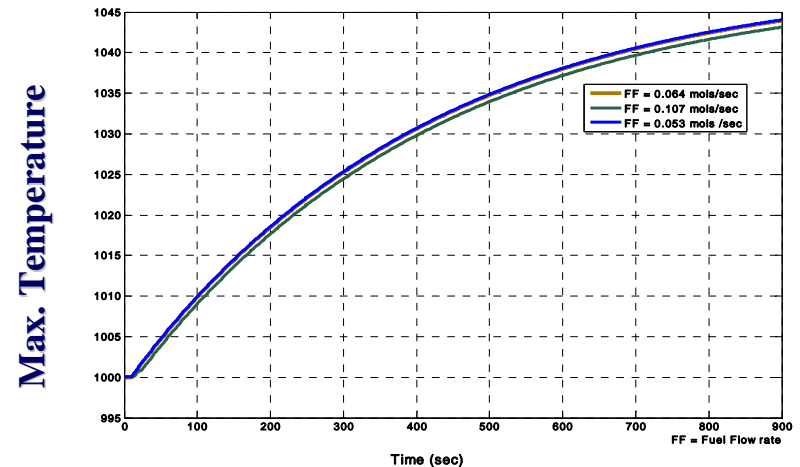
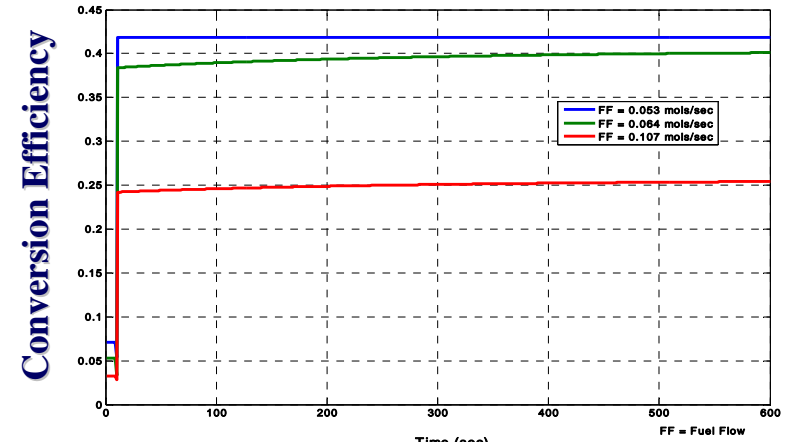
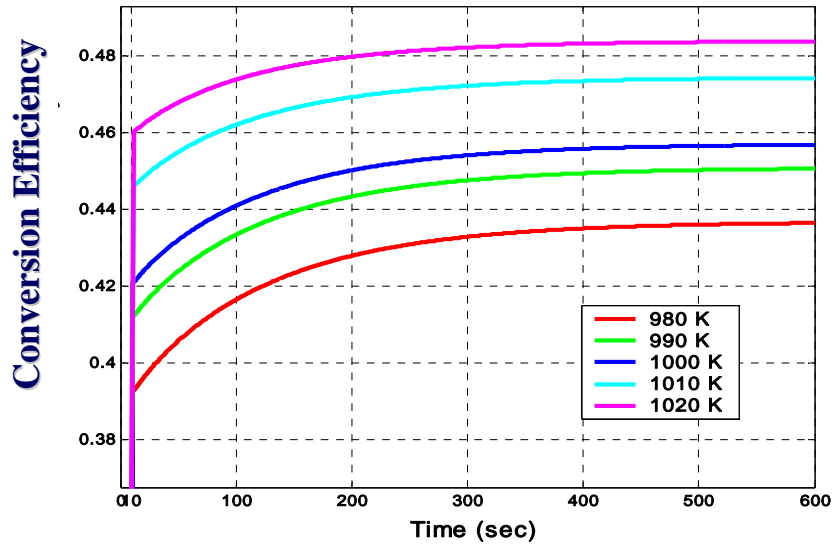
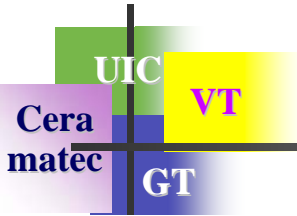


■ The lower the load power factor

- The higher is the SOFC stack current and current ripple
- The higher is the hydrogen utilization



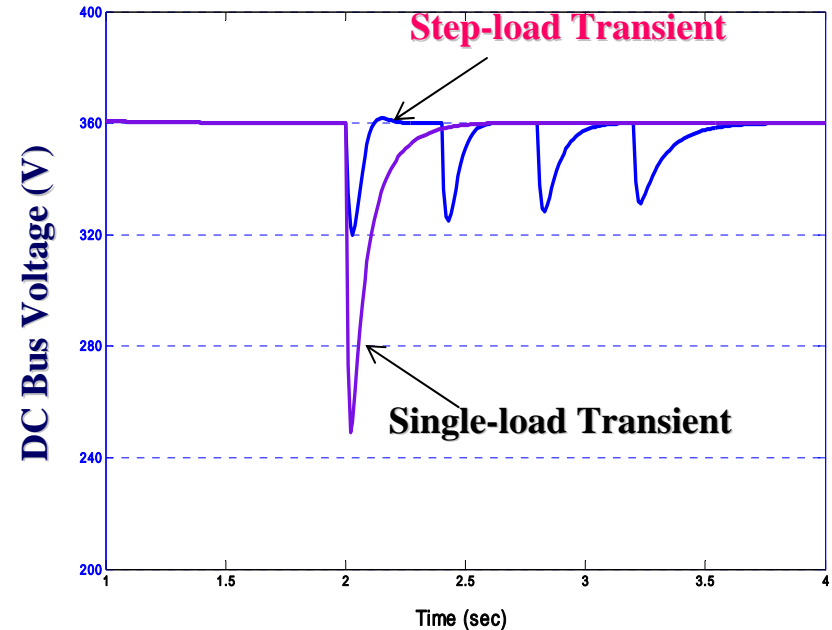
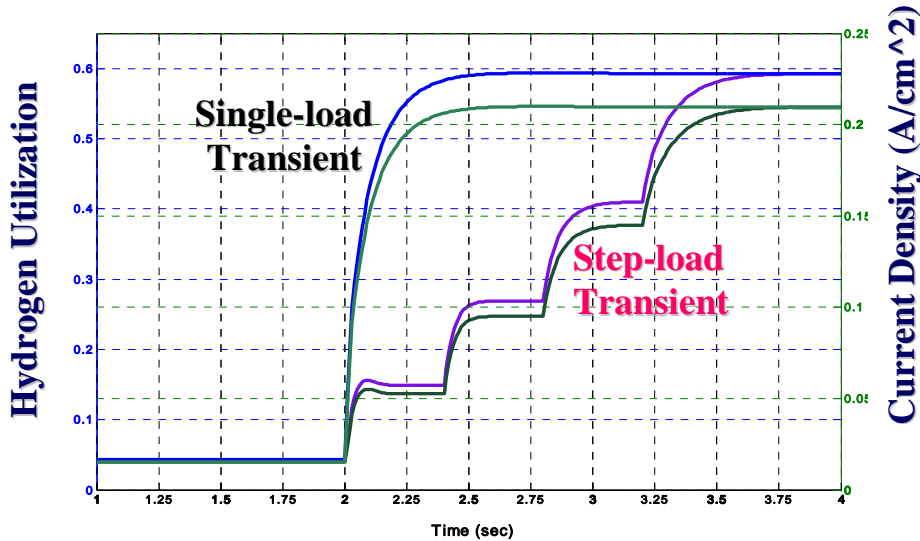
# Impacts of Parametric Variations on the Effects of Load Transient



- Operating temperature increase
  - ASR decreases exponentially with increase in the temperature
  - Lesser potential drop
  - Higher efficiency

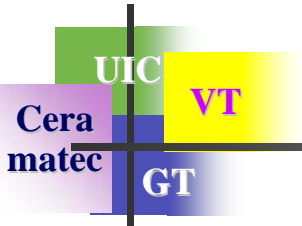
- Fuel flow rate increase
  - Slight decrease in the temperature
  - Decrease in the efficiency

# Effect of step-load transient vs. single-load transient



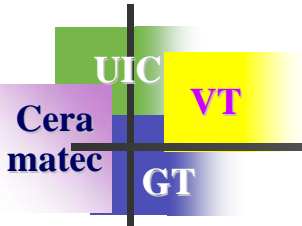
- Step-load transient leads to
  - Significant reduction in the drop of the DC bus voltage
  - Reduction in increase of the hydrogen utilization and current density during the transient
    - Reduction in the battery size

# Conclusion



- **1D PSOFC model appears to be a good choice to study the load transient effects to reduce computation time without compromising accuracy. But, to accurately study the characteristics including thermal stress, temperature, strength, and the reliability prediction should be based on the PSOFC 2D model;**
- **On a similar note, the state-space averaged model of PES is better suited for the study of load-transient effects from computational efficiency standpoint;**
- **Fully-controlled BOPS model may accurately emulate the actual system but, for spatio-temporal studies on a basic PC, a reduced-order lookup-table model based on the comprehensive model is a more effective choice;**
- **Step-load transients as compared to single load-transient reduces the harmful effects on the SOFC and improves the performance of the PES, which may lead to reduction in the sizes of energy-buffering components (e.g., battery or PHT) and hence, the cost and weight of the power system.**

# Future Works



- Build a complete look-up table model for the BOPS to enhance faster and accurate simulation
- Experimental validation of the obtained simulation result on a PSOFC stack
- Investigate the electrical feedback effects on the material properties of the PSOFC and prediction of life of the PSOFC
- Build an optimal hybrid controller for the PSOFC system to optimize the stack performance while enhancing the reliability of the PSOFC