Modeling of Electrical Interactions with SOFCs

Project Investigators

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Student Acknowledgement

- R. Burra and K. Acharya (U of I)
- Diego Rancruel (VT)
- Robert Williams (GT)

SECA Modeling & Simulation Team – Integration Meeting
February 19-20, 2003
Sacramento, CA

PERC
U of I

CFC/BT
GTRI

EMI
VT

Acknowledgement

- DoE SECA
- Don Collins (NETL)
- Engineous Software
- Joe Hertvigsen (Ceramatech)
- Jonathan Felton (PSE, UK)
- Lee Johnson and Ken Ruan (Synopsys Inc.)

R&D Objectives

- Develop fully transient nonlinear, unified models for SOFC planar configurations, different PESs and application loads, and a variety of BOPS components
- Demonstrate the feasibility of integrating these models into an overall systems-analysis and optimization tool (Phase I)
- Develop a prototypical software package (Phase II) for industry to understand the dynamical and stead-state system interactions among of SOFC stack, power electronics, and BOPS and system optimization
- Conduct parametric studies (Phase I) and optimizations (Phase II) to determine control strategies and their effects on the cell reliability, efficiency, and power density; as well as system response and configuration, and component designs.

Applicability to SECA

- A “Unique” “Simple-to-Use” Tool for “Rapid” Prototype SOFC Power-Conditioning System Design and Marketability
- Resolving the “Steady-State” and “Transient” Dynamics of the SOFC, Power-Electronics Interface, BOPS for
  - Stationary Loads
  - Non-Stationary Loads
  - Higher Power Distributed Power Systems
- Optimization and Control Enhancement
  - Designing control for optimal bandwidth
  - Cost-effective design
- “Multi-Disciplinary” “Industry +Academic” Expertise for SOFC Power-Conditioning System Design:
  - University of Illinois – PES
  - Virginia Tech – BOPS
  - Georgia Tech – SOFC

  Synopsys Inc. (SABER – 30000 models)
  gPROMS (PSE - Optimizer + Nonlinear Solvers)
  iSIGHT – (Engineous - System Integration)
  TOPAZ – (Ceramatech - FEA for SOFC thermal and current-density distribution)

DoE SECA Tasks Timeline – Phase I

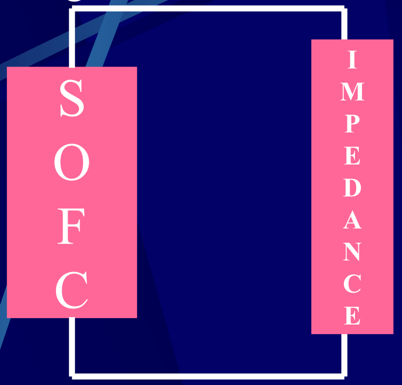
	Phase I											
	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
Task 1.0 Planar SOFC Model Development	🟥	🟥	🟥	🟥	🟥							
Task 2.0 Model of Power-Electronic Interface			🟥	🟥	🟥	🟥	🟥					
Task 3.0 Load Profile Development	🟥	🟥	🟥									
Task 4.0 BOPS Model Development, Implem. & Valid.	🟥	🟥	🟥	🟥	🟥							
Task 5.0 SOFCSS Model Implementation Environ.	🟥	🟥	🟥									
Task 6.0 Integration of PES, SOFCSS, & BOPS Models					🟥	🟥	🟥	🟥				
Task 7.0 Analysis of System Stability and Dynamics							🟥	🟥	🟥	🟥		
Task 8.0 Parametric Studies of Best-Practice Ctl. Strat.								🟥	🟥	🟥	🟥	
Task 9.0 Final Report and Phase II Proposal											🟥	🟥

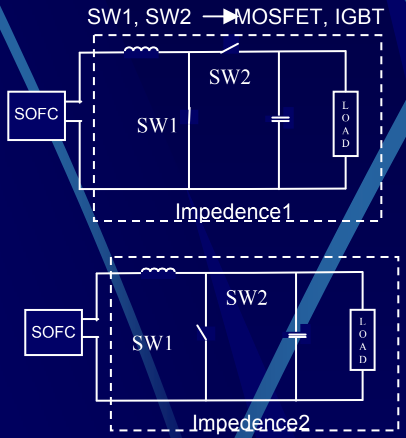
Methodology

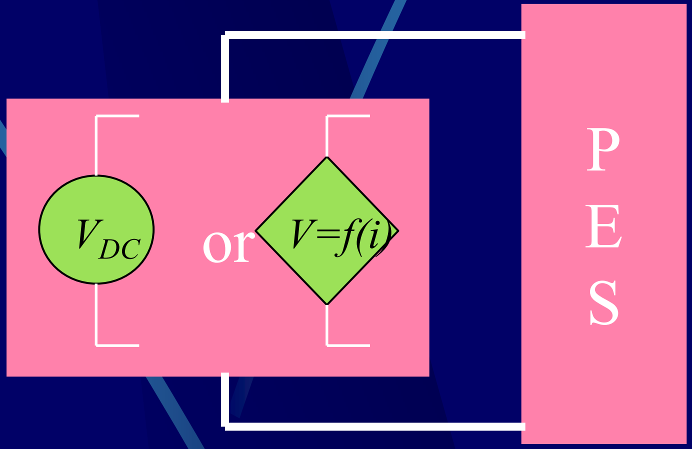
Power-Electronics System (PES)

Fuel Cell Power-Conditioning System

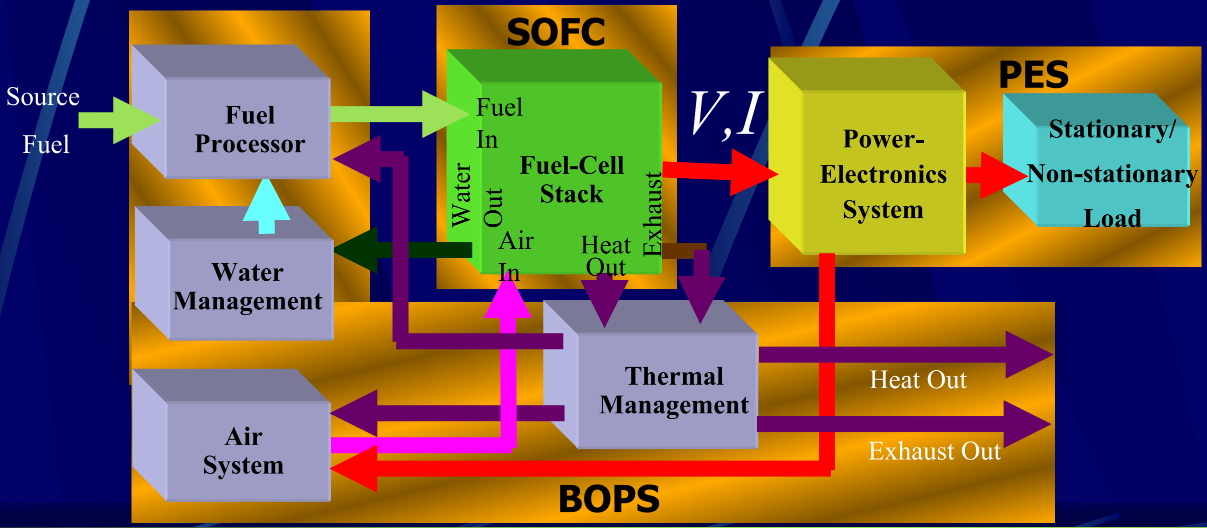
- ***Conventional Modeling Techniques***
  - Fuel cell manufacturers typically model the FC feeding a constant impedance
  - Power Electronic Engineers typically model the FC as a dc voltage source or a current controlled voltage source feeding the PES





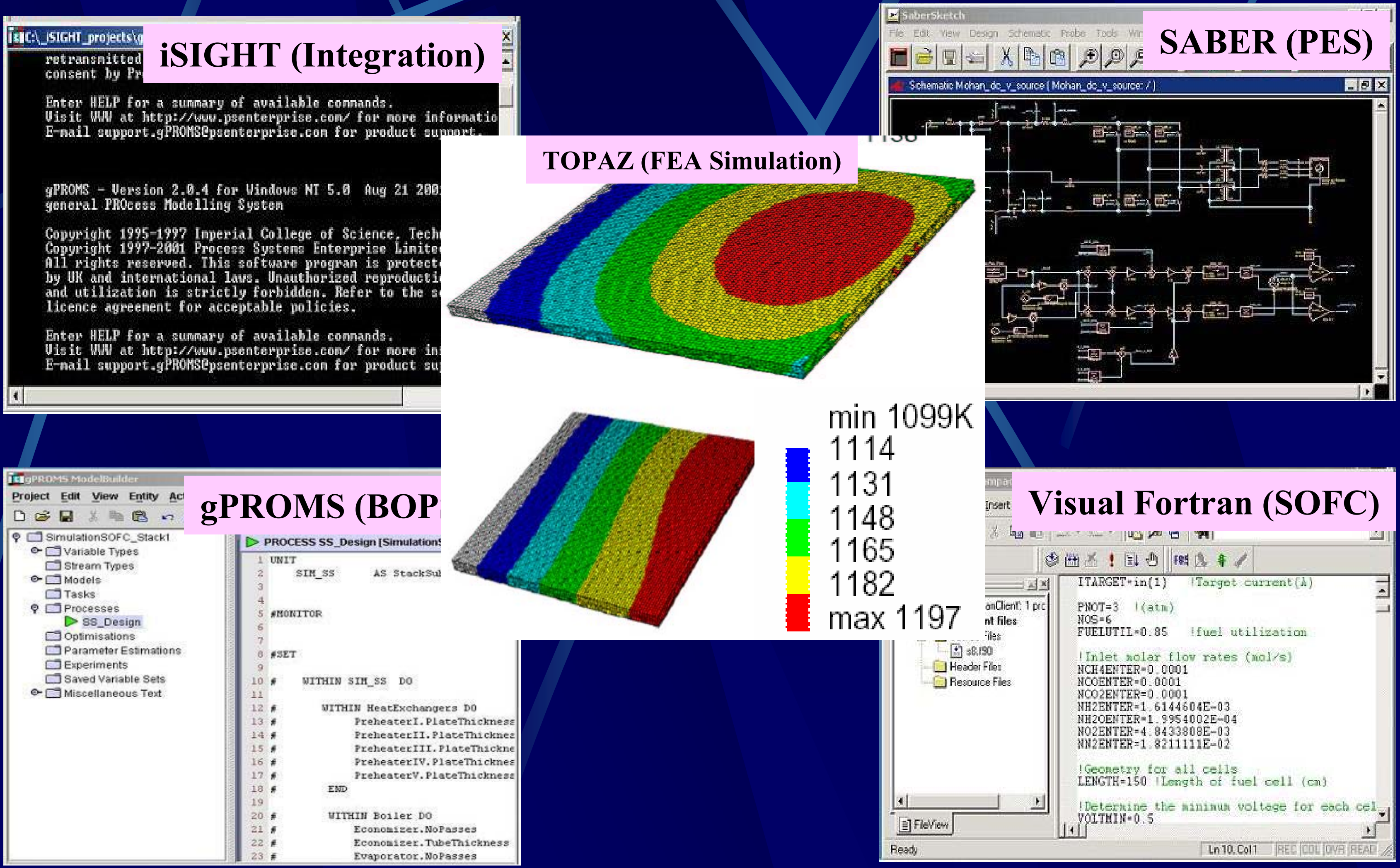


- ***Our Approach***



$$\begin{bmatrix} V \\ I \end{bmatrix} = f(BOPS, PES, LOAD)$$

Proposed Simulation Platform for Fuel-Cell System



iSIGHT (Integration)

```
retransmitted
consent by Pr

Enter HELP for a summary of available commands.
Visit WWW at http://www.psenterprise.com/ for more informatio
E-mail support.gPROMS@psenterprise.com for product support.


gPROMS - Version 2.0.4 for Windows NT 5.0  Aug 21 200
general PROcess Modelling System

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E-mail support.gPROMS@psenterprise.com for product su
```

SABER (PES)

TOPAZ (FEA Simulation)

gPROMS (BOP)

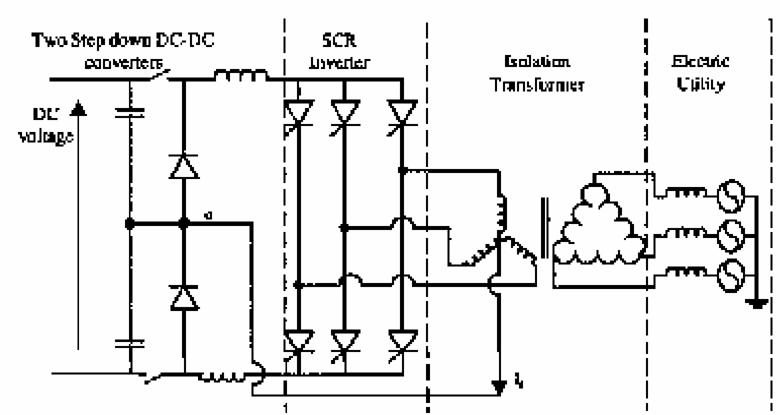
```
UNIT
    SIM_SS      AS StackSu


#MONITOR


#SET

#    WITHIN SIM_SS  DO

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

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

Visual Fortran (SOFC)

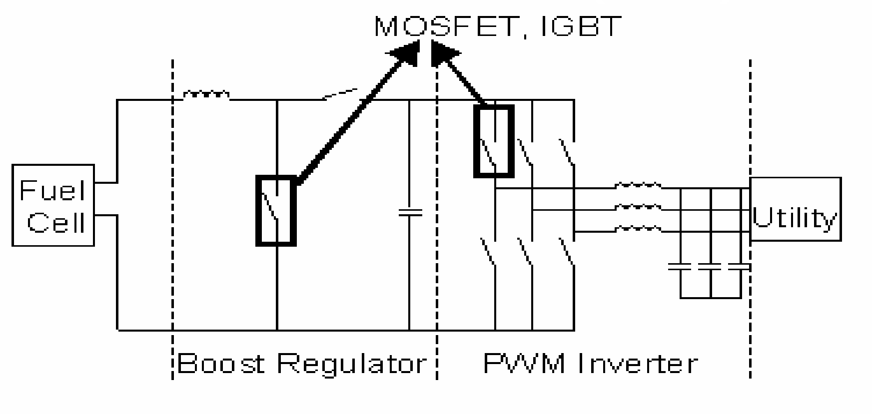
```
ITARGET=in(1)    !Target current(A)

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

!Inlet molar flow rates (mol/s)
NCH4ENTER=0.0001
NCOENTER=0.0001
NCO2ENTER=0.0001
NH2ENTER=1.6144604E-03
NH2OENTER=1.9954002E-04
NO2ENTER=4.8433808E-03
NN2ENTER=1.8211111E-02

!Geometry for all cells
LENGTH=150 !Length of fuel cell (cm)

!Determine the minimum voltage for each cel
VOLTMIN=0.5
```

Power-Electronics Topologies

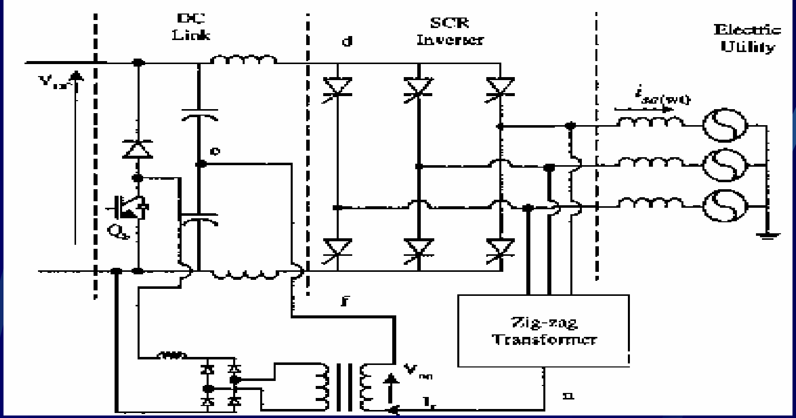
Line Commutated



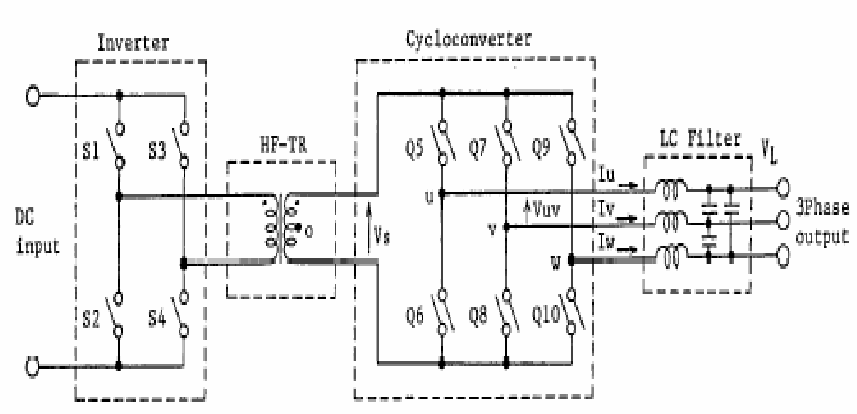
Self Commutated (PWM)



Line Commutated

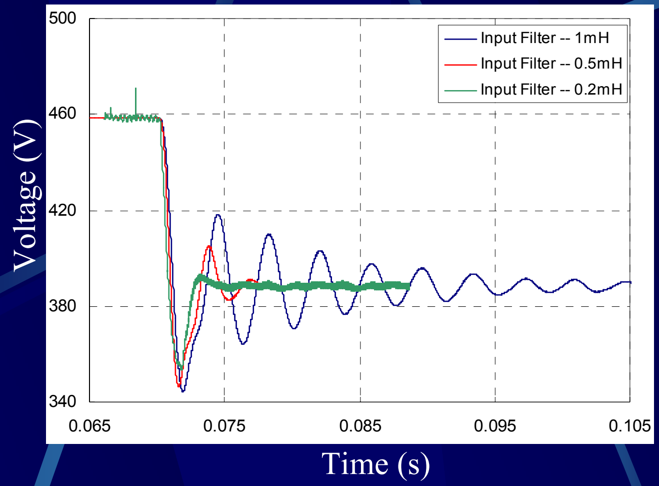


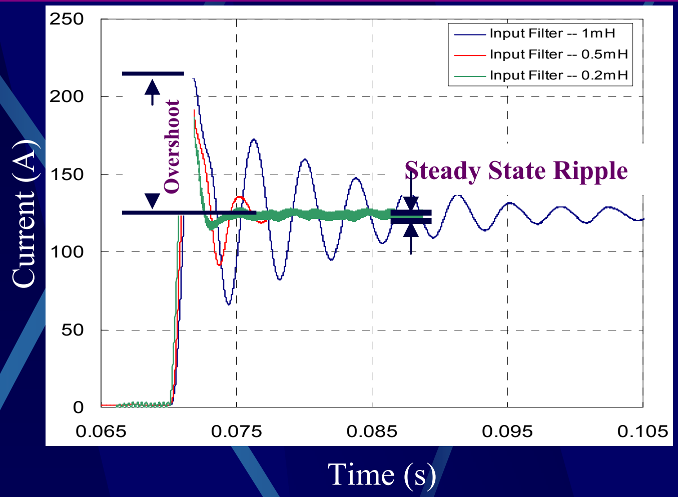
Transformer Assisted

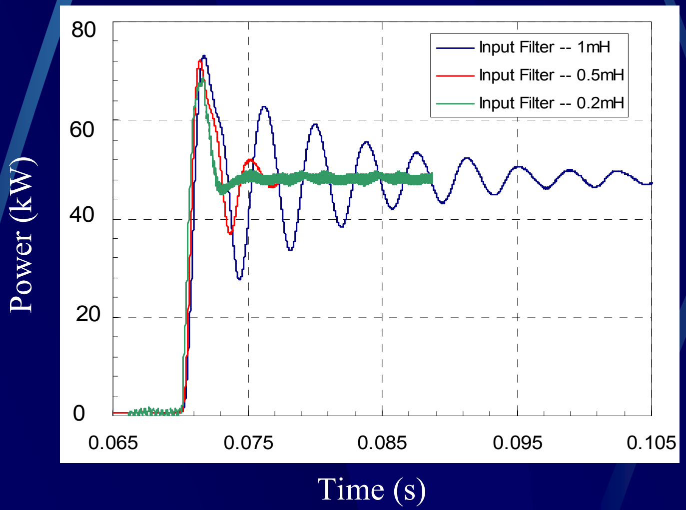


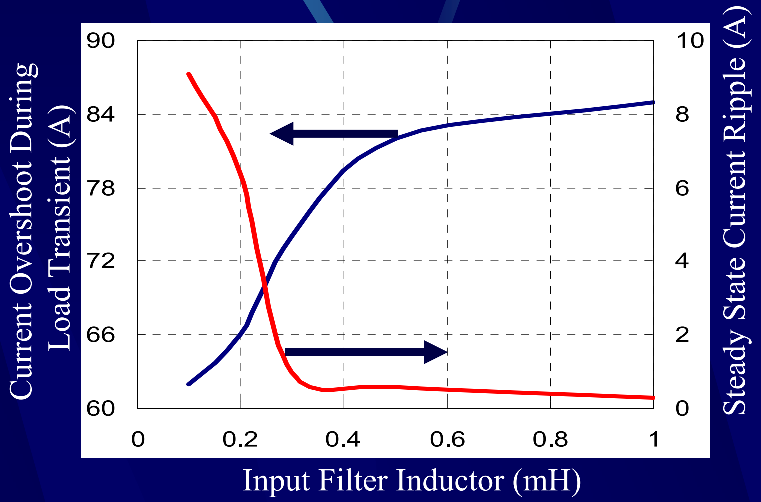
- Variation in topologies effect the current and voltage ripple dynamics of the SOFC, cost, and dynamic response

Fuel-Cell Transients With Variations in Input Filter









- Steady state ripple decreases with increase in input filter size, but load transient overshoot increases
- Transient and steady state power ripple could subject the fuel cell to thermal cycles
- Therefore, an optimum value of input filter should be chosen to reduce the degrading effect on the SOFC

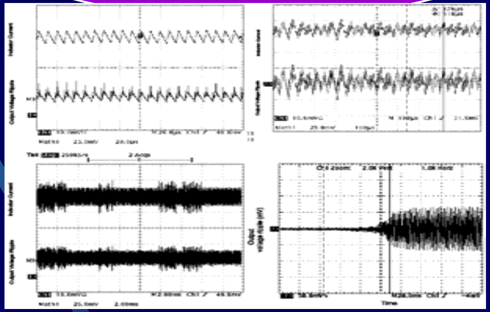
Project Status at UIC

Tasks Accomplished

PES

Tasks to be Accomplished

Nonlinear Behavior
- Circuit parameters
- Load



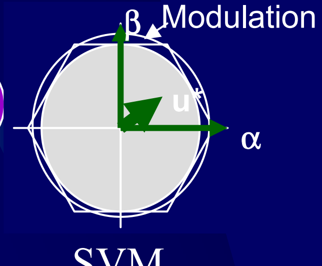
Topological Variations

SOFC load transient response

SOFC steady state response

Parametric variations

Control Strategies
- Local/global
- Modulation Schemes

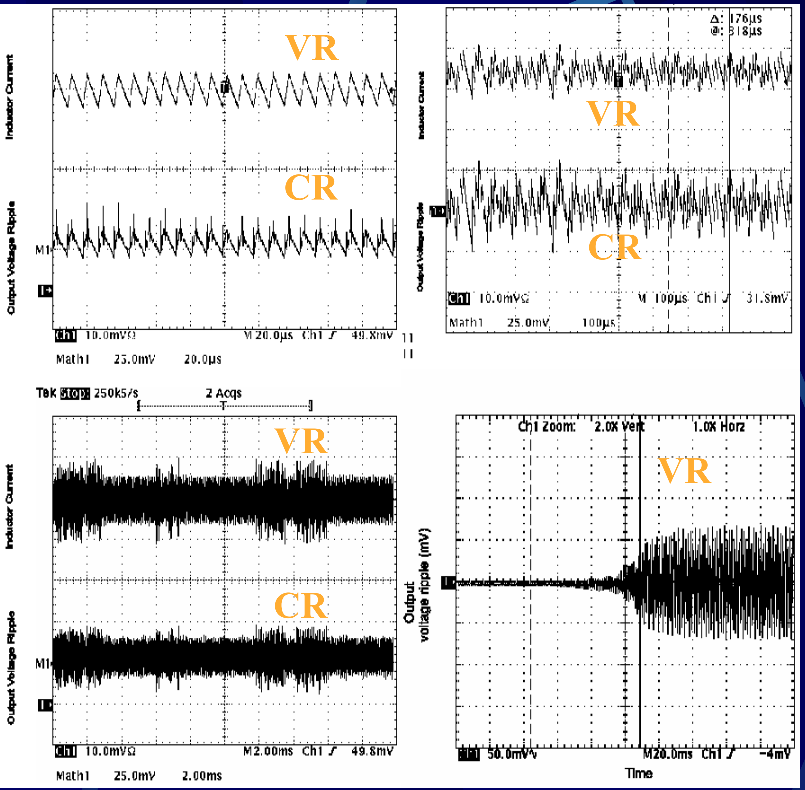


SVM

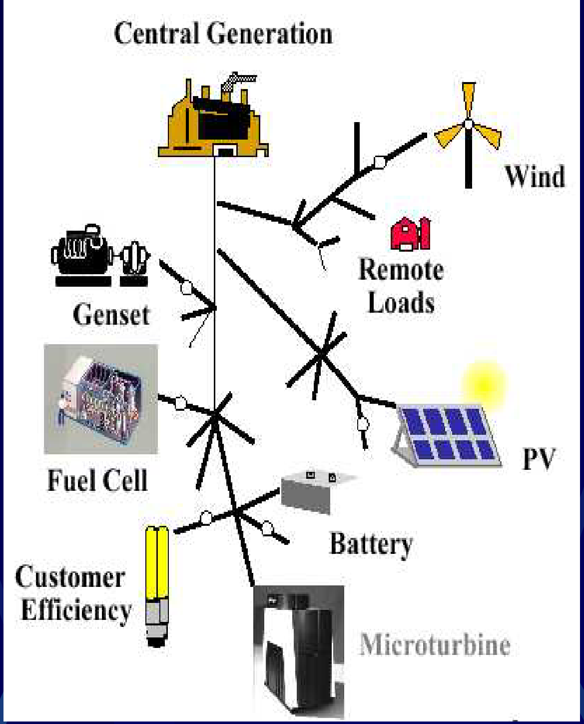
Energy Storage Distribution & Optimization

Illustrations

Nonlinear Behavior of a DC-DC Converter

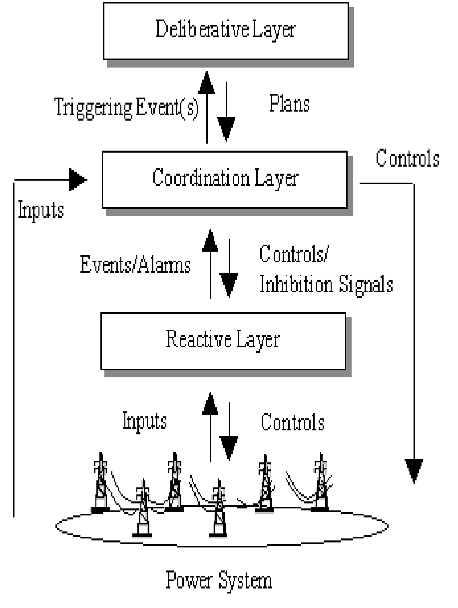


- By simply varying “only one” parameter (load in this case), the voltage and current ripples of the converter change drastically. In reality, more than one parameter can vary simultaneously.

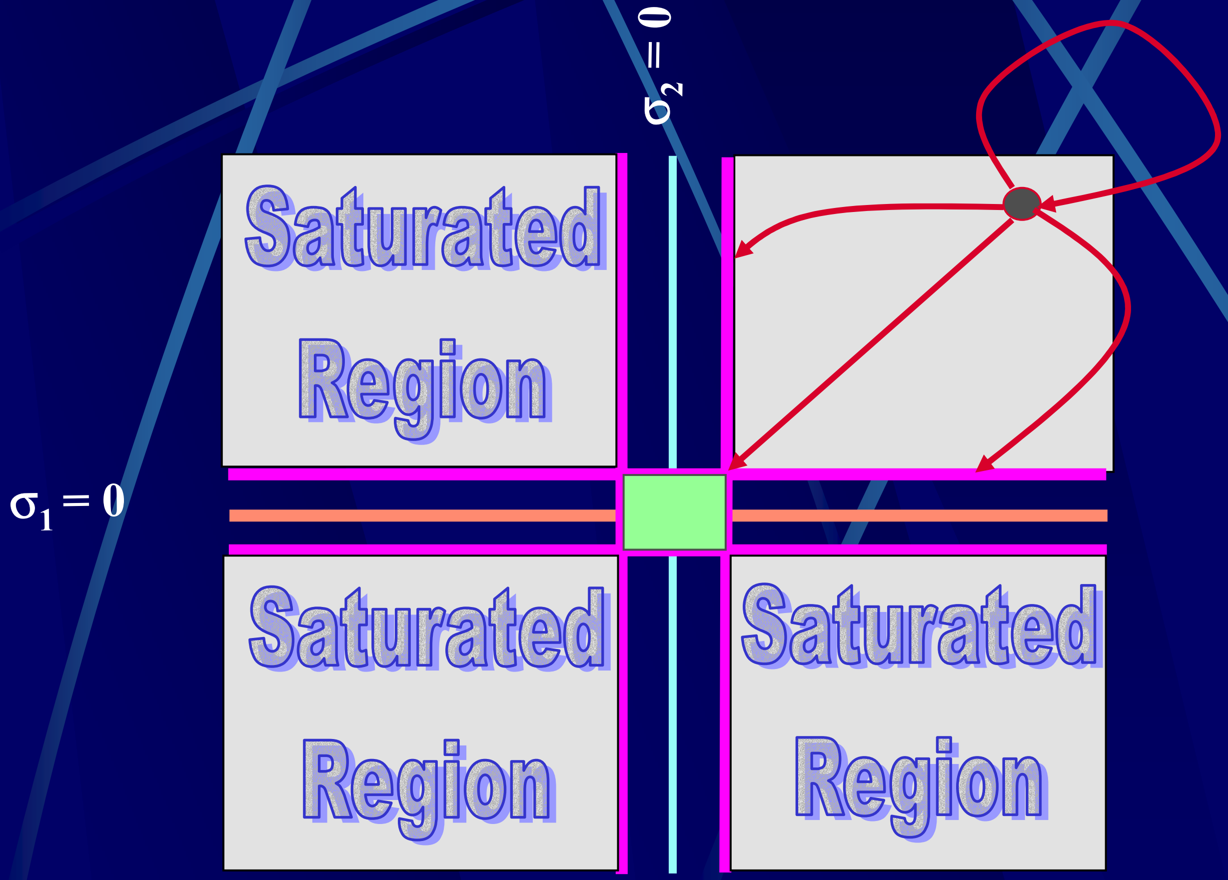


Multi-Objective Control and Optimization for Hybrid IPNs

DoE SECA + NSF CAREER



Idea Behind A New Fast Hybrid Control For Protecting the SOFC during Load Traneints

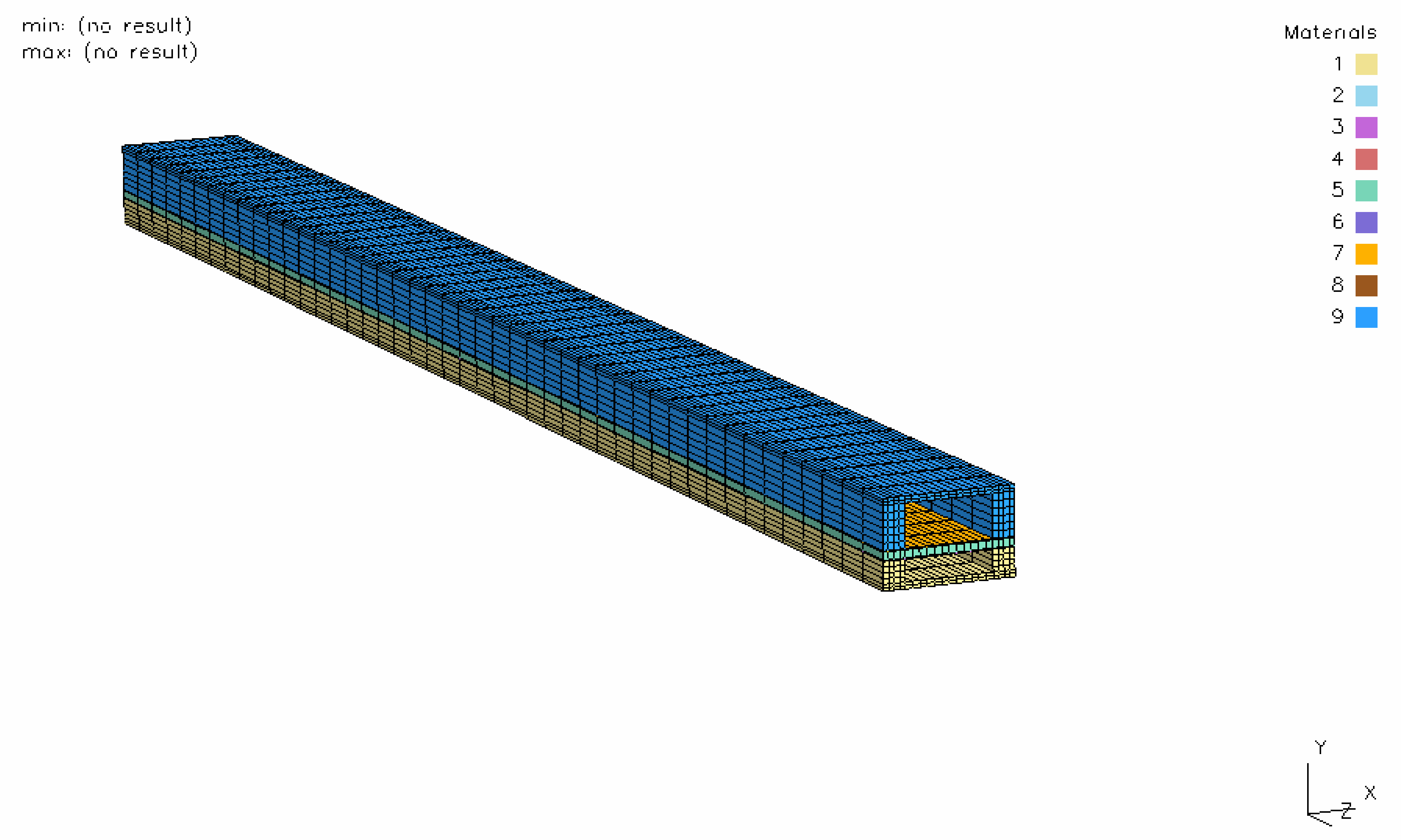


Hybrid Strategy

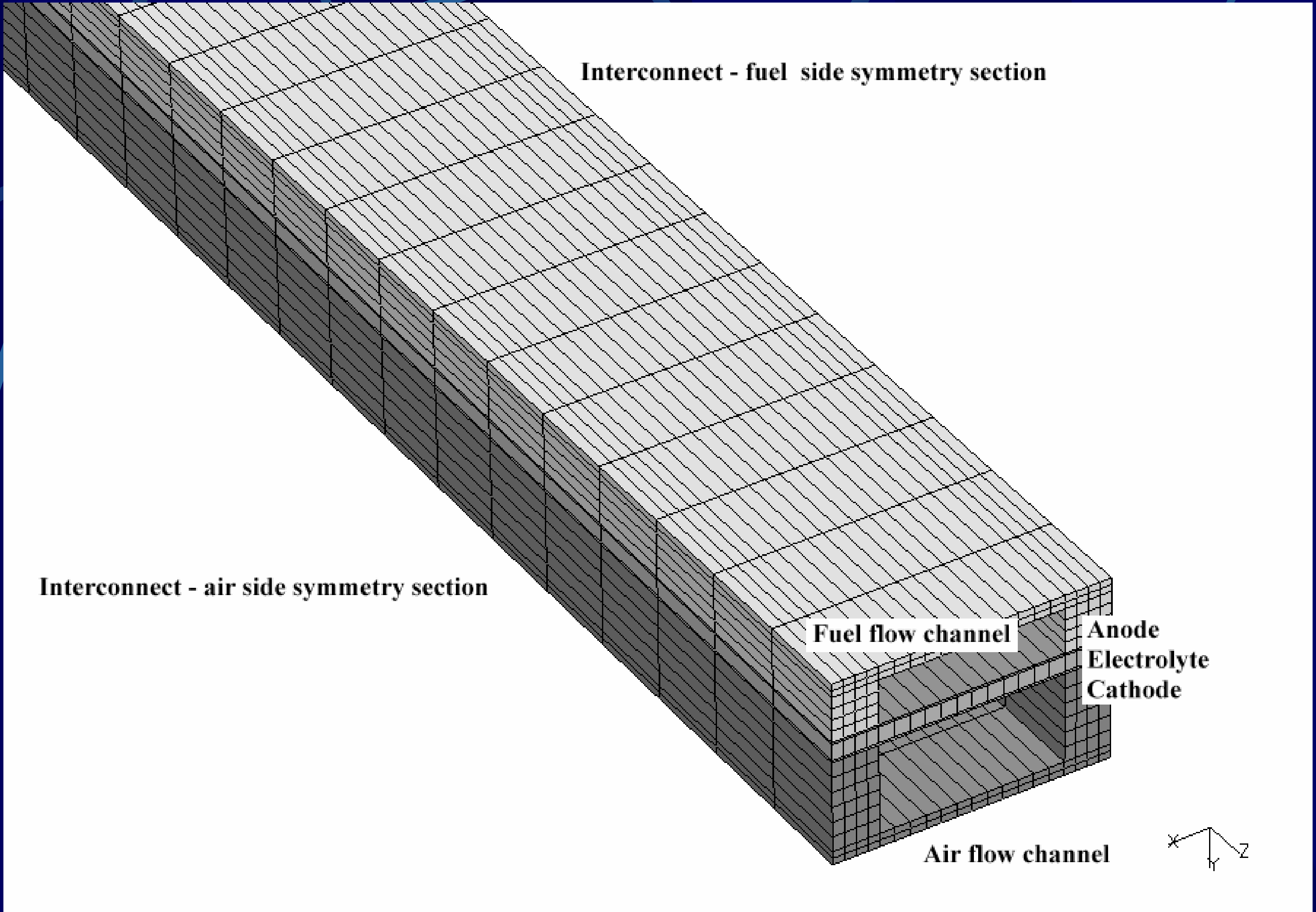
Control the dynamics of
unsaturated
and
saturated
regions separately

Integrating TOPAZ

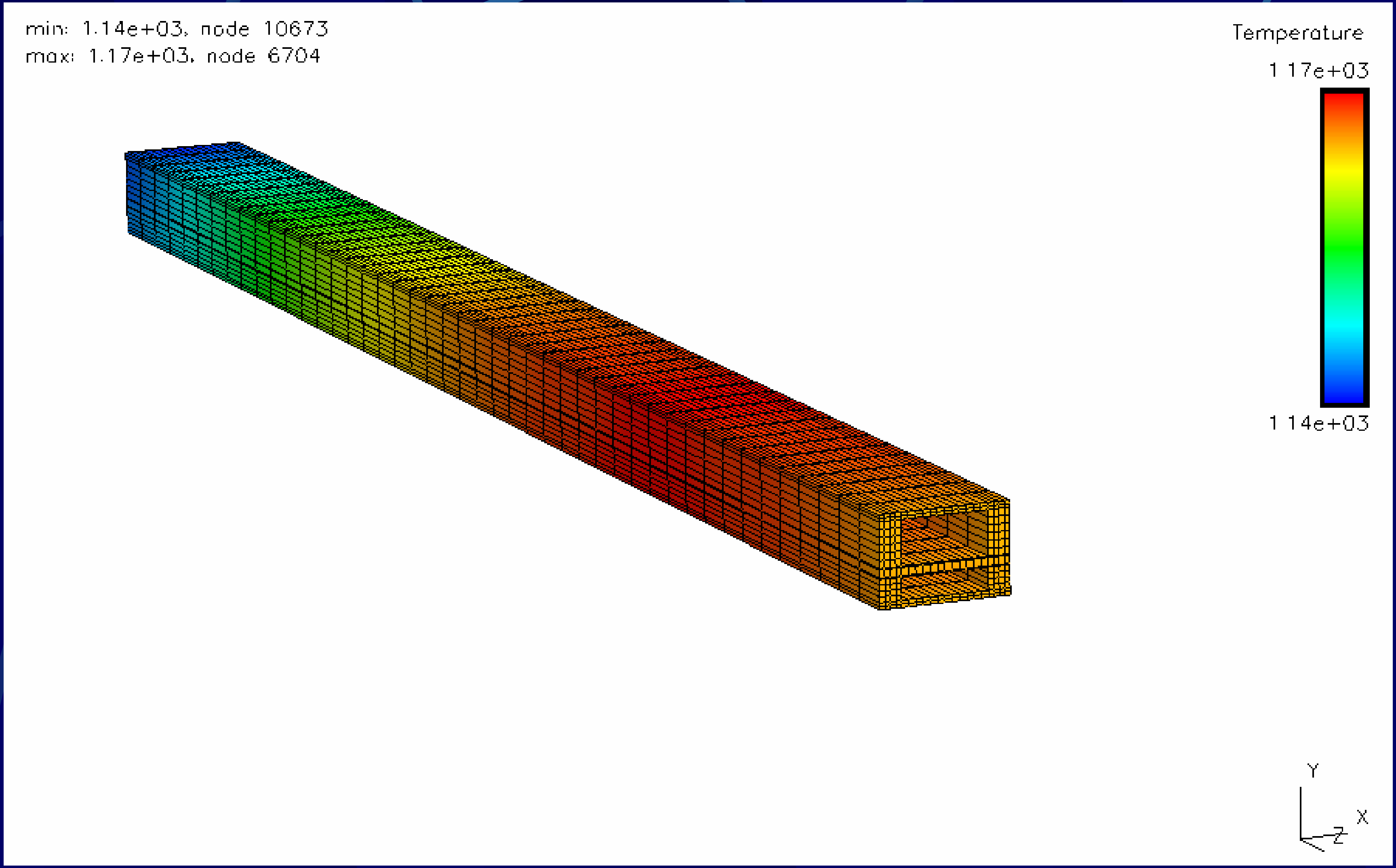
Co-flow SOFC Symmetry Section Mesh



Co-flow SOFC Symmetry Section Mesh

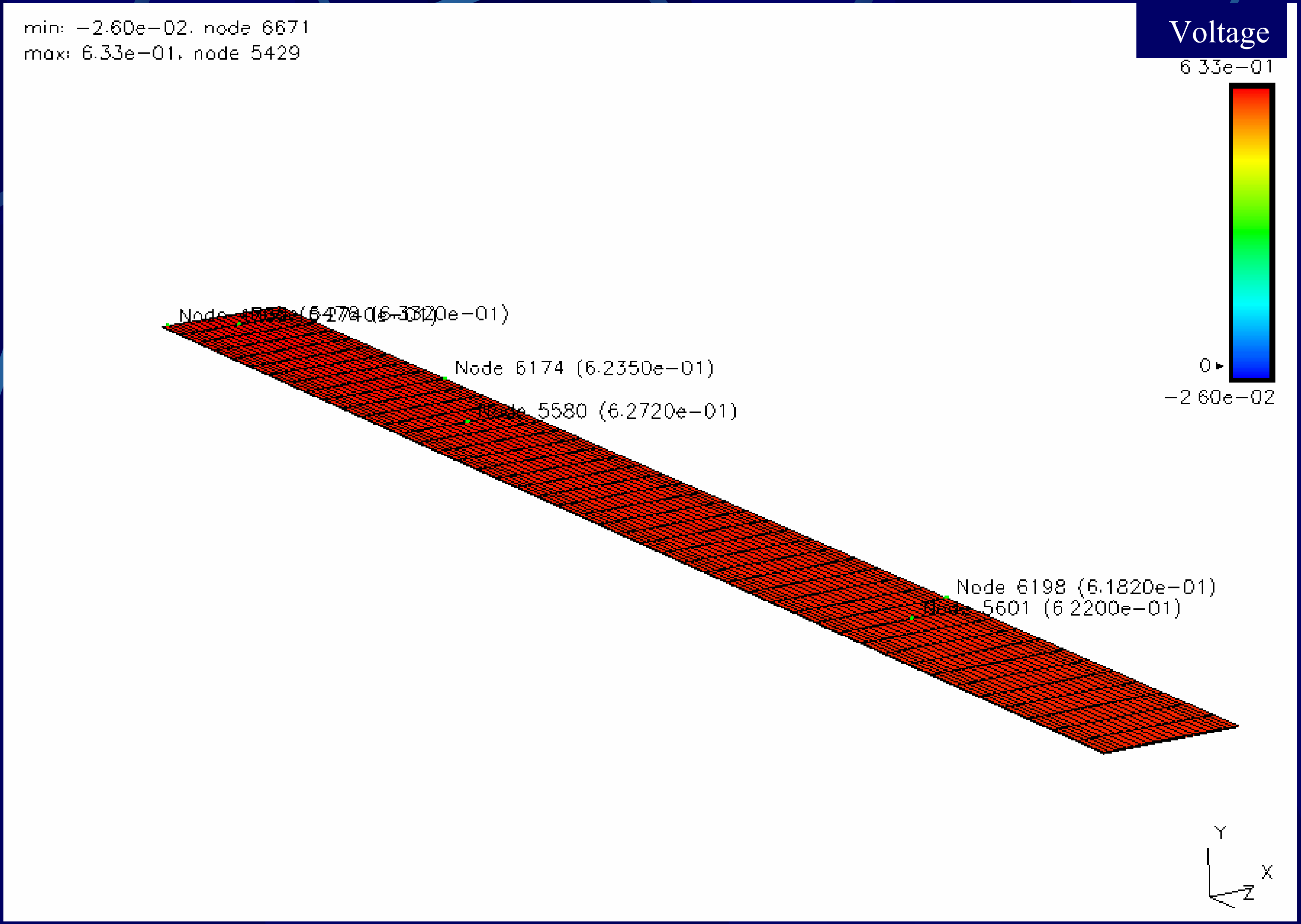


Model Temperature Distribution

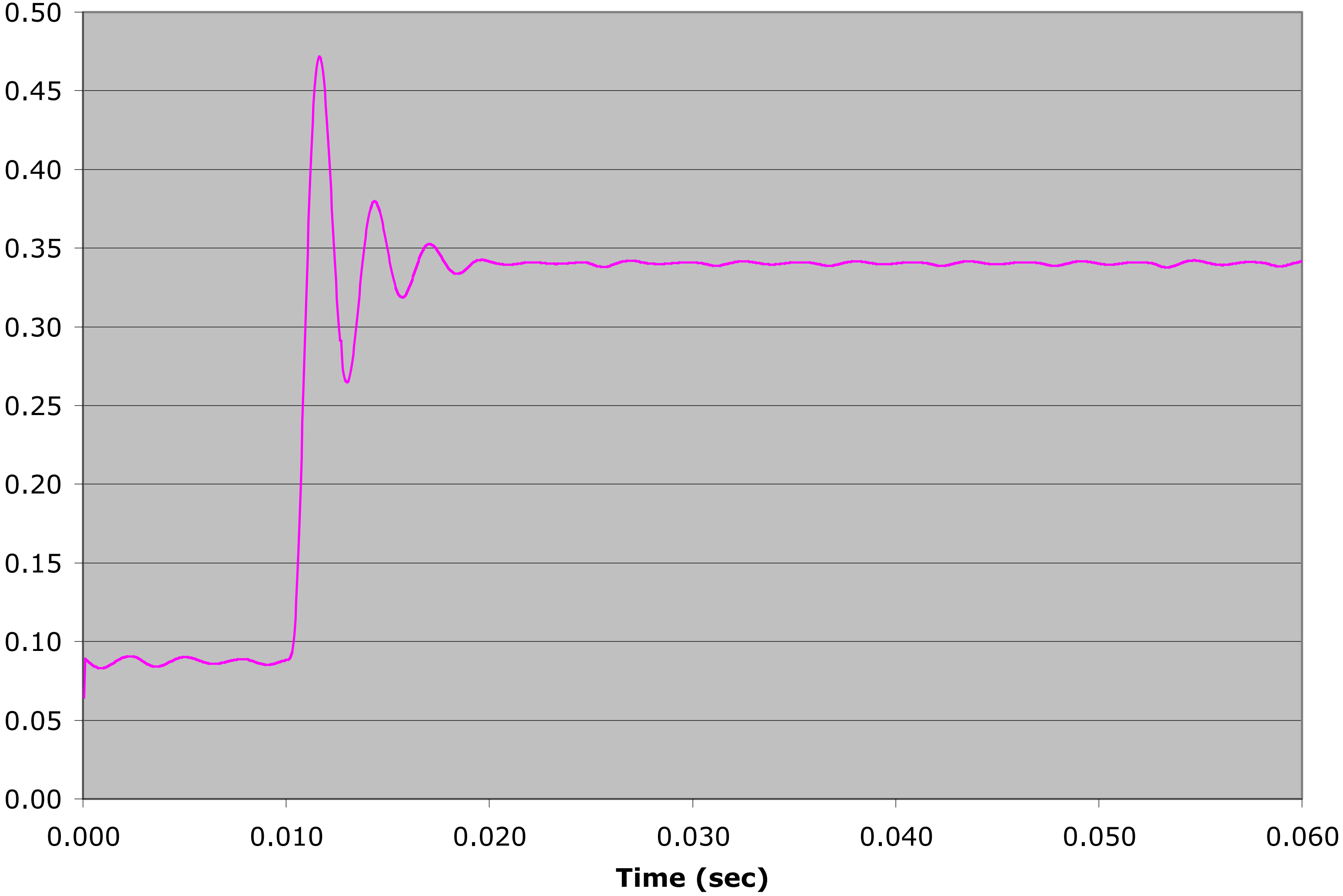


min: 1.14e+03, node 10673
max: 1.17e+03, node 6704

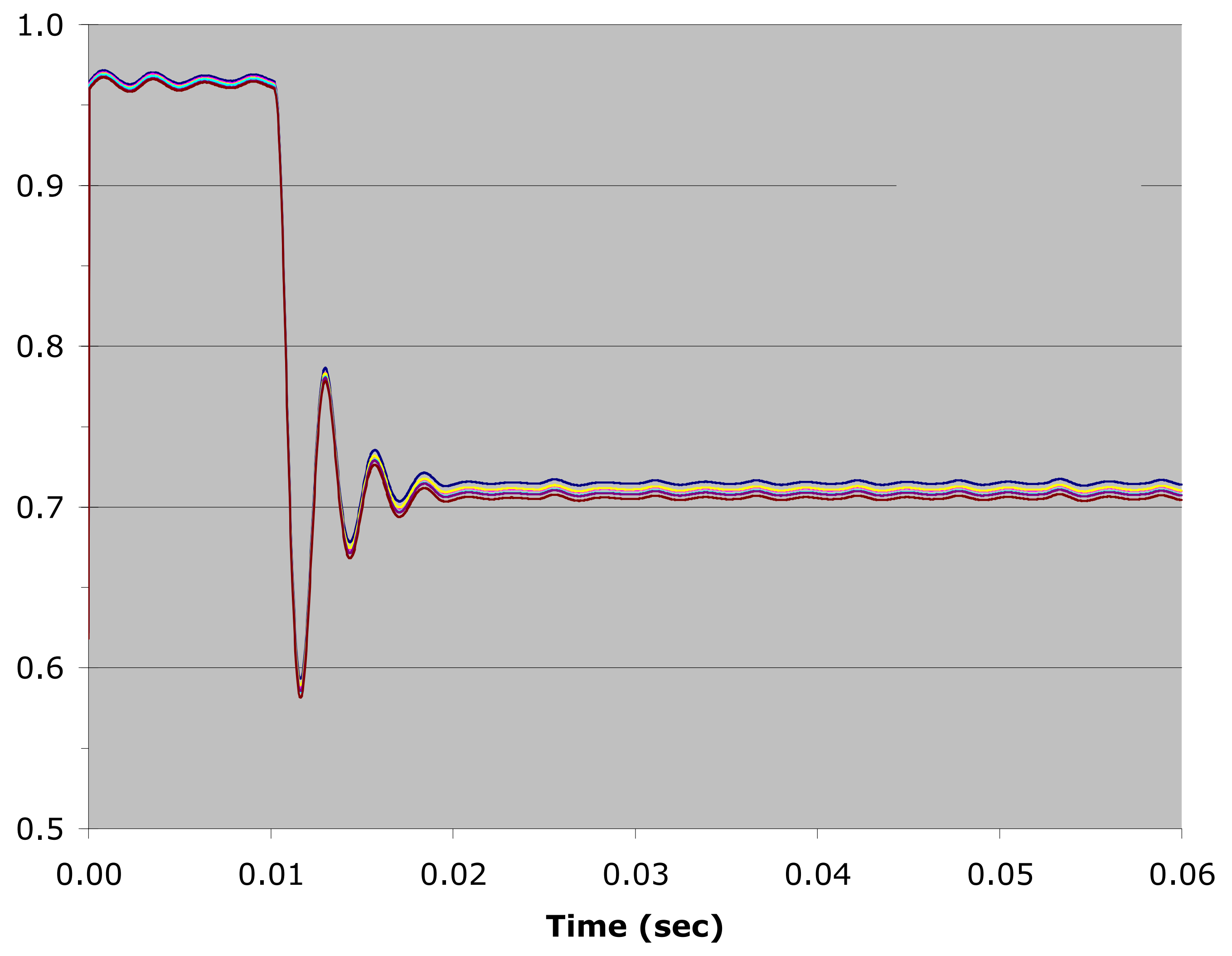
Selected Nodes on Electrode Mesh



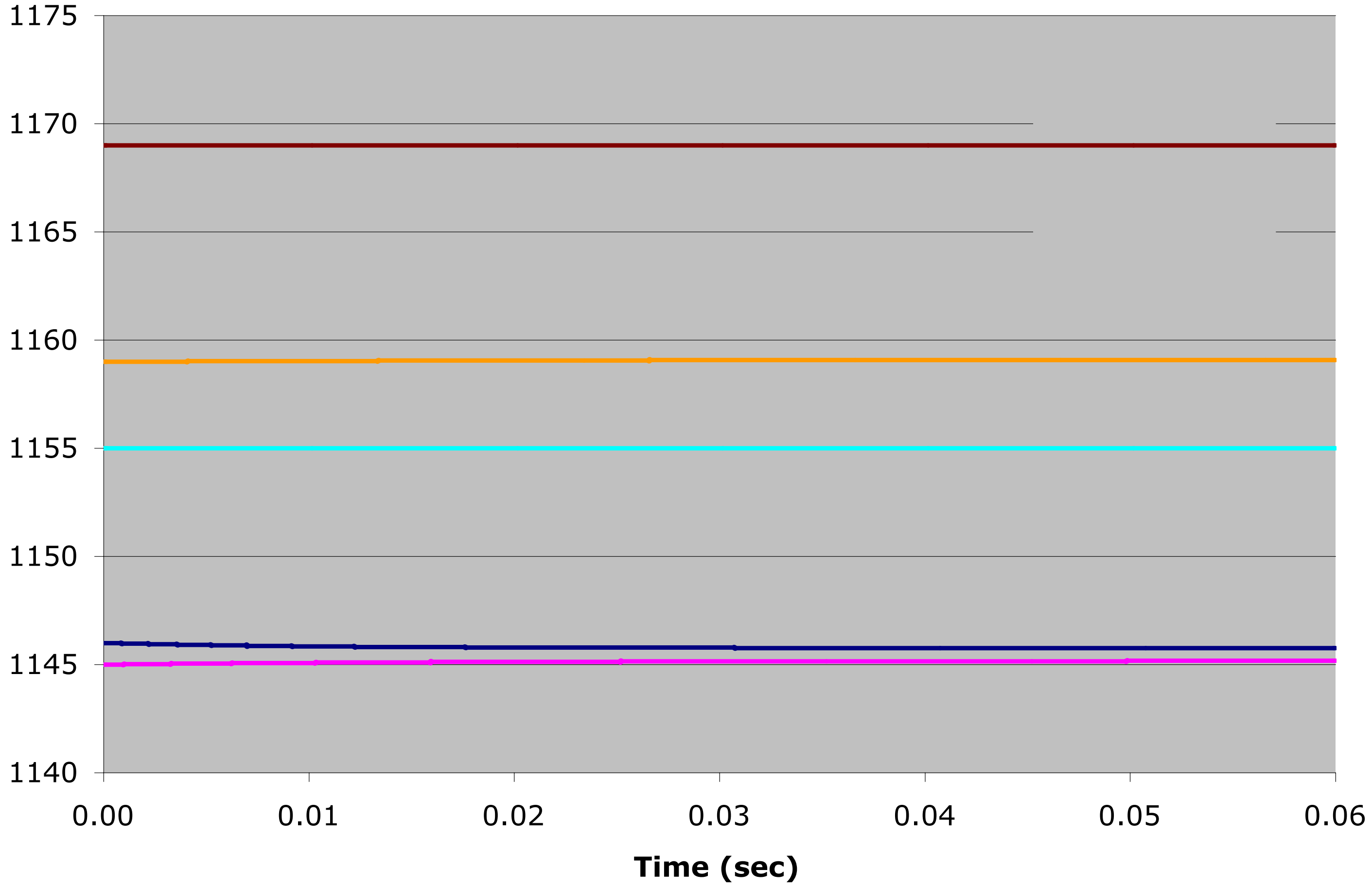
Current Response to Imposed Voltage



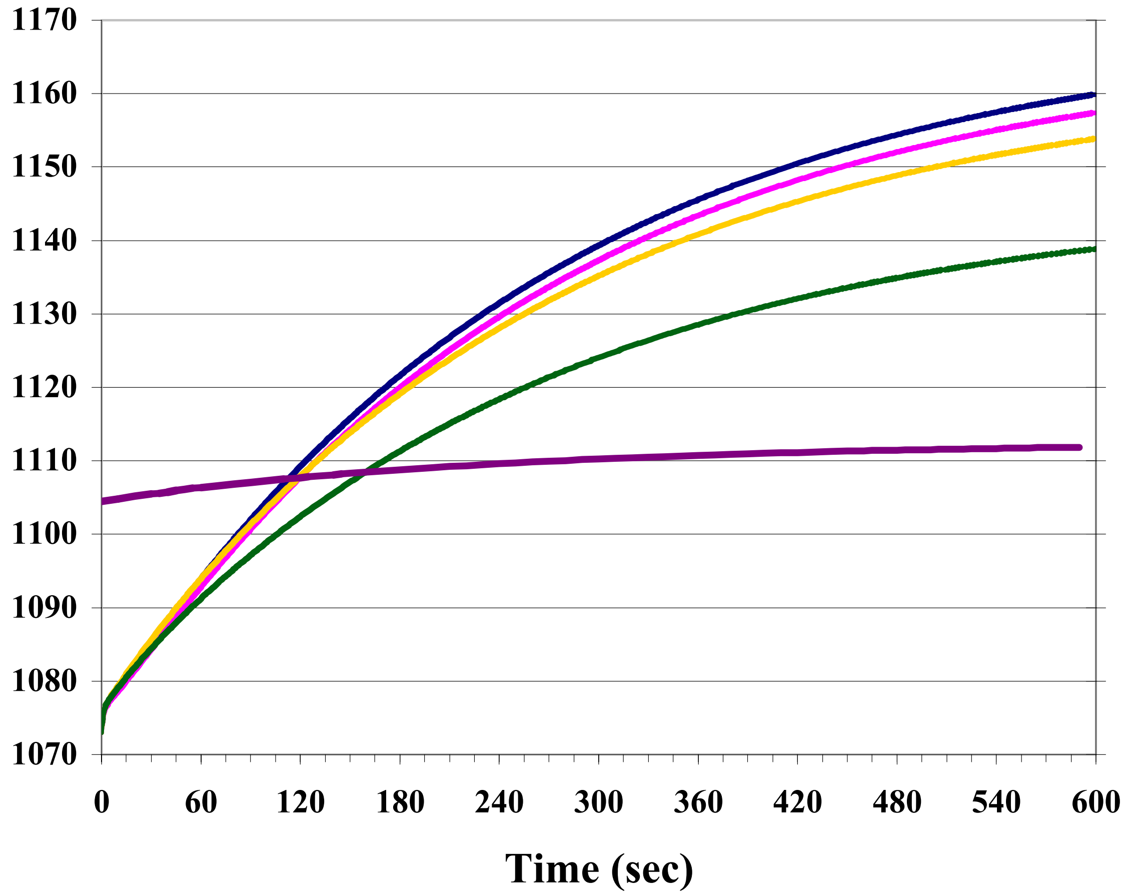
Interior Nodal Voltage Response



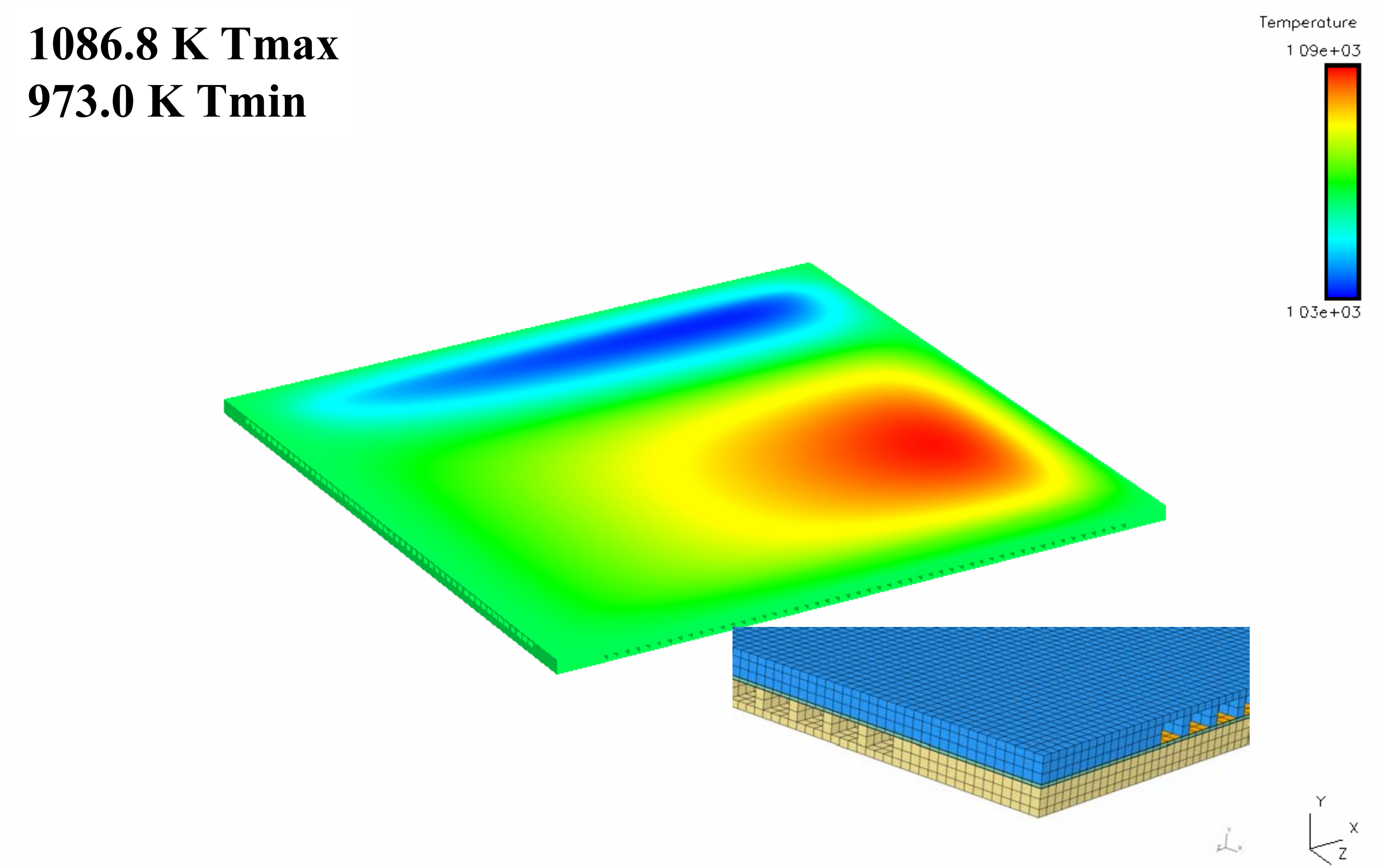
Negligible Thermal Response in 60 msec



Typical Step Load Thermal Response



Cross-Flow Temperature Distribution

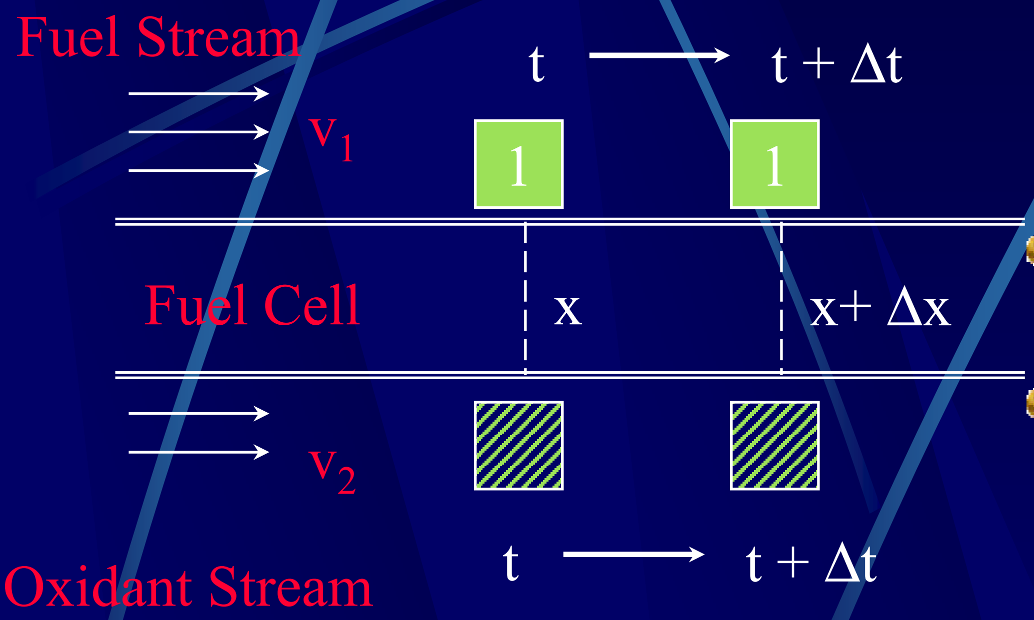


1086.8 K Tmax
973.0 K Tmin

Internal reforming
External radiation boundaries

Solid-Oxide Fuel Cell Modeling

Transient SOFC Response to Electrical Stimulus: Modeling Approach



Fuel Stream

$t \longrightarrow t + \Delta t$

v_1

1

1

Fuel Cell

x

$x + \Delta x$

v_2

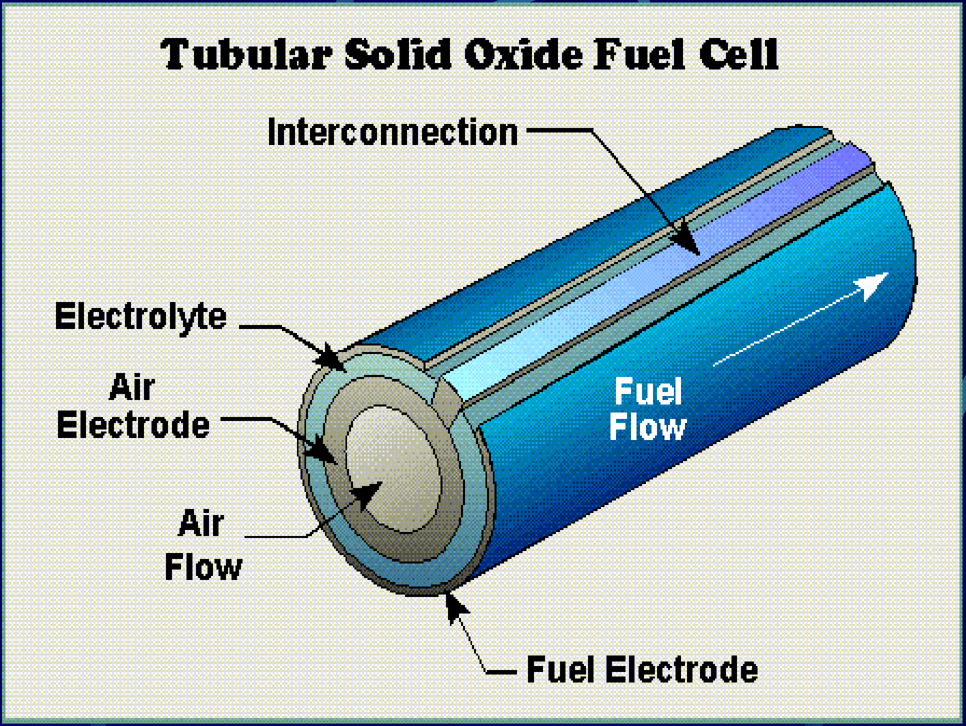
$t \longrightarrow t + \Delta t$

Oxidant Stream

- Reactants’ inlet flow rates and properties are invariant during relatively short transient episode
- Quasi-steady state electrochemistry
- Lagrangian extension of validated steady state model to track ***fuel*** parcels that travel over electroactive area

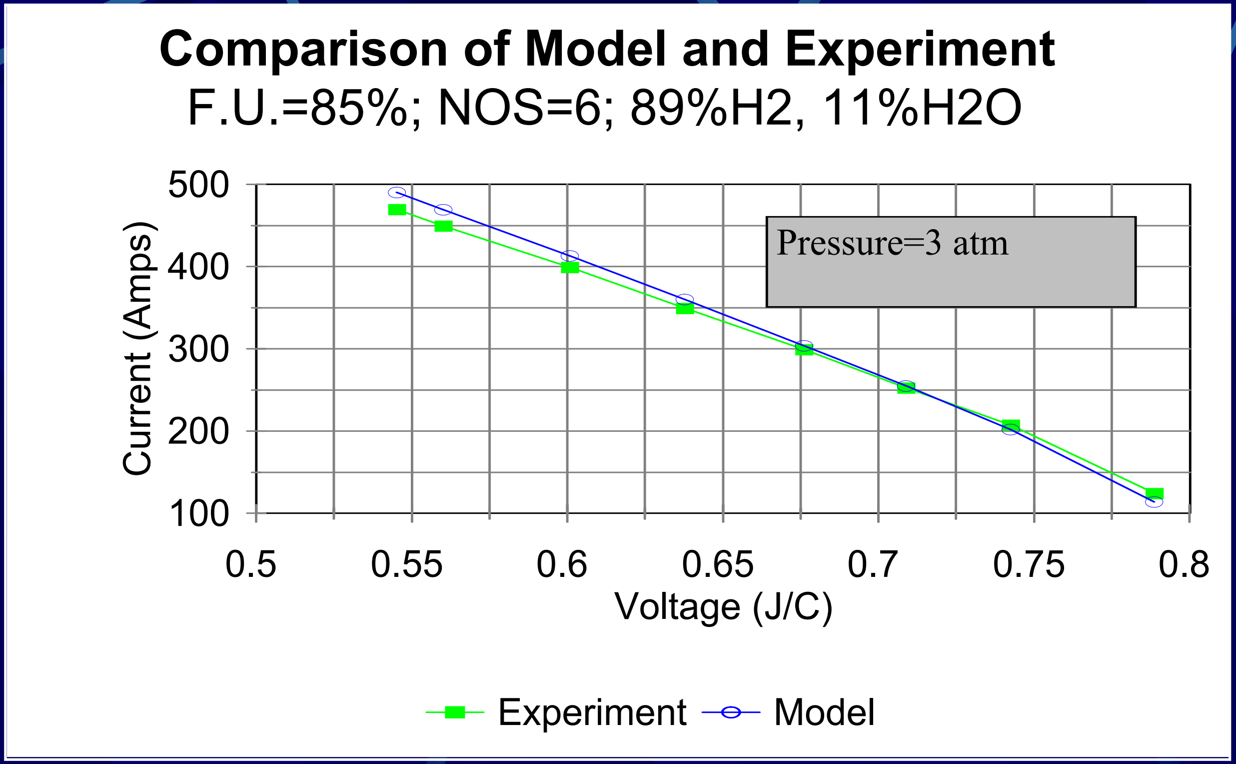
$$\eta_{element}(t+\Delta t) = \eta_{field}(x+\Delta x,\ t+\Delta t)$$

SOFC Example: SWPC TSOFC “Bundle”



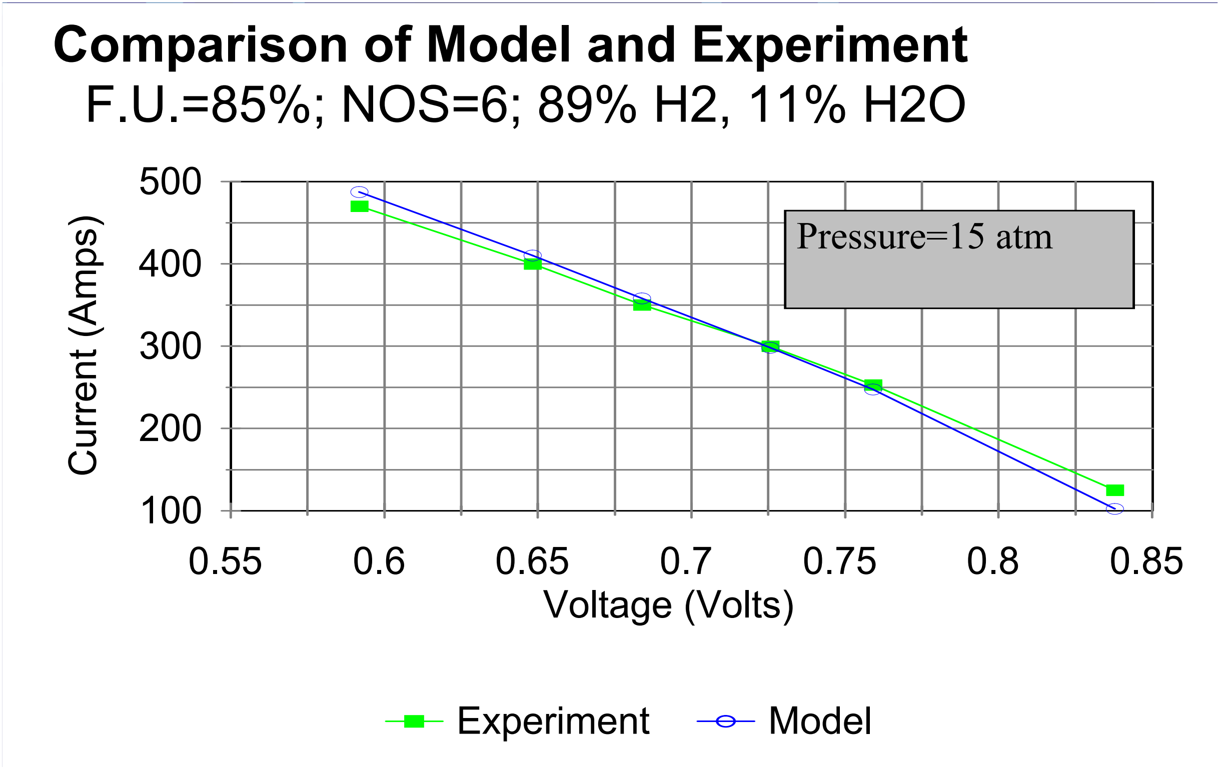
- 3 (parallel) x 8 (series) stack producing single-digit kilowatts
- Field tested
- Complementary simulation to the “flat planar” designs under SECA support
- Design with experimental data available limited extent

Steady-State Validation



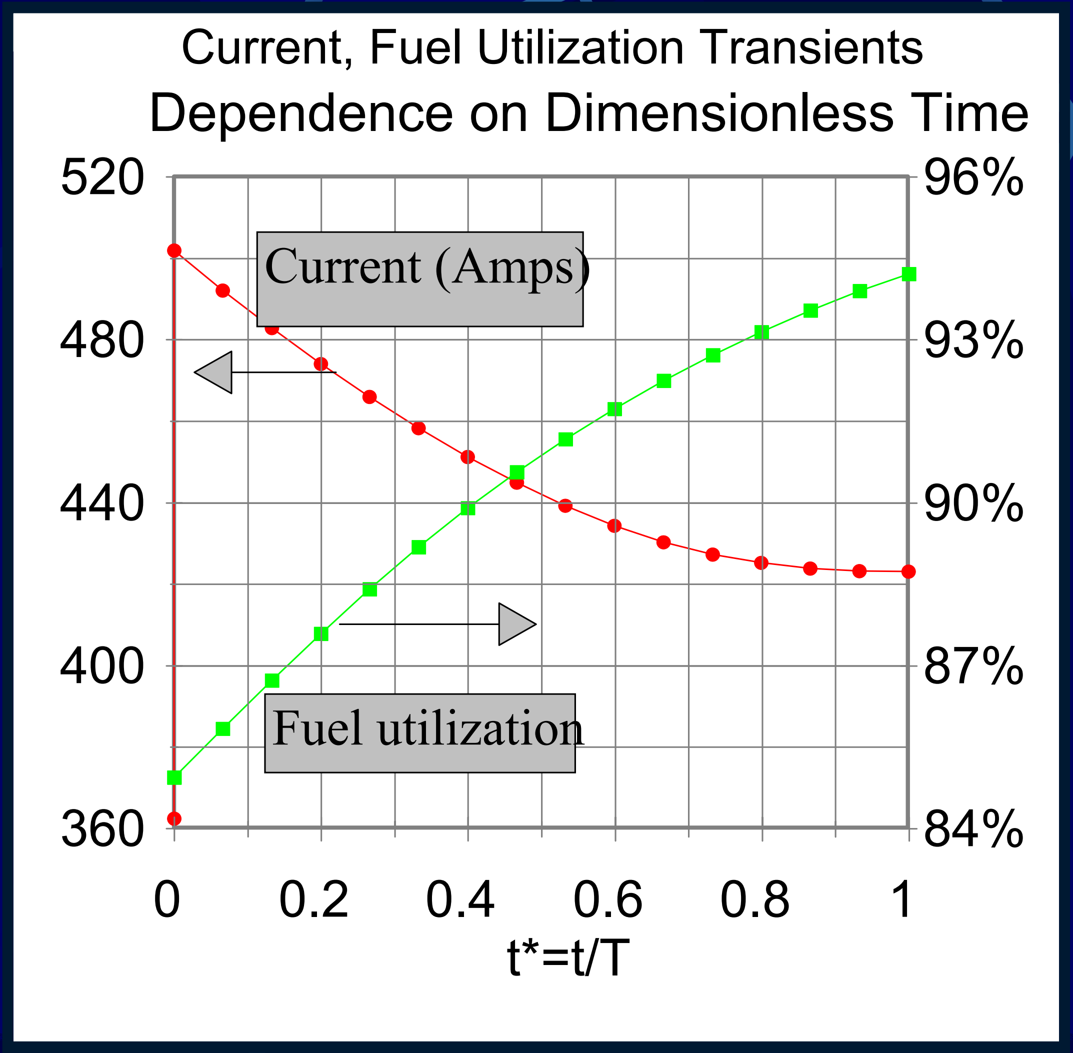
Accuracy to within 3-5%

Steady-State Validation: Cont.'d



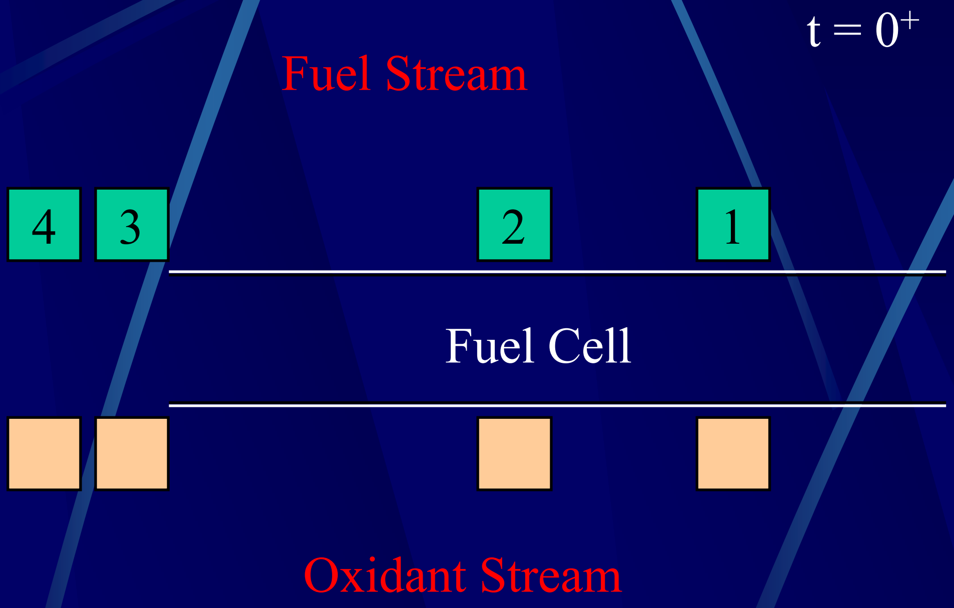
Accuracy to within 3-5%

Impact of Electrical Stimulus: Potentiostatic Control (Power Increase)



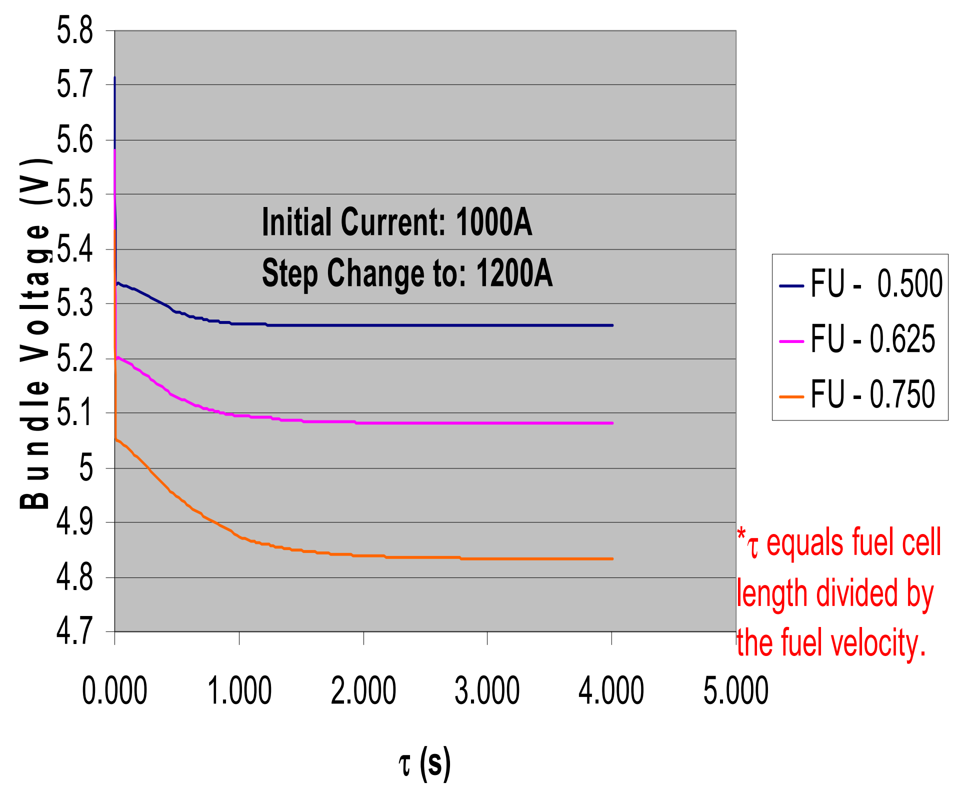
- Current spikes up, yet the fuel supply remains invariant due to the *decoupling* of the cell
- Fuel utilization thus increases; this causes current (and power) to decrease from $t^*=0^+$ values, until a new steady state "match" occurs at the new voltage ($t^*=1$)
- Attainment of steady state at the time constant $\{T=L_{cell}/v_{fuel}\}$

Impact of Electrical Stimulus: Potentiostatic Control (Cont.'d)



- Reactants' inlet flow properties are the same
- The fuel elements' exit properties depend upon their locations at $t^*=0^+$
- Steady state is regained when element 3 exits ($t^*=1$), because every successive element will then pass along the cell "seeing" only the new operating potential

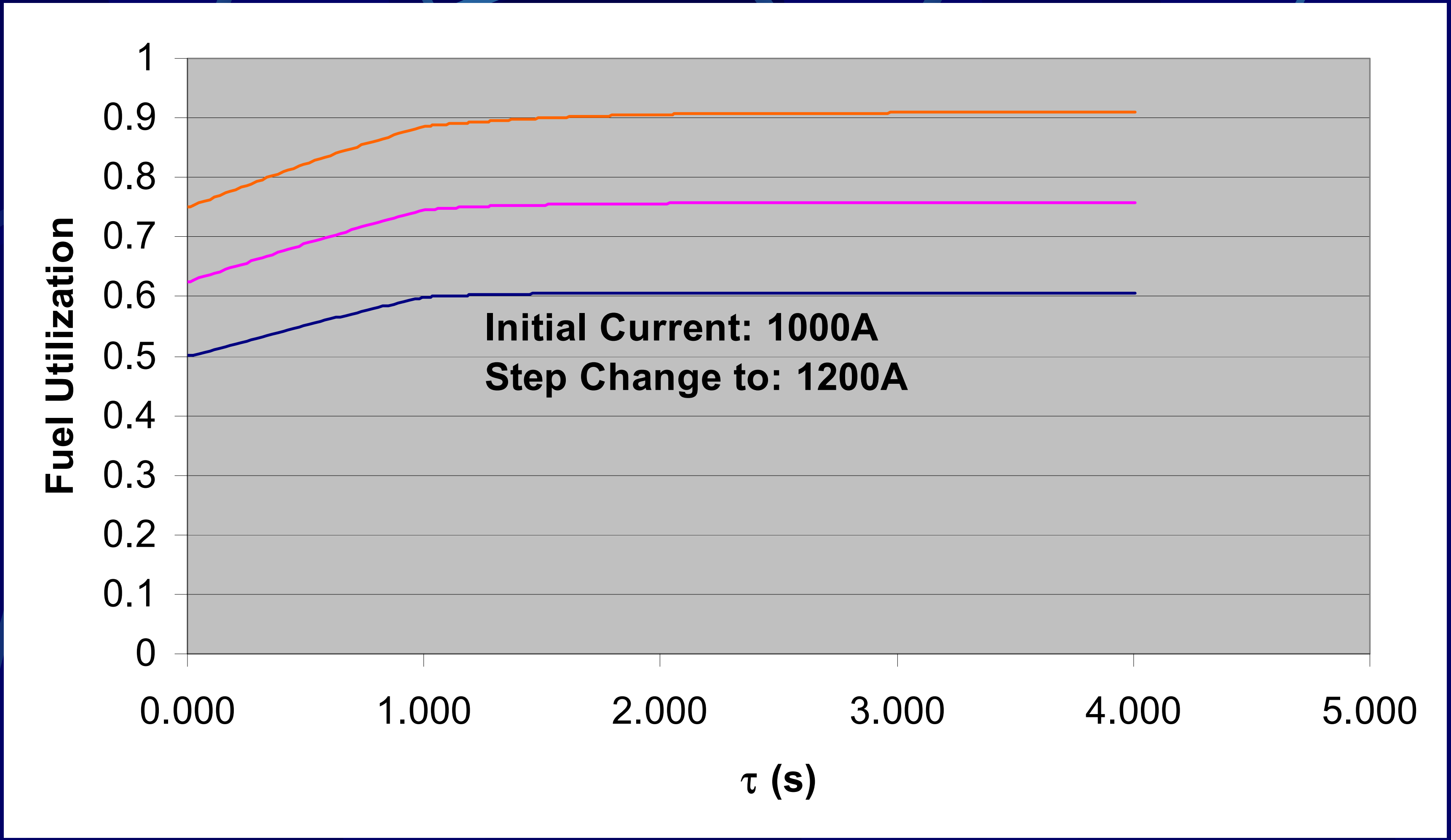
Impact of Electrical Stimulus: Galvanostatic Control (Power Increase)



*τ equals fuel cell length divided by the fuel velocity.

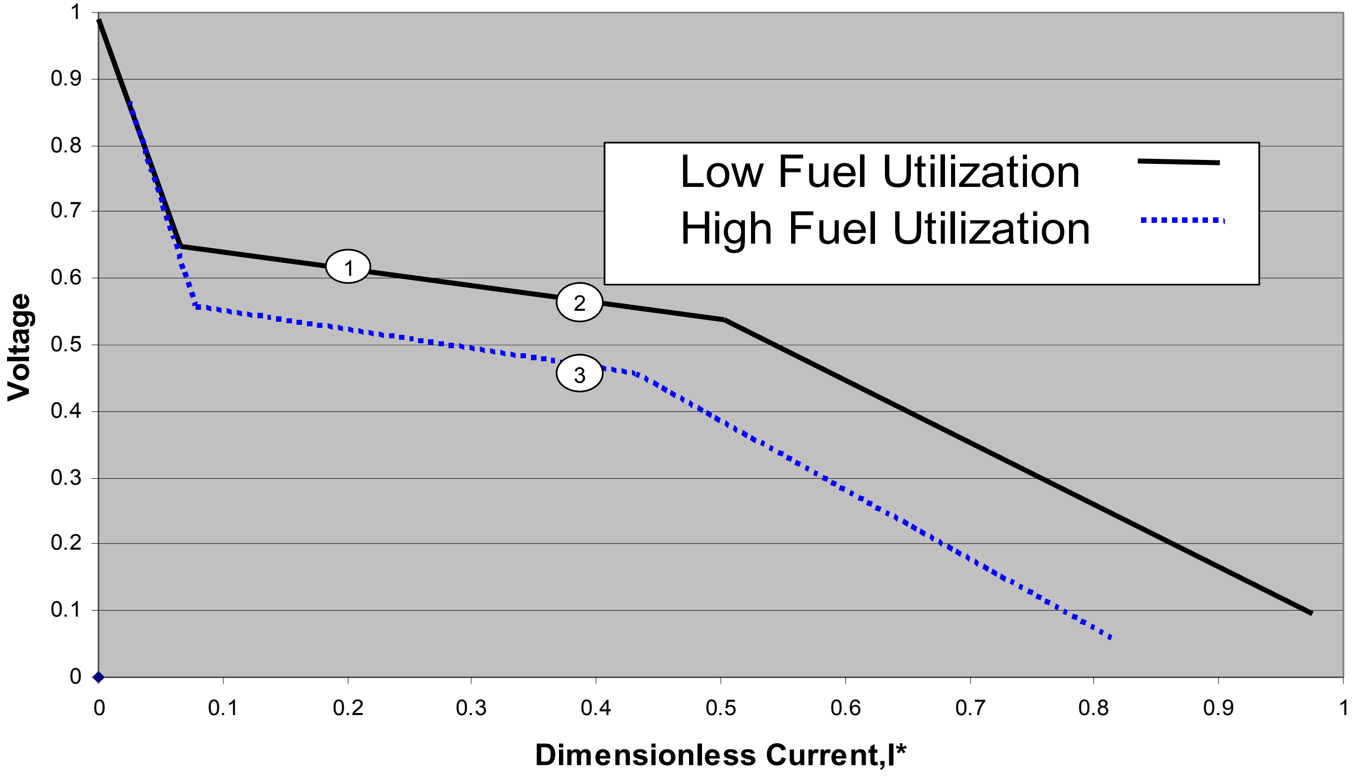
- Multiple voltage reductions are "seen" by the reactant streams
- Transient is thus longer by multiples of the time constant
- Larger initial fuel utilizations prolong the relative transient due to enhanced fuel depletion effects

Illustration of Respective Fuel Utilization Trends {20% Increases}

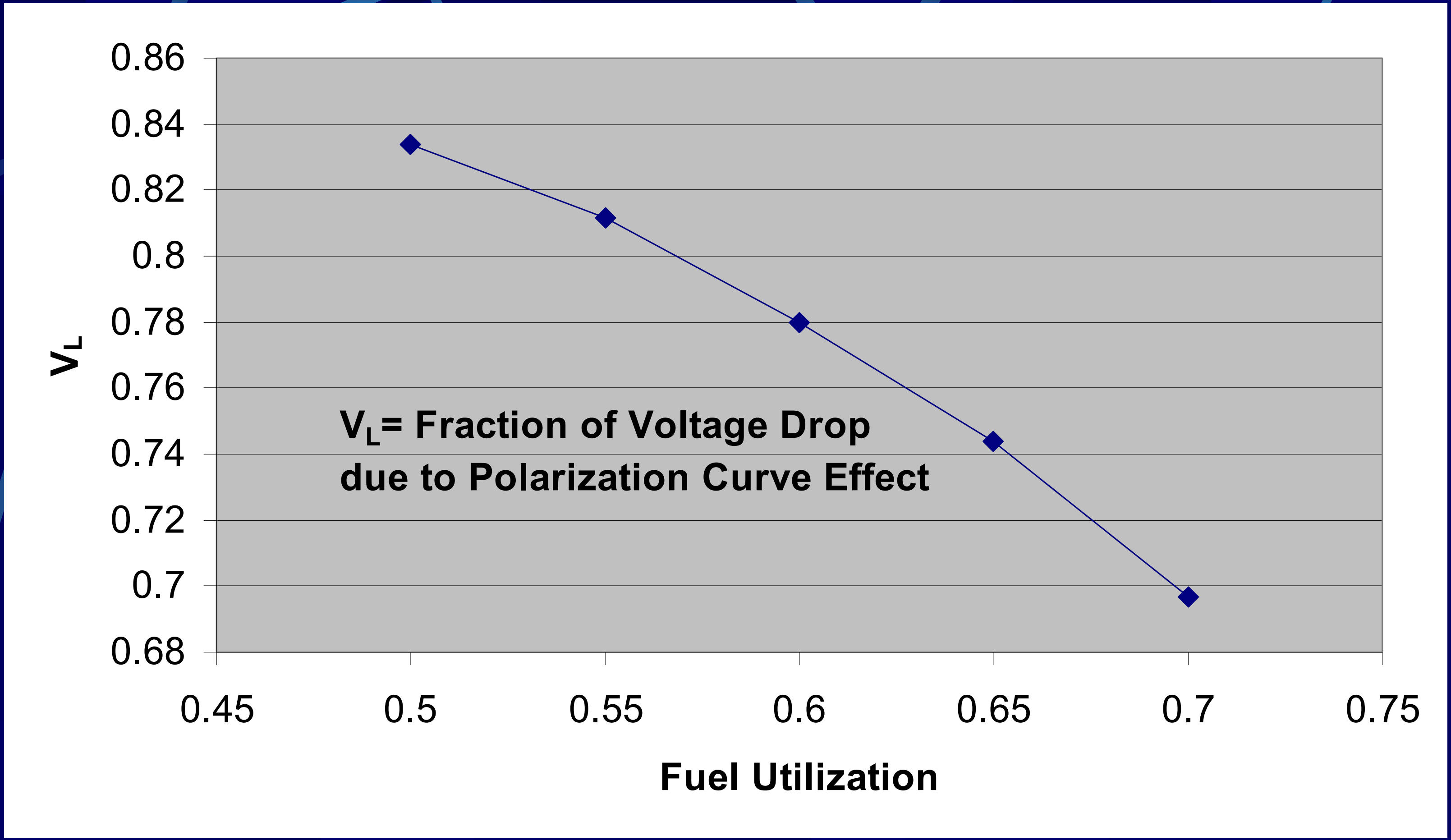


Initial Current: 1000A
Step Change to: 1200A

Dual Mode Potential Loss: Polarization Curve Effect & Reactant Depletion

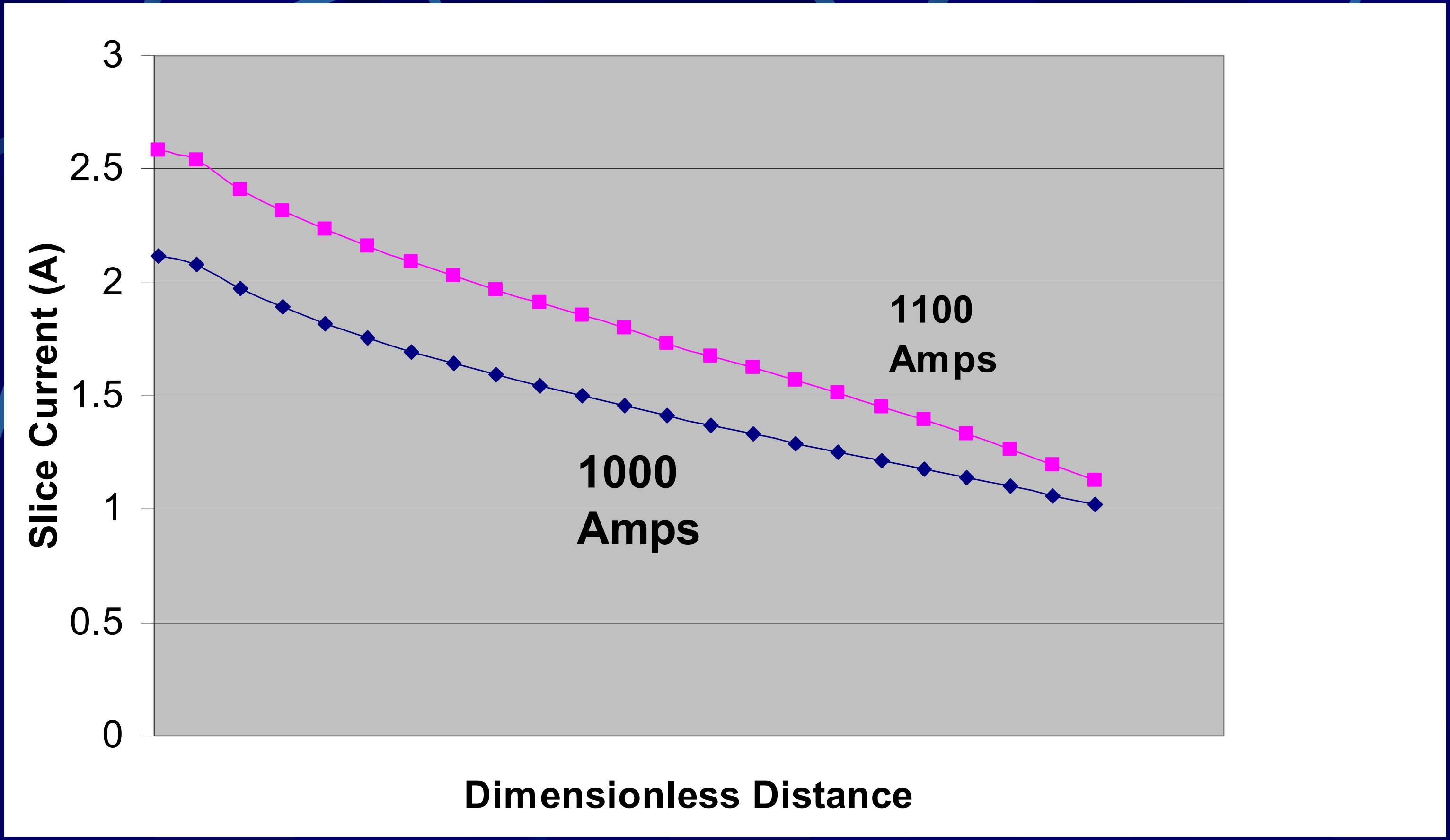


“Polarization Curve Effect” Less Dominant at Higher Initial Fuel Utilizations



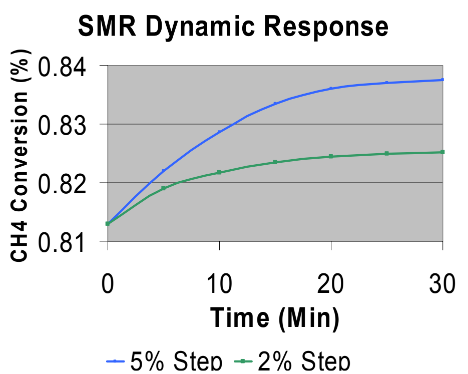
V_L= Fraction of Voltage Drop due to Polarization Curve Effect

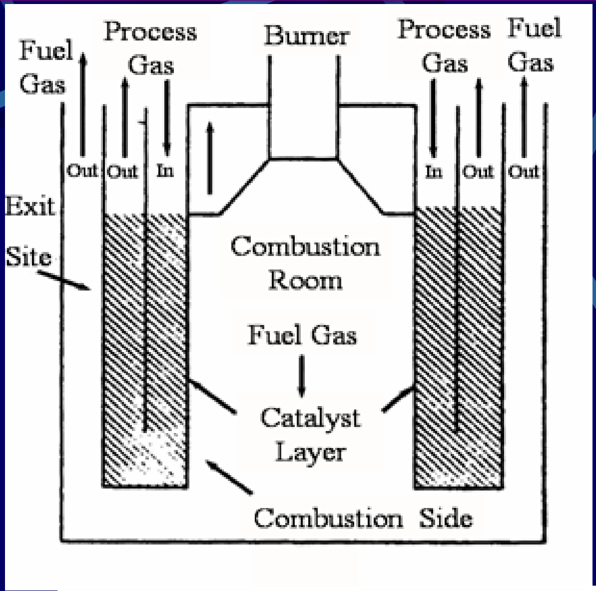
Variations in Current Density Distribution via Load Fluctuation



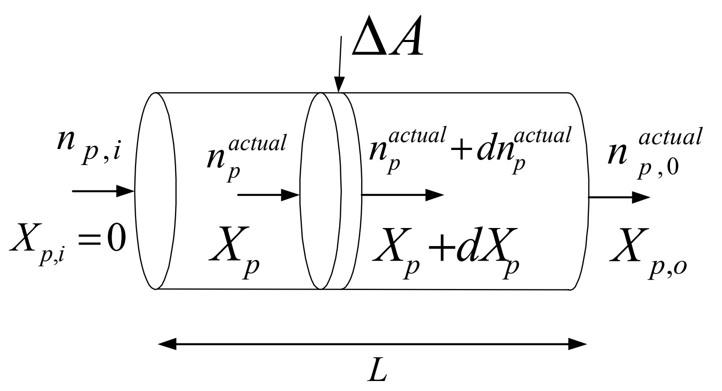
Balance-of-Plant System (BOPS)

SOFC Based APU: Steam Methane Reformer Component





The mass balance on a control volume



MODEL DESCRITION

Assumptions

- ➢Axial dispersion and radial gradient are negligible
- ➢Reforming and combustion gases behave ideally in all sections of the reactor
- ➢Gas flow pattern through the channels is plug flow
- ➢Demethanation and water gas shift reactions are kinetically controlled
- ➢Reaction kinetics are adequately described by a pseudo-first-order rate equation
- ➢Bed pressure drops are neglected
- ➢Uniform Temperature through each catalyst particle

MODEL PHYSICS AND DYNAMICS

SMR reaction:

$$CH_4 + H_2O \rightarrow 3H_2 + CO \qquad CO + H_2O \rightarrow H_2 + CO_2$$

SMR kinetics:

$$-r_{CH_4} = k_o^{SMR} \exp\left(-\frac{EA_{SMR}}{RT_{avg}^{SMR}}\right) P_{CH_4} \qquad L = \frac{n_{CH4,i}^{smr}}{\pi D_o} \int_{X=0}^{X=X_{CH4}} \frac{dX}{-r_{CH4}}$$

SMR dynamic mass balance:

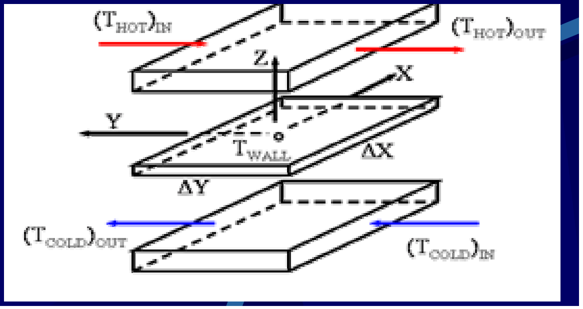
$$\frac{\partial(-vC)}{\partial z} - r_{CH4}e_B = \frac{\partial C}{\partial t}$$

SMR dynamic energy balance:

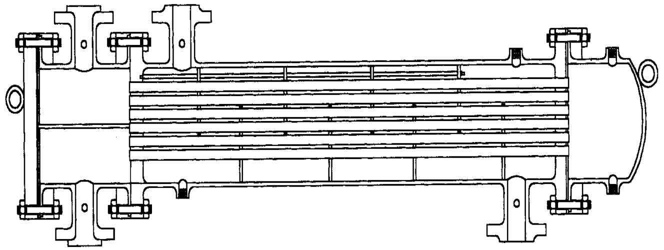
$$\frac{\partial(FC_pT)^2}{\partial z} + \sum_{i=1}^{2} F(-\Delta H)\frac{\partial X}{\partial z} + h_1 \pi d_i (T_w - T) + h_c A_c \frac{\pi d_i^2}{4}(T_c - T) = \frac{\pi d_i^2}{4} C_p \frac{\partial(\rho T)}{\partial t}$$

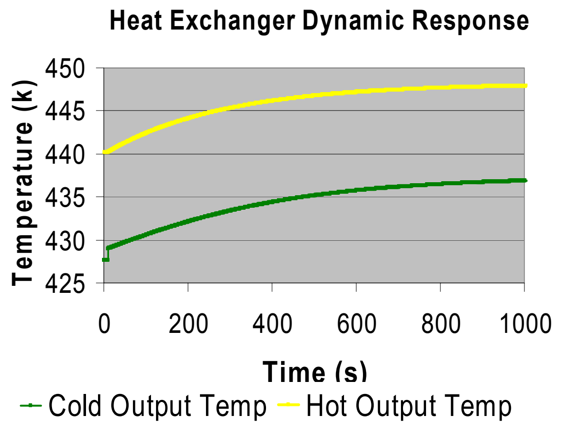
SOFC Based APU: Heat Exchanger and Steam Generator Components

COMPACT HX



STEAM GENERATOR





MODEL DESCRITION

➢Compact Heat Exchanger: Energy and mass balance are performed
  - ✓Plate-fin type with a single-pass, counter-flow arrangement
  - ✓One-dimensional flow
  - ✓Wall temperature in each section is a function of time only (spatially constant)
  - ✓Heat exchanger is adiabatic overall
  - ✓Heat transfer models based on Shah (1981) and Kays and London (1998)
  - ✓Effectiveness-NTU method applied in order to relate the geometric models to the thermodynamic ones
  - ✓Fluid thermal capacitance is negligible compared to the wall's

➢Steam Generator
  - ✓Cross-flow, shell-and-tube heat exchanger (single-pass shell and two tube passes)
  - ✓Consists of an economizer, an evaporator and a superheater
  - ✓Tube-side heat transfer coefficient: Correlation for fully developed laminar or turbulent flow for the economizer and superheater. Correlation of Kandlikar (1989) for the evaporator
  - ✓Shell-side heat transfer coefficient: Correlation suggested by Kern (1950)

MODEL PHYSICS AND DYNAMICS

Heat transfer:

$$\varepsilon = 1 - \exp\left[\left(\frac{1}{C_r}\right)(NTU)^{0.22}\left\{\exp\left[-C_r\,(NTU)^{0.78}\right]-1\right\}\right]$$

$$UA = \frac{1}{\dfrac{1}{(\eta_o Ah)_h} + \dfrac{1}{(\eta_o Ah)_c}}$$

$$NTU = \frac{UA}{C_{min}}$$

$$h = jGC_p Pr^{-2/3}$$

Energy Balance:

$$(mC_p)_h \frac{\partial T_h}{\partial t} - (wC_p)_h L_y \frac{\partial T_h}{\partial y} + (\eta hA)_h (T_h - T_W) = 0$$

$$(mC_p)_c \frac{\partial T_c}{\partial t} + (wC_p)_c L_y \frac{\partial T_c}{\partial y} + (\eta hA)_c (T_c - T_W) = 0$$

$$(mC_p)_W \frac{\partial T_W}{\partial t} = (\eta hA)_h (\overline{T}_h - T_W) + (\eta hA)_c (\overline{T}_c - T_W) = 0$$

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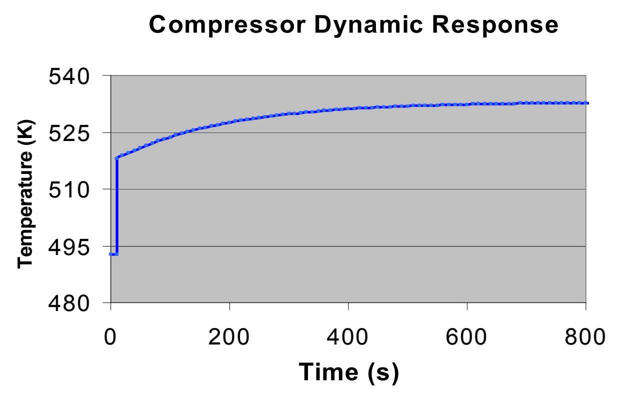
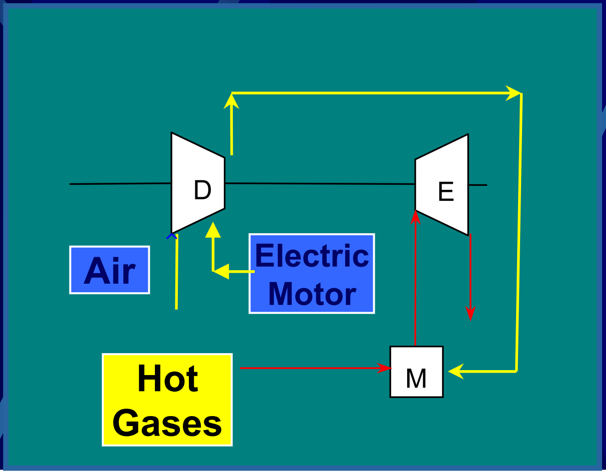
SOFC Based APU: Compressor and Turbine Components


Compressor Dynamic Response



MODEL DESCRITION

- Compressor/Expander
    - ✓Two energy balances performed to determine the input power required for a certain pressure ratio and percentage of that power recovered
    - ✓Heat transfer coefficient to the environment is constant
    - ✓The internal heat transfer coefficient is flow dependant and a function of the hydraulic diameter
    - ✓Performance maps for the steady state condition were used
    - ✓Thermal capacitance of the casing, impeller, and inlet ducts is approximated to a single thermal mode Tm

Heat transfer:

$$\Delta T_{Work} = \frac{T_1}{\eta_c}\left[\left(\frac{P_2}{P_1}\right)^{\frac{\gamma-1}{\gamma}} - 1\right]$$

$$\Delta T_{\dot{q}} = \frac{(hA)_1}{(W_2 C_p)}\left[\left(\frac{T_1+T_2}{2}\right) - T_m\right]$$

$$T_2 = T_1 - \Delta T_{\dot{q}} + \Delta T_{Work}$$

Energy Balance:

$$(mC_p)\frac{\partial T_m}{\partial t} = (hA)_1\left[\left(\frac{T_1+T_2}{2}\right) - T_m\right] - (hA)_o(T_m - T_{amb})$$

$$\frac{\partial N}{\partial t} = \frac{\Delta W_k}{I \cdot N}$$

$$\Delta W_k = W_{kt} - W_{kc} - W_{km}$$

- W_{kt} is the turbine power output, W_{kc} is the compressor power input, W_{km} is the mechanical loss

Latter Phase I/ Phase II Activities

- Expansion of transient performance modeling
  - Bridge the transient simulation algorithms to prototype/ pre-prototype "flat planar" SOFC modules
  - Simulate "real world" load following and fluctuations via superposition of step changes in electrical variables
  - Enhanced integration with balance-of-plant reactants supply and power conditioning subsystems

- Investigation of current ripple impact upon reliability
  - *Electrochemical* "fatigue"/degradation due to multiple charge-discharge cycles associated with current ripple
  - *Thermal* "fatigue" associated with oscillations in current density distribution

SOFC Based APU: Balance of Plant Sub-System (BOPS) Summary

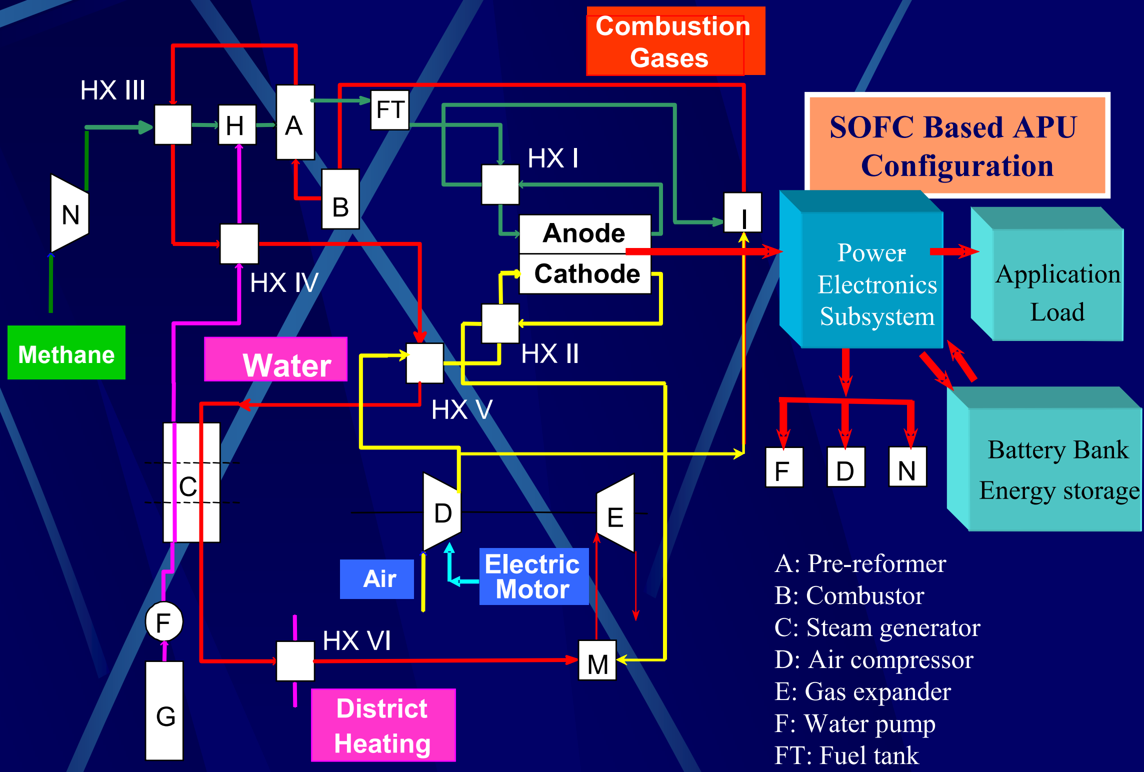
PHASE I : TRANSIENT MODELING OF THE SOFC BASED APU'S BOPS

TASKS ALREADY PERFORMED

- ➢Sub-system interactions definition (fuel cell stack, power conditioner, and balance of the plant).
- ➢Definition of BOPS and system configurations
- ➢Development of dynamic thermodynamic, heat transfer, and physical models for each component of the BOPS
  - ✓Compressor, expander, heat exchangers, steam generator, reformer, fuel storage
- ➢Implementation of models in a dynamic programming environment using state-of-the-arte transient numerical solver
  - ✓Compressor, expander, heat exchangers, reformer

TASKS TO BE PERFORMED

- ➢Implementation of models in a dynamic programming environment
  - ✓Steam generator, fuel storage
- ➢Integration of BOPS component models into a BOPS sub-system model
- ➢Integration of the PES, SOFCSS, and BOPS models
- ➢Analysis of system stability and dynamics
- ➢Parametric studies (trade-off analysis) of best-practice control strategies



A: Pre-reformer
B: Combustor
C: Steam generator
D: Air compressor
E: Gas expander
F: Water pump
FT: Fuel tank
G: Water tank
H: Pre-reforming mixer
I: Combustor mixer
M: Air-Comb gas mixer
N: Methane compressor
HXI: Fuel preheating HX
HXII: Air preheating HX
HXIII: Methane preheating HX
HXIV: Steam preheating HX
HXV: Air Recuperator
HXVI: District heating HX

PHASE II : SYSTEM CONTROL STRATEGIES

- ➢Application of large-scale optimization using decomposition
- ➢Determination of optimal control strategies based on their effects on system reliability, performance and response

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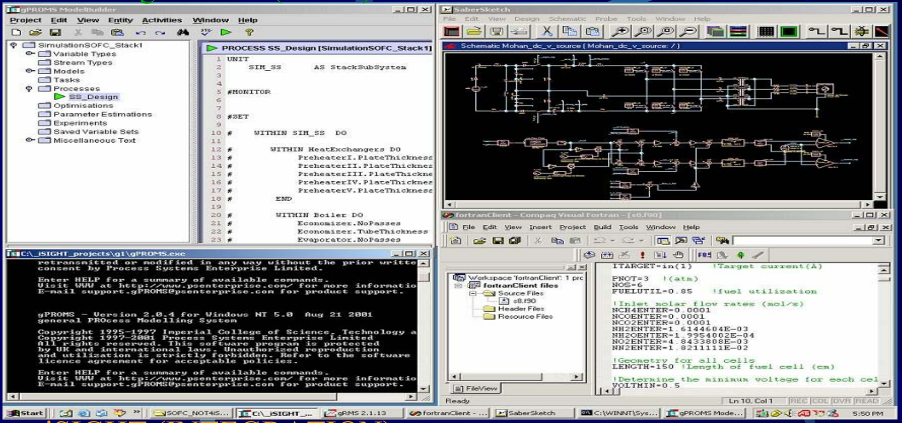
Summary: SOFC Based Power-Conditioning System

SOFTWARE SYSTEM INTEGRATION

gPROMS (BOPS) SABER (**P**ower-**E**lectronics **S**ystem)



```
UNIT
    SIM_SS       AS StackSubSystem


#MONITOR


#SET

#    WITHIN SIM_SS  DO

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

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

```
retransmitted or modified in any way without the prior writte
consent by Process Systems Enterprise Limited.

Enter HELP for a summary of available commands.
Visit WWW at http://www.psenterprise.com/ for more informatio
E-mail support.gPROMS@psenterprise.com for product support.


gPROMS - Version 2.0.4 for Windows NT 5.0  Aug 21 2001
general PROcess Modelling System

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licence agreement for acceptable policies.

Enter HELP for a summary of available commands.
Visit WWW at http://www.psenterprise.com/ for more informatio
E-mail support.gPROMS@psenterprise.com for product support.
```
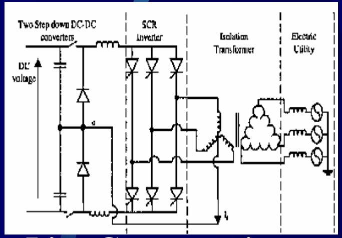
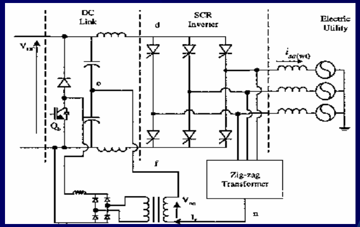

```
ITARGET=in(1)     !Target current(A)

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

!Inlet molar flow rates (mol/s)
NCH4ENTER=0.0001
NCOENTER=0.0001
NCO2ENTER=0.0001
NH2ENTER=1.6144604E-03
NH2OENTER=1.9954002E-04
NO2ENTER=4.8433808E-03
NN2ENTER=1.8211111E-02

!Geometry for all cells
LENGTH=150 !Length of fuel cell (cm)

!Determine the minimum voltage for each cel
VOLTMIN=0.5
```

iSIGHT (INTEGRATION) VISUAL FORTRAN (SOFC)

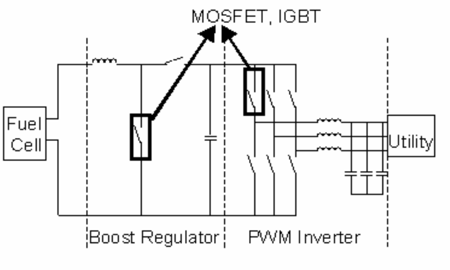
PES TOPOLOGIES



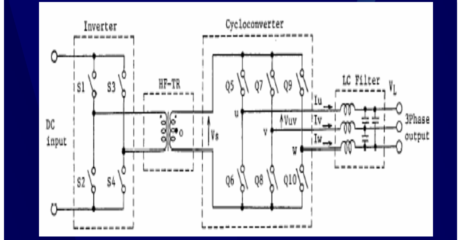
Line Commutation



Line Commutation



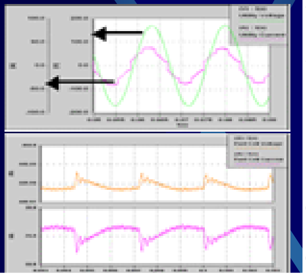
Self Commutation (PWM)

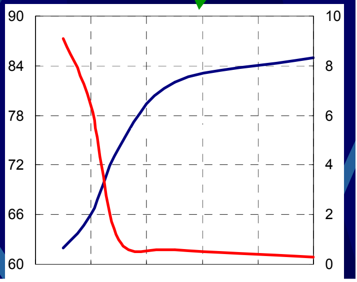


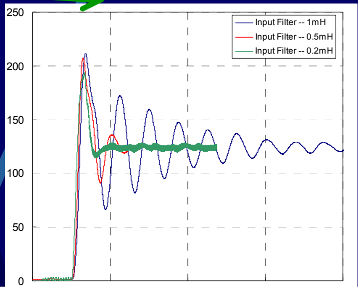
Transformer Assisted

(PES+SOFC) ANALYSES

Steady State **Parametric** **Transient**







PHASE I (Industrial Support: Synopsys Inc., Ceramatech, Engineous Software, PSE)
(Communication: Delphi, ORNL, IFC)

- Completed
  - Modeling of PES interfaces for stationary applications
  - Integration of PES and preliminary SOFC models
  - Multi-software platform integration
- In Process (and carry on to Phase II)
  - Integration of PES and SOFC models with BOPS model
  - Modeling of PES interfaces for non-stationary applications
  - Load profiling
  - Parametric studies and bifurcation analyses related to ripple dynamics
  - Impact of steady-state and transient ripple dynamics "for any given PES topology" on the current-density and thermal distribution inside a SOFC (with Ceramatech)
  - PES and BOPS control and energy-conservation techniques to alleviate the impact of load transients on SOFC

PHASE II

- Experimental validation of theoretical predictions to determine the accuracy of models and methods and predictions of analyses and control strategies
- System optimization (based on cost, durability, performance, and response): distributed control strategies, energy-conservation techniques, ripple dynamics for a given topology vs thermal and current-density distribution inside a SOFC
- Optimal PES for stationary and non-stationary application loads and experimental verification

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