SECA 2003 Core Technology Program Review Meeting

Model Tool Development & Application at NETL

a) NETL/Fluent Fuel Cell Model
b) Effects of Dynamic Loads on SOFCs

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Albany, NY

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Sponsor: SECA Program

DEPARTMENT OF ENERGY • UNITED STATES OF AMERICA

CFD Tools--Technical Issues

- **Success in the commercialization of SEC technology will depend on:**
  - – reducing manufacturing costs
    - Improve power density (~0.5 W/cm^2)
  - – producing a <u>usable</u> technology...
    - success in durability (>40,000 hours)
    - success in energy conversion efficiency
      - Manage flow distribution
      - Manage current distribution
      - Manage thermal stress distribution

- **One-Dim codes fine for performance prediction, but not “distribution design/management”.**

R&D Objective

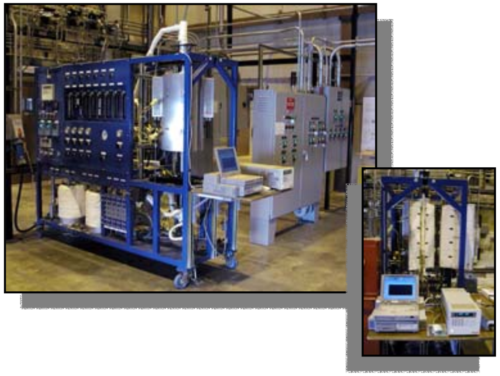
Develop modeling tools that can provide developers with detailed information on cell performance

to enable

design solutions for optimal performance and lifetimes

Approach

- **Develop and validate detailed fuel cell model**
  - Use commercial CFD code as underlying platform
    - FLUENT code is parallel, unstructured mesh, with well-validated models for fluid flow, heat transfer, species transport
    - Industry-accepted code already in use by SECA developers
    - Output compatible with ANSYS
  - Validate the code using experimental data
    - Single cell and cell stack data



Approach (cont.)

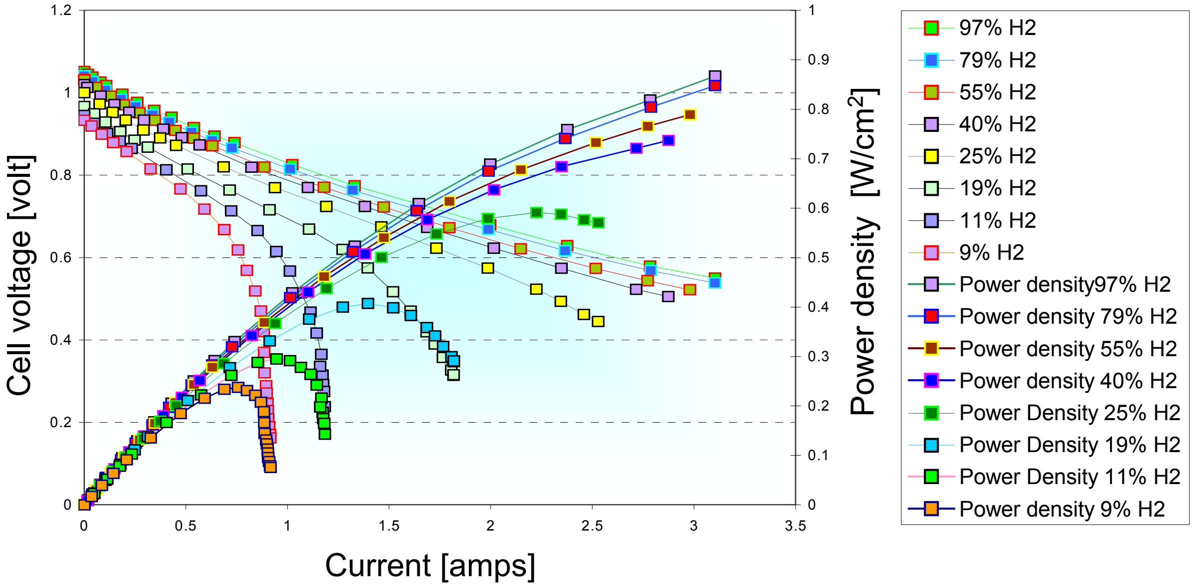
- **FLUENT handles all aspects of the hydrodynamics, species transport and heat transfer in the flow channels and the porous electrodes (anode and cathode).**
- **A User Defined Function (UDF) is used to model**
  - electrochemical reactions
  - potential field in the electrically conducting zones
- **The model is parallelized and shows identical scaling to normal Parallel FLUENT. The fuel cell model is only a small computation**
- **Includes treatment for CO/H2 electrochemistry**
- **The model has been tested for stack configurations**

Results

- **Electrochemical UDF code has been developed to provide electrochemical analysis suitable to**
  - analyze a wide range of fuel cell concepts
  - evaluate sensitivity to manufacturing tolerances and failure modes (e.g., effect of regional loss of connection b/t electrode and interconnects)

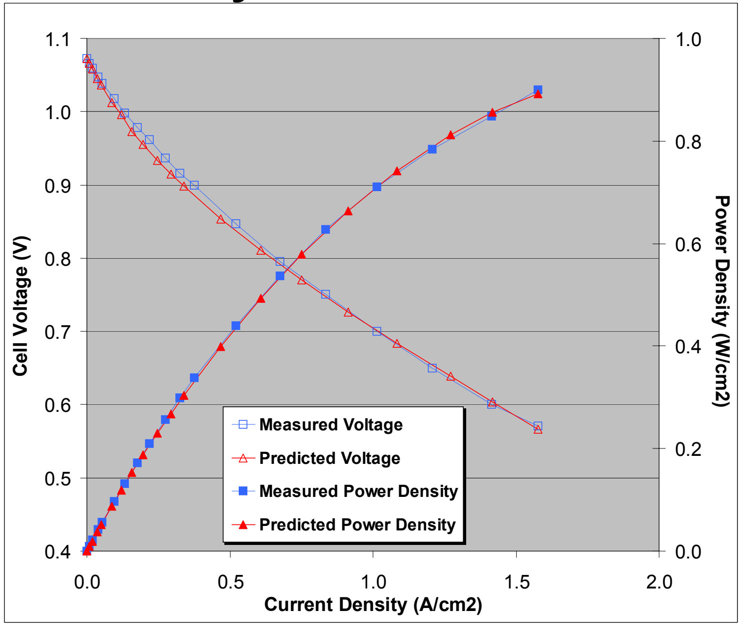
- **Tool now being validated using ‘standardized’ cells in collaboration with UoU.**

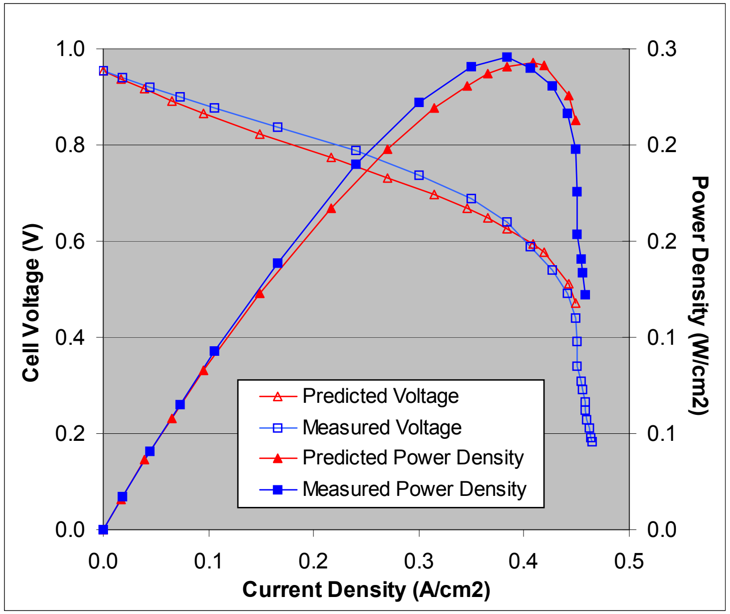
NETL Data: Standard Cell (UoU), 800C, varying fuel composition (H2, N2, H2O)



Productivity and Results

- **Preliminary Validation of model**

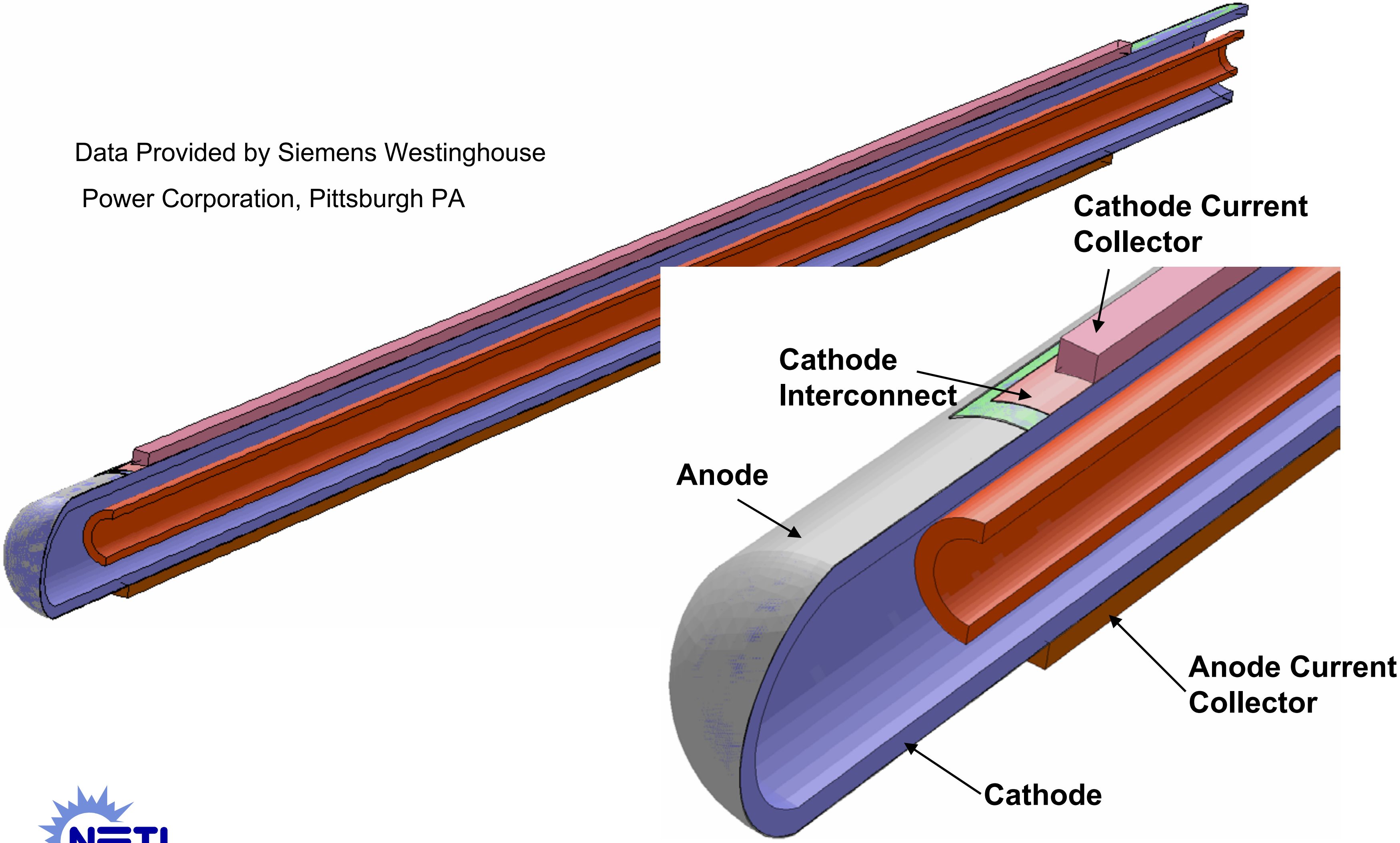




- **Standard Cell: 800C, 97%H2, 3% H2O**
- **Best fit with data:**
  - Electrolyte resisitivity = **1.9 ohm-m**
  - Cathode Exchange Current Density = **1000 A/m^2**
- **Data for varying electrolyte thickness will provide more accurate values**

- **Standard Cell: 800C, 9% H2, 3%H2O, Balance N2**
- **Best fit based on qualitative agreement with data:**
  - Tortuosity in both regions = **3.3**

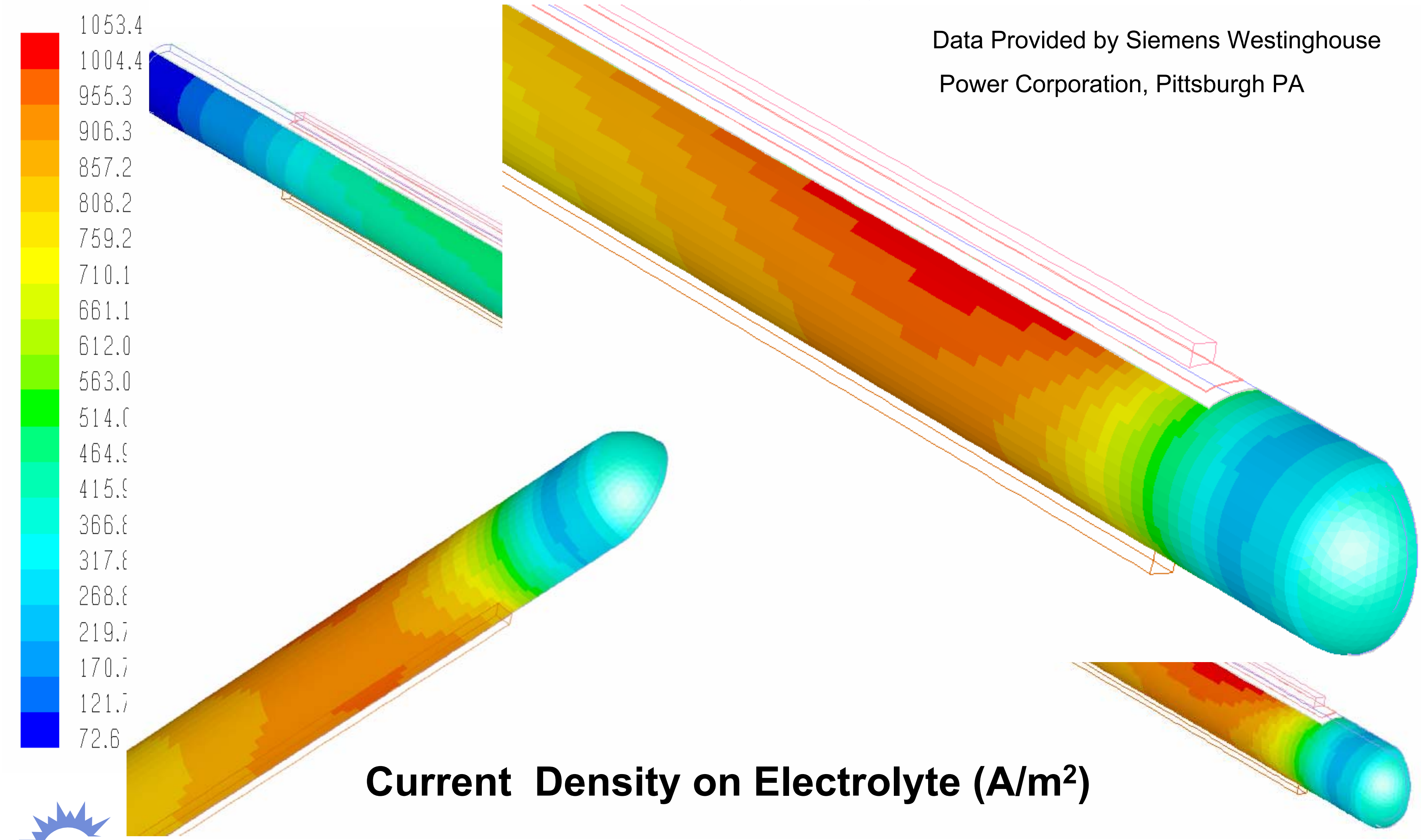
Results (cont.)



Data Provided by Siemens Westinghouse

Power Corporation, Pittsburgh PA

Results (cont.)

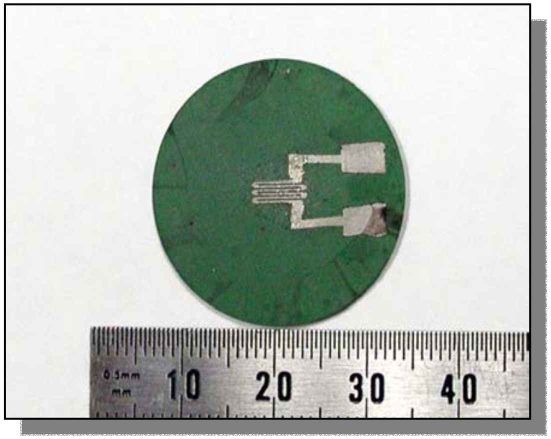


Data Provided by Siemens Westinghouse Power Corporation, Pittsburgh PA

Current Density on Electrolyte (A/m^2)

Other Related Results (cont.)

- **Sensors for Fuel Cell Diagnostics**
  - High-temperature thin film sensors to measure temperature, strain and heat flux
  - Sensors can be applied to fuel cell anodes and cathodes, embedded on electrolyte, or applied to stack hardware such as seals and interconnects
  - Measure fuel cell strain
  - Measurements can be used for stress and temperature model validation



URI strain gage applied to SOFC anode

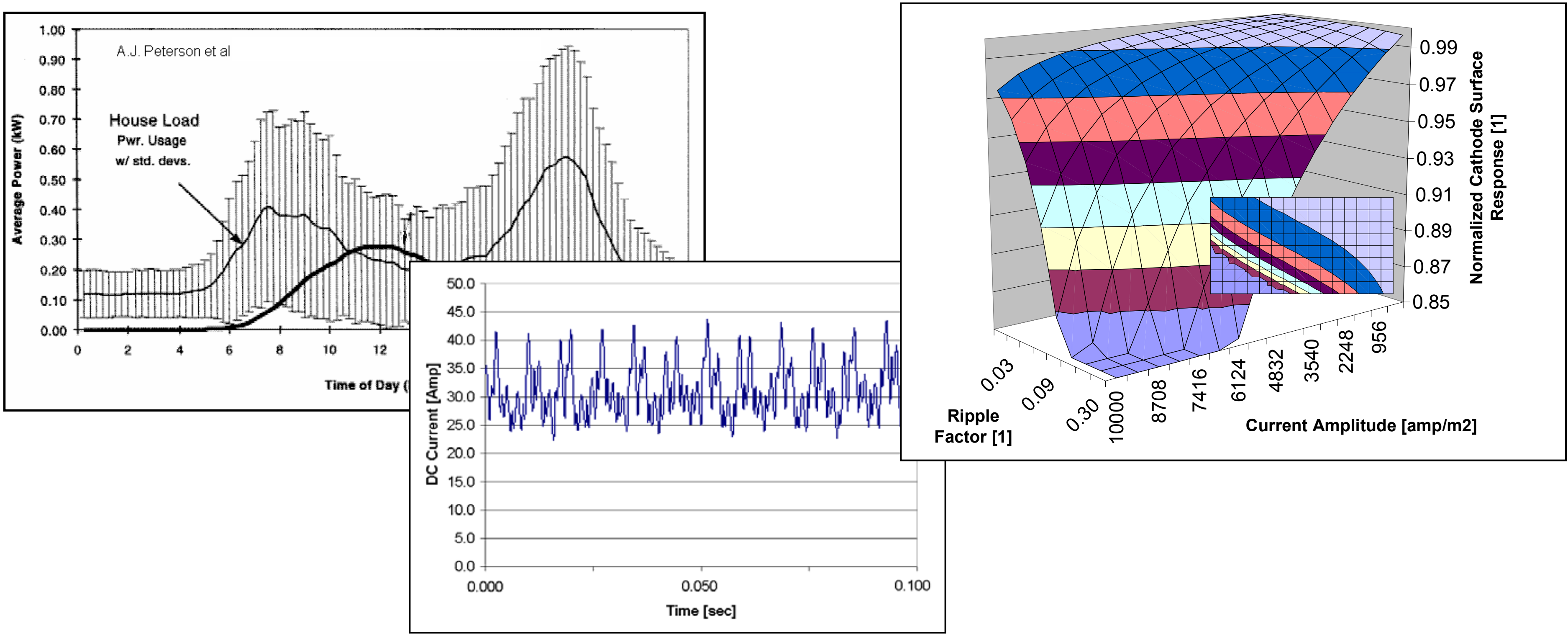
Applicability to SOFC Commercialization

- Providing basic engineering tools suitable for detailed cell and stack analysis.
- Capability enables fuel cell designers to better predict and manage flow, current and temperature distributions.

FY04 Work Plans

- **Continued Validation (Q1-Q4/FY04)**
  - NETL data (button and full-size cells)
  - SW data
  - UTRC data
- **Transient Application of SOFC Model (Q1/FY04)**
- **Release to SECA Vertical Teams (Q2/FY04)**
- **Internal Reforming Model (Q2/FY04)**
- **Link NETL SOFC Model with ANSYS (Q3/FY04)**
  - validation
  - application

Dynamic Analysis

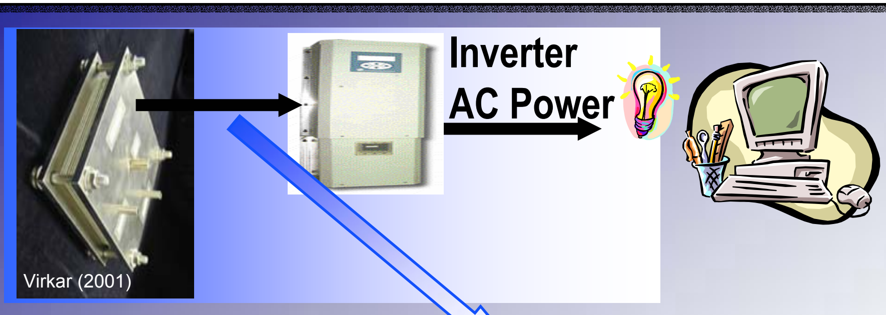


Technical Issues

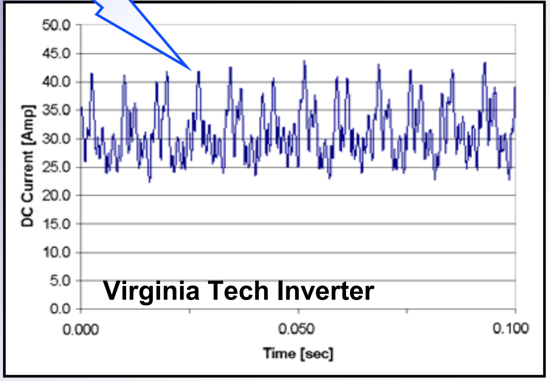
- **Success in the commercialization of SECA technology will depend on:**
  - reducing manufacturing costs
  - producing a usable technology...
    - success in durability (>40,000 hours)
    - success in energy conversion efficiency
    - success in managing dynamics
      - less than XX minute startup (pick a number!)
      - safe and failure-free shutdown
      - load transients
      - …

Technical Issues (cont.)

Power Conditioning Induced Load Dynamics



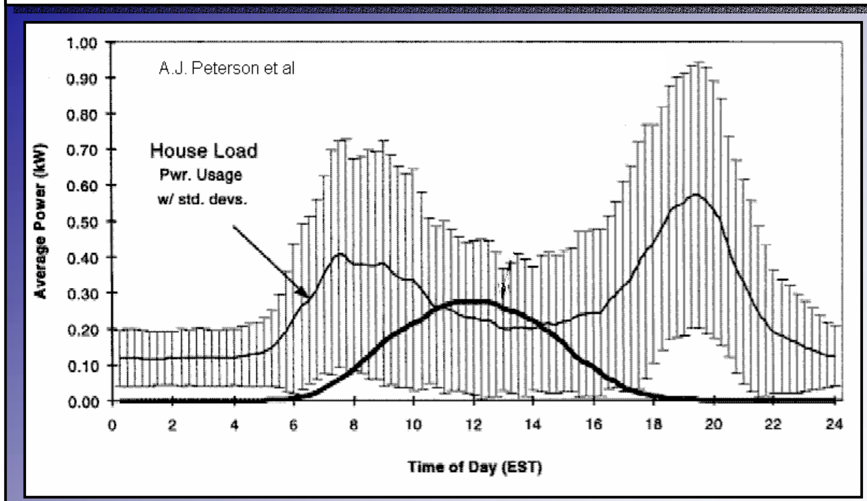
Lesster (2000) filtering for low ripple is costly.



Research questions:

- how do dynamic loadings compare to steady?
- at what amplitude/cut-off frequency will such oscillatory loadings have negligible impact?

Application Induced Load Dynamics



- Commonly use fast energy storage device (batteries)
- Minimize system cost (e.g., batteries) by allowing fuel cell load dynamics

Background (cont.)

- A literature search on *fuel cell dynamics* yields little helpful information.
- Dynamic concerns at the cell level have not yet been addressed.
- Riso Nat. Lab studied impacts of steady loading on degradation. Jorgensen et al. (2000) indicate current loading causes degradation in cell materials.
- Degradation mechanisms (steady or non-steady loaded) not clear, Badwal (2001).
- Most prior transient studies focused on cell thermal behavior under heat-up, or employed simple lumped models for system studies (no detailed and coupled electrochemistry).

Technical Investigations

- **Transient loads**
  - Application load driven
  - Inverter driven
- **Experimental**
  - Button cells
  - 10cmx10cm cells
- **Modeling**

- **Understanding to be acquired**
  - Details of cell operation
    - Y(x,y,t)
    - T(x,y,t)
    - $\sigma(x,y,t)$
  - Deviation in behavior from steady-state loads

Technical Challenges for Investigating Effects of Dynamic Loads

- **Need improved understanding on resultant transient behavior in and around PEN to improve durability.**
- **Detailed electrochemical codes not ready for transient studies.**
- **Detailed transient studies can be time consuming.**
- **SOFC test conditions are challenging.**
- **Long duration tests often required to assess degradation.**
- **Reliable experimental results/conclusions require repeatability in specimen fabrication and test setup.**
- **Identifying correct degradation mechanisms is not easy even for steady-state loads.**

R&D Objective

Understand the impact of dynamic loads on the cell level reactant histories, thermal transients, component stress, and fuel cell degradation

to enable

design solutions for optimal startup and lifetimes

Technical Approach

- **Modeling**
  - Goal: Identify impact of dynamic loads on species concentration and temperature changes to help quantify deviation from SS loads
  - Apply existing (NETL developed) one-dimensional models
    - Investigate spatial transient behavior over a cell (cell performance model)
    - Investigate electrode response due to ripple (electrode transport model)
    - Guide experimental analysis by providing estimates for experimental load conditions

Technical Approach (cont.)

- **Experimental**
  - Work with external partners to acquire ‘standardized’ button cells (repeatable fabrication, well characterized). UoU-button.
  - Use existing SOFCEL facility to run both steady-state (baseline) and dynamic (20-30% ripple) loadings.
  - Apply AC impedance and galvanostatic/potentiostatic techniques to identify performance changes.
  - Consult with materials experts to help with materials measurements and identifying material degradation mechanisms (PNNL, ORNL):
    - SEM - identify material structural changes
    - XRD - material phase changes
    - XPS – material phase changes

Technical Approach (cont.)

- Results published in conference and journal articles.

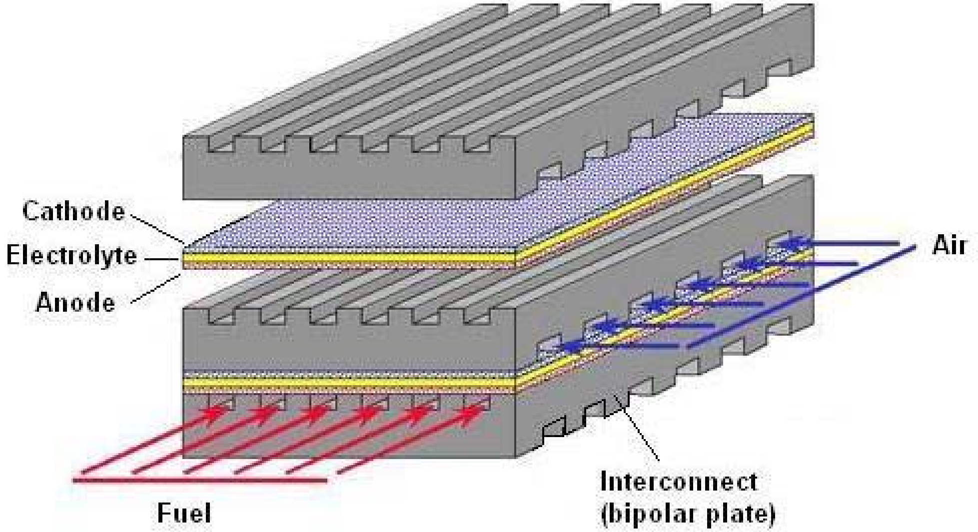
Results

- Applied existing Electrode Model and Cell Models to help begin understanding transient issues for SOFC technology.

- Journal article (Gemmen (2003))
- Conference presentation (Gemmen et al. (2003))

10cm x 10cm Cell Dynamic Model

- **Based on 1-D code**
  - Liese, Gemmen et al. (1999)
- **Fully coupled electrochemistry and flow (V, T, species, i’’)**
- **Cross Flow Geometry**
  - Anode supported
  - 8 x 8 channels



- **Active Area: 10cm x 10cm**
- **Nominal Steady Load Conditions**
  - Cell voltage=0.77 volt
  - Current density=0.74A/cm^2
  - Power=0.57W/cm^2
  - Temperature=860^{o}C
  - FU=0.81
  - AU=0.11

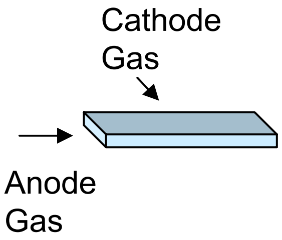
- **Cases studied**
  - 0) Load change (incr./decr.)
  - 1) Idle (no load) to Steady State Load
  - 2) Introduce Ripple following Steady State Condition at 1
  - 3) Unload event

Case 2: Ripple Case

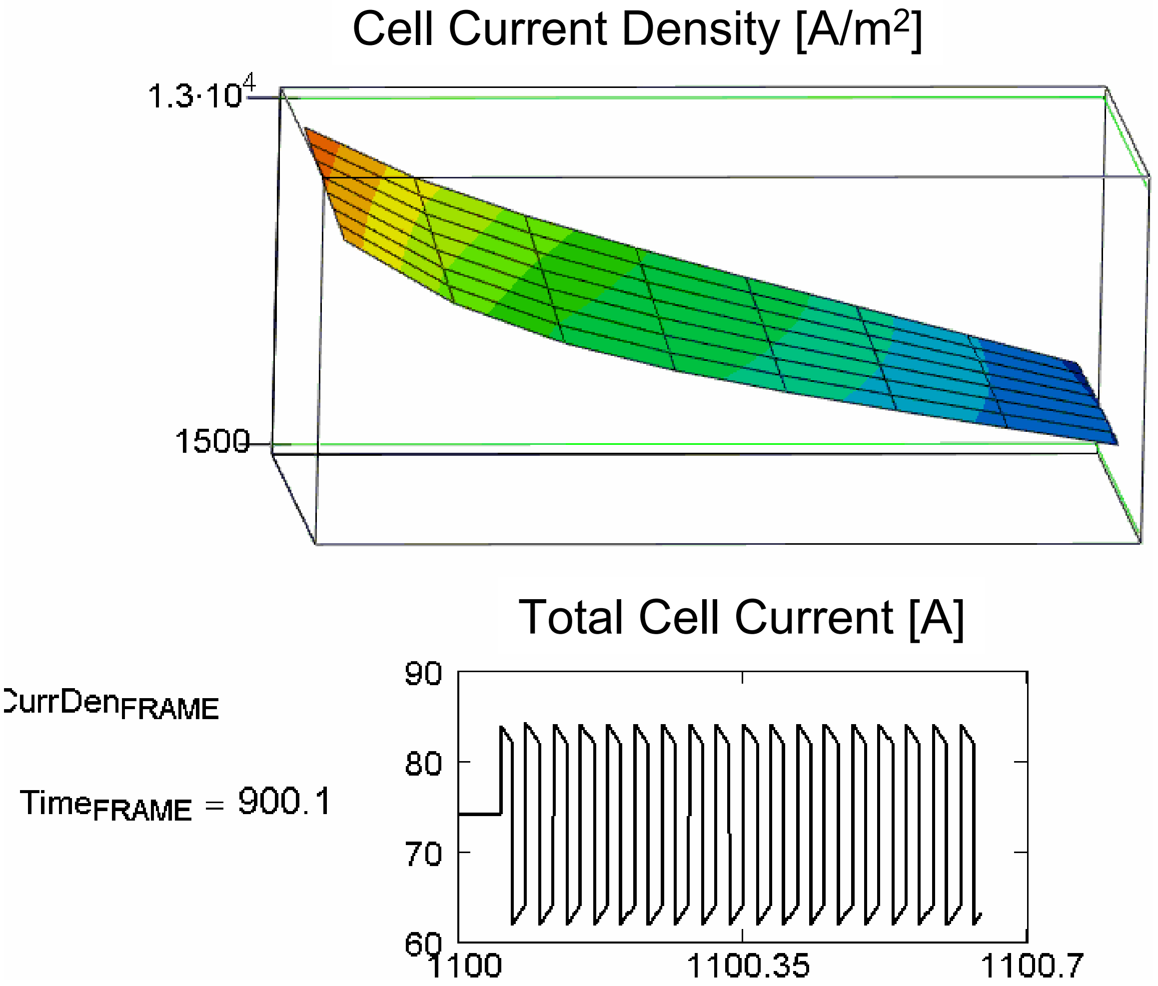
- **Following Steady State Load…Impose Ripple**
  - Voltage controlled (0.77+/-0.015)

Case 2: Cell Current Density

(10cm x 10cm; 30Hz Ripple; voltage driven; 8x8 nodes)

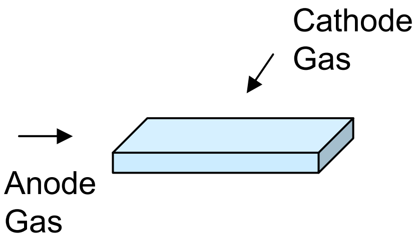


- **Current density response due to ripple is nearly uniform over cell, with minor asymmetric secondary response.**

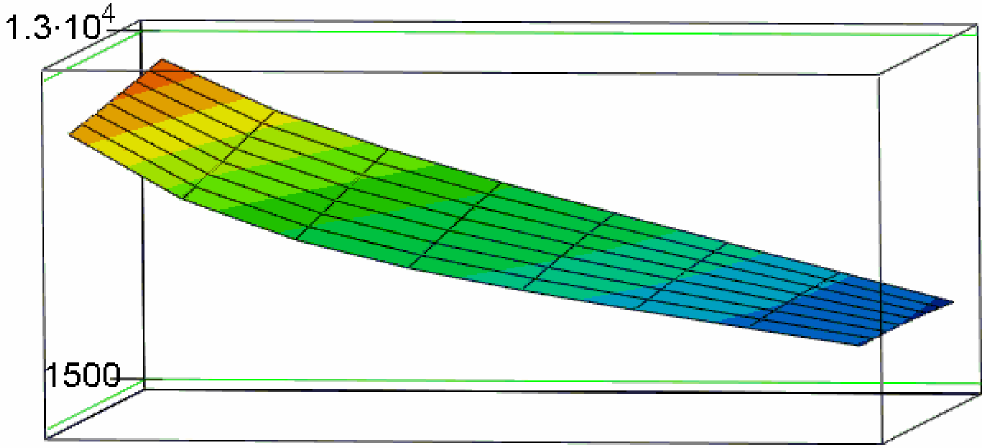


Case 2: Cell Current Density

(10cm x 10cm; 120Hz Ripple; voltage driven; 8x8 nodes)



Cell Current Density [A/m^2]

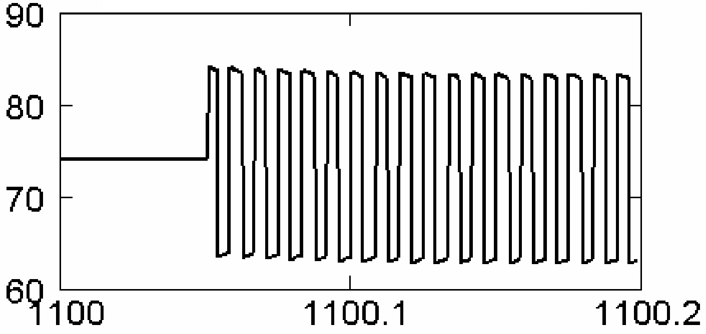


- **120Hz case similar to 30Hz case, with slightly weakened secondary.**

urrDen$_{\text{FRAME}}$

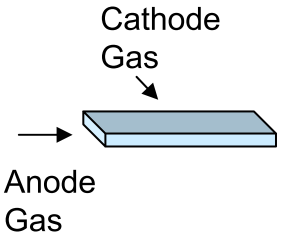
Time$_{\text{FRAME}}$ = 900.100

Total Cell Current [A]

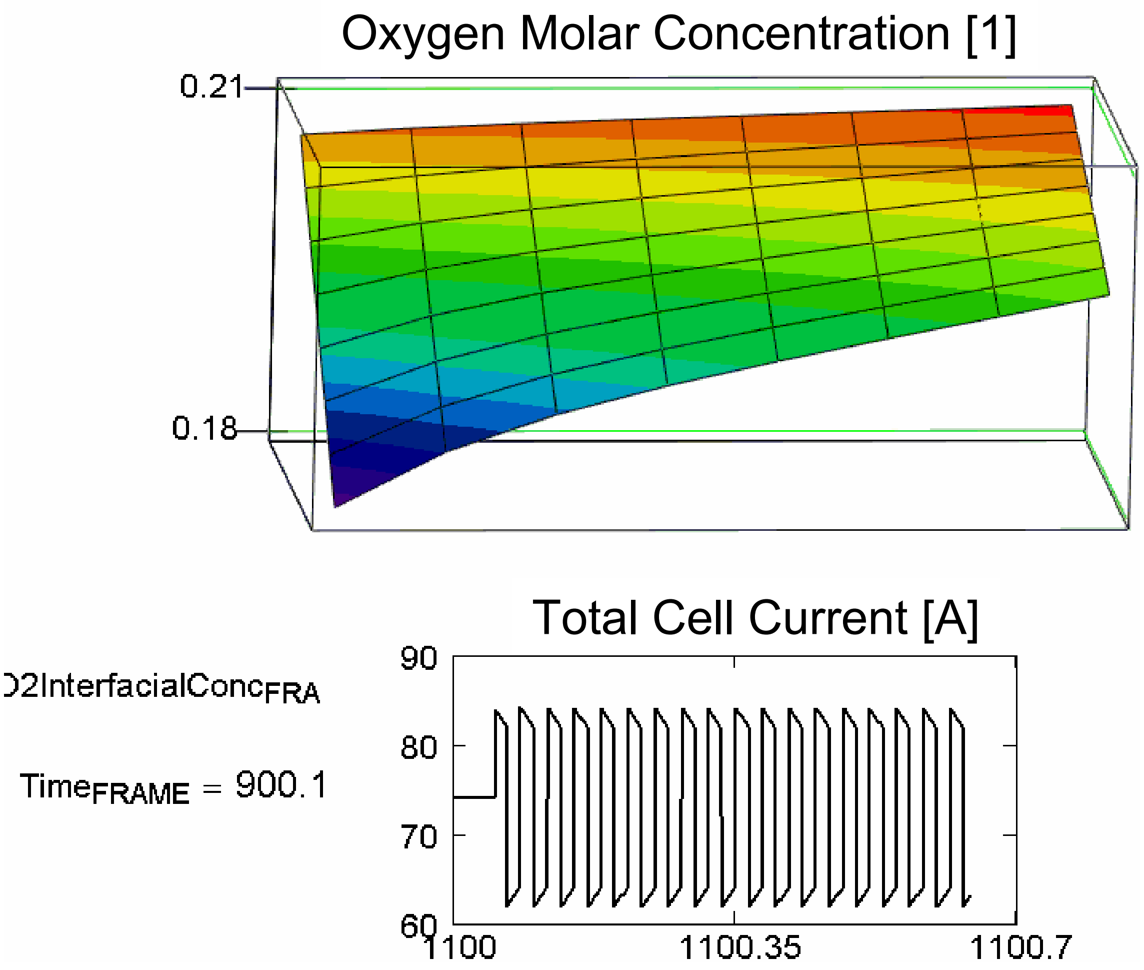


Case 2: Oxygen Interfacial Concentration

(10cm x 10cm; 30Hz Ripple; voltage driven; 8x8 nodes)

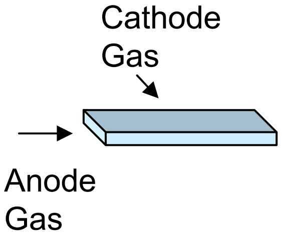


- **O2 response due to 30Hz ripple is like a wave, with largest oscillation at the exit.**

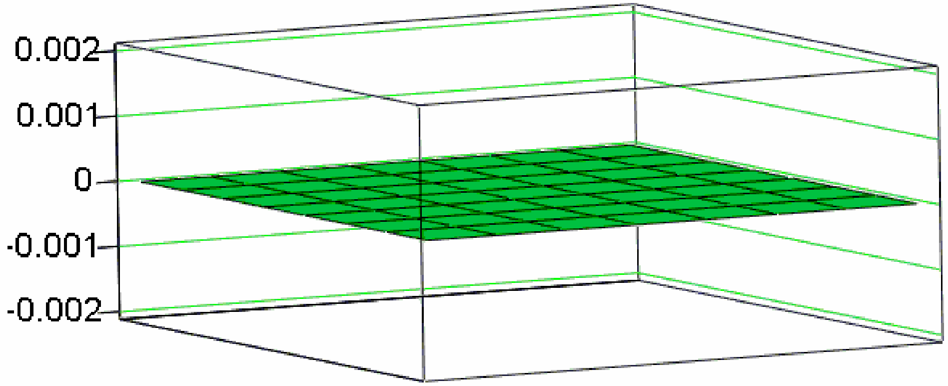


Case 2: Oxygen Deviation from Steady State

(10cm x 10cm; 30Hz Ripple; voltage driven; 8x8 nodes)



Oxygen Molar Concentration [1]

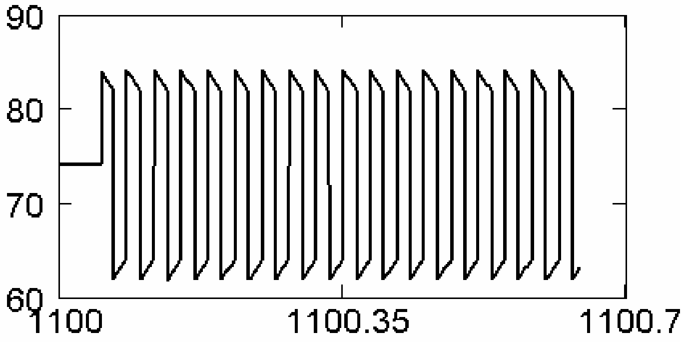


- **Ave. O2 concentration toward exit nodes appears increased compared to SS condition. Needs to be investigated further.**

DeltaO2FRAME

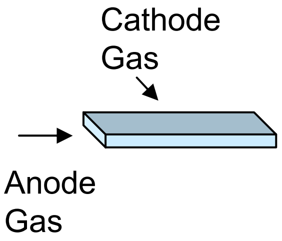
TFRAME = 1080.100

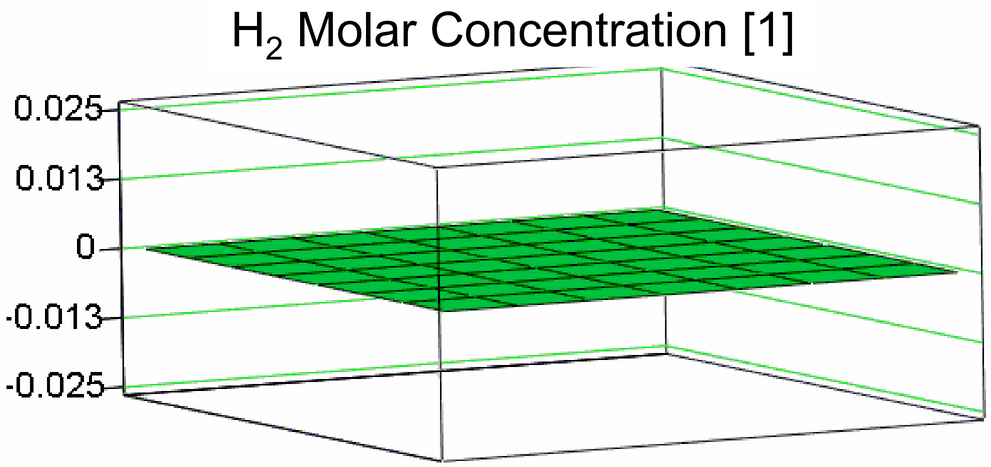
Total Cell Current [A]



Case 2: Hydrogen Deviation from Steady State

(10cm x 10cm; 30Hz Ripple; voltage driven; 8x8 nodes)





DeltaH2FRAME

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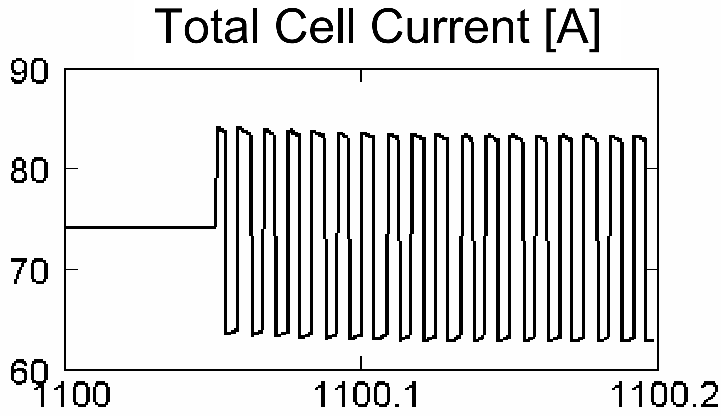
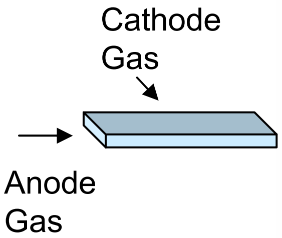
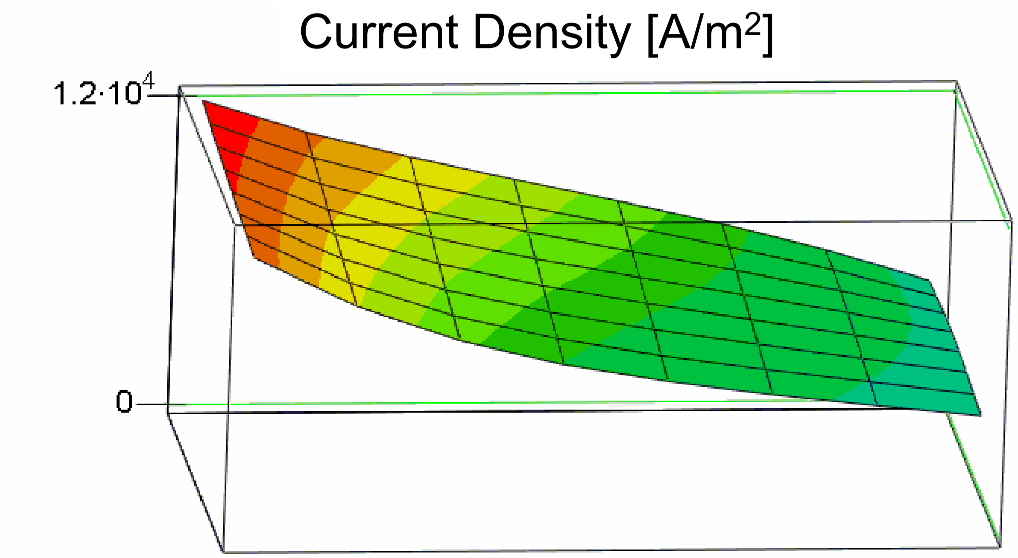


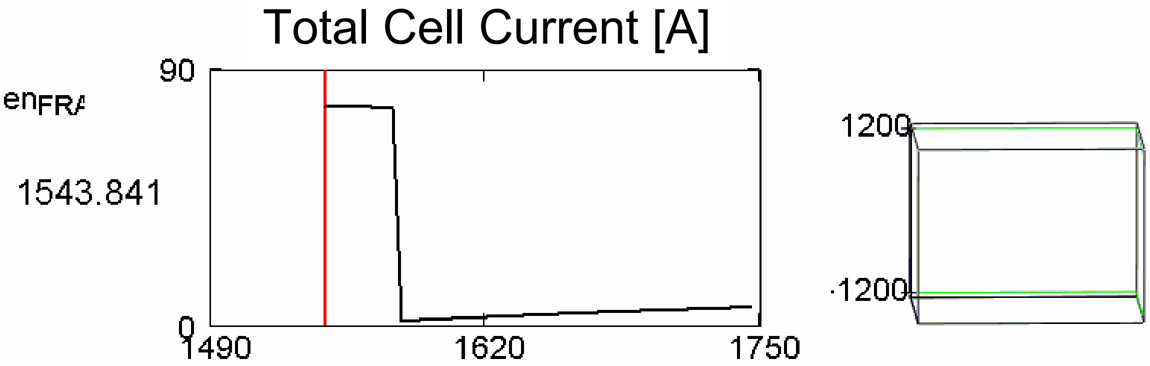
- **Ave. H2 concentration toward air inlet side appears increased compared to SS condition. H2 concentration toward air exit side appears decreased compared to SS condition.**

Case 3: Unload

(10cm x 10cm; 8x8 nodes)







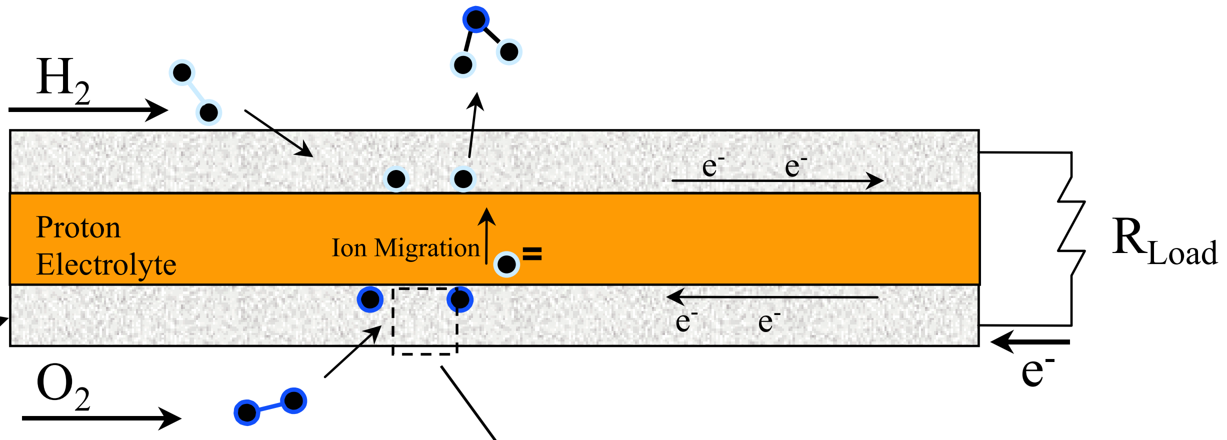
- **Upon unload, current density over portions of the surface reverse (electrolysis) as cell attempts to reach new thermal and specie equilibrium.**

Conclusions (Full Cell Transient Studies)

- For frequencies above 120Hz, response of fuel cell is mostly uniform over cell surface.
- For frequencies below 120Hz, oxygen response begins to become ‘wave-like’, while hydrogen response is mostly uniform over cell surface.
- Current density response is mostly uniform for all cases studied (little frequency dependency).
- Ripple induces a slightly modified time-average response to hydrogen (more H2 conc. at air inlet side, less at exit side).

- Certain dynamic conditions (unloading) can cause current reversal over portions of the cell.

1-Dim. Electrode Model Results



- 0.017 in. thick
- 40% porosity

$$\varepsilon \frac{dY_j}{dt} + u\nabla Y_j = D'\nabla^2 Y_j$$

$$\frac{dP_j}{dt} = \frac{RT_s}{V_s}\left(n_i Y_{j\_i} - n_o Y_{j\_o} - \frac{I(t)N}{Z_j F}\right)$$

$$D' = D\frac{\varepsilon}{\tau} \qquad u = N/\rho\varepsilon^{2/3}$$

D=Knudsen+Molecular Diffusion
N=Molar Flux
ρ=Molar density

Ripple Model

- **Assume steady DC current component and a square wave ripple component imposed at the electrode/membrane interface:**

  $I(t) = A*S[1+x*sq(\omega*t)]$

  where,

  A = current amplitude factor [amp/m^2]

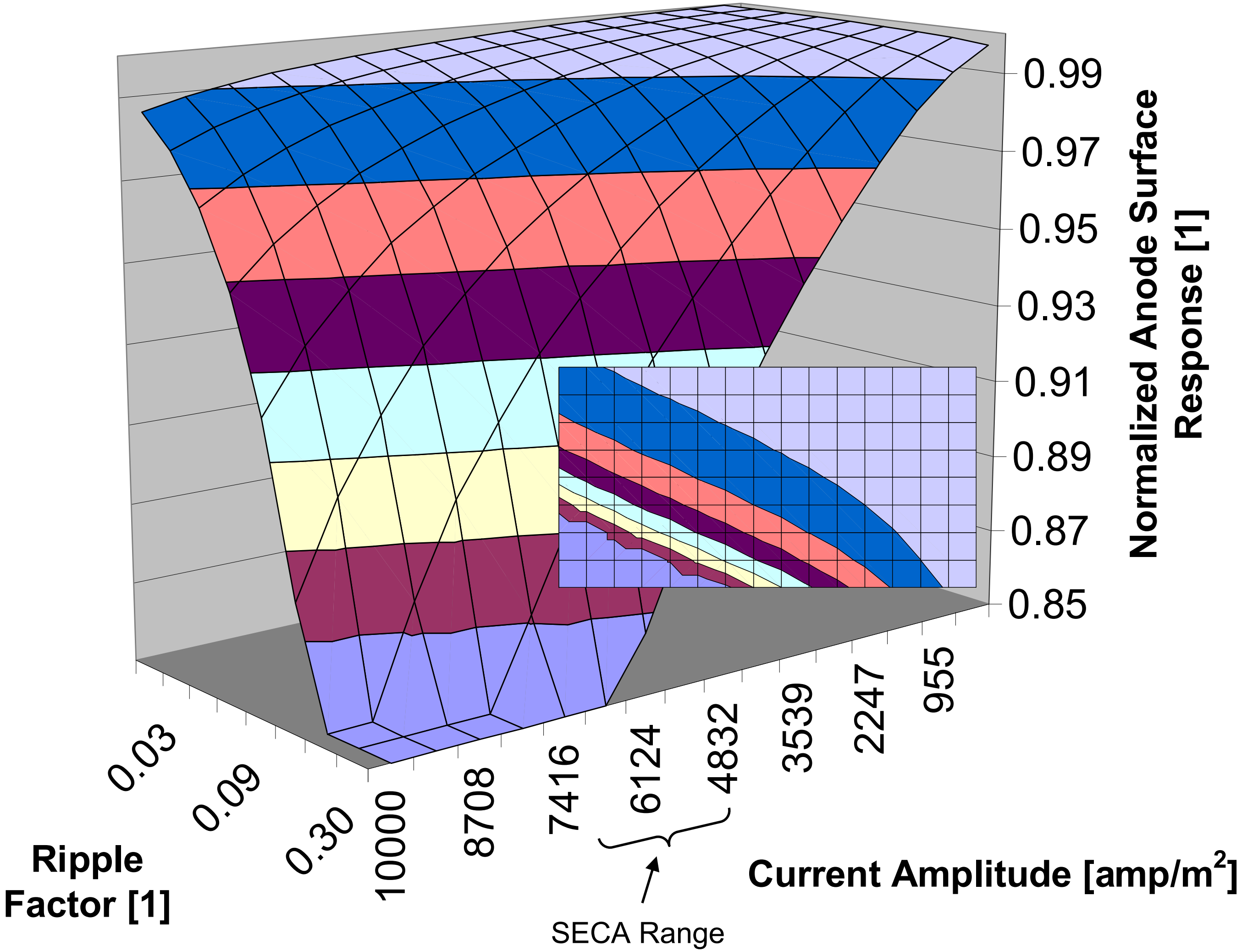
  S = active area [m^2]

  x = ripple factor [1]

  $sq(\omega*t)$ = square wave of unity amplitude and frequency ω.

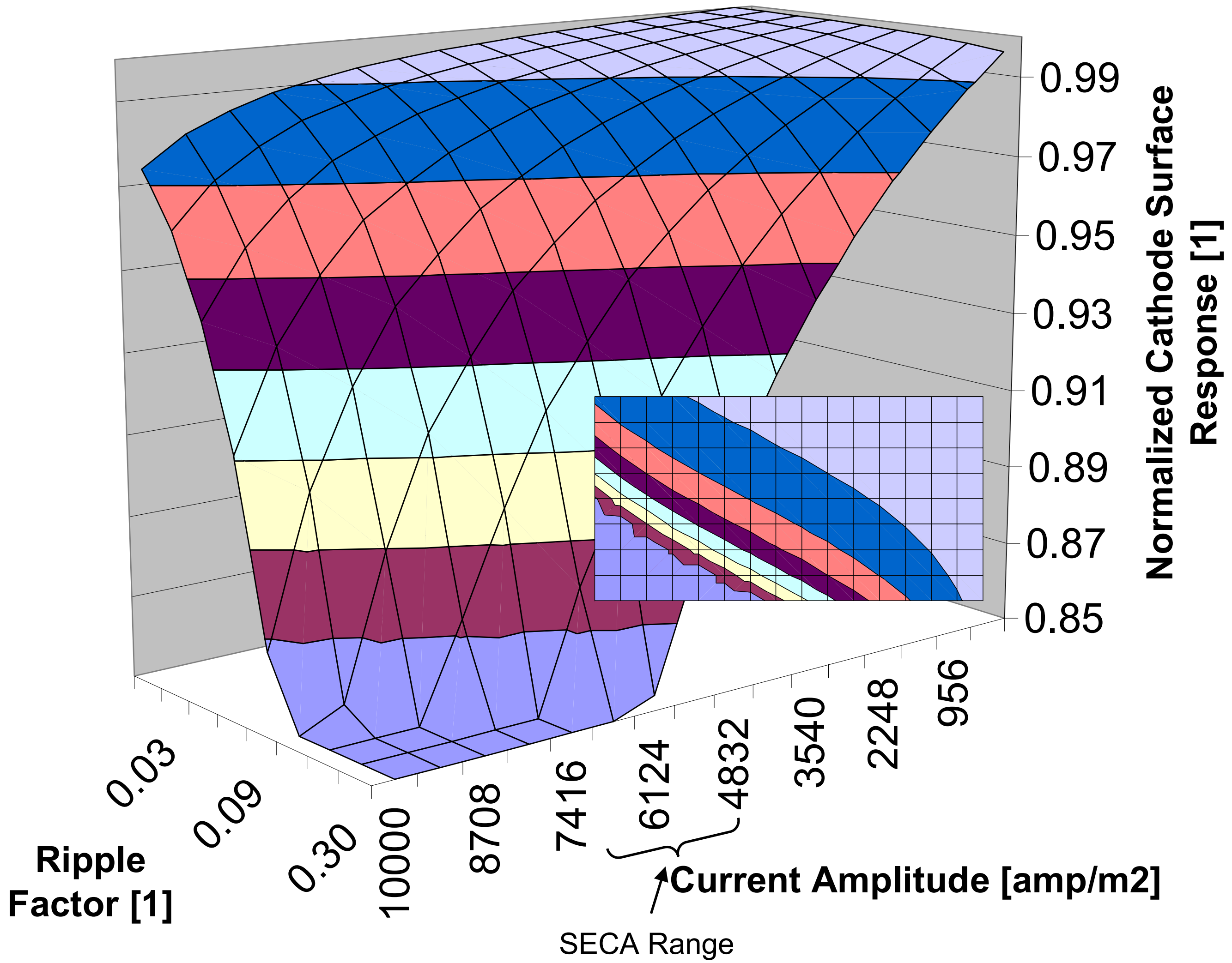
Impact of Inverter Dynamic Load

Anode Electrode Model H2 Response (120 Hz fixed 0.8 utilization)

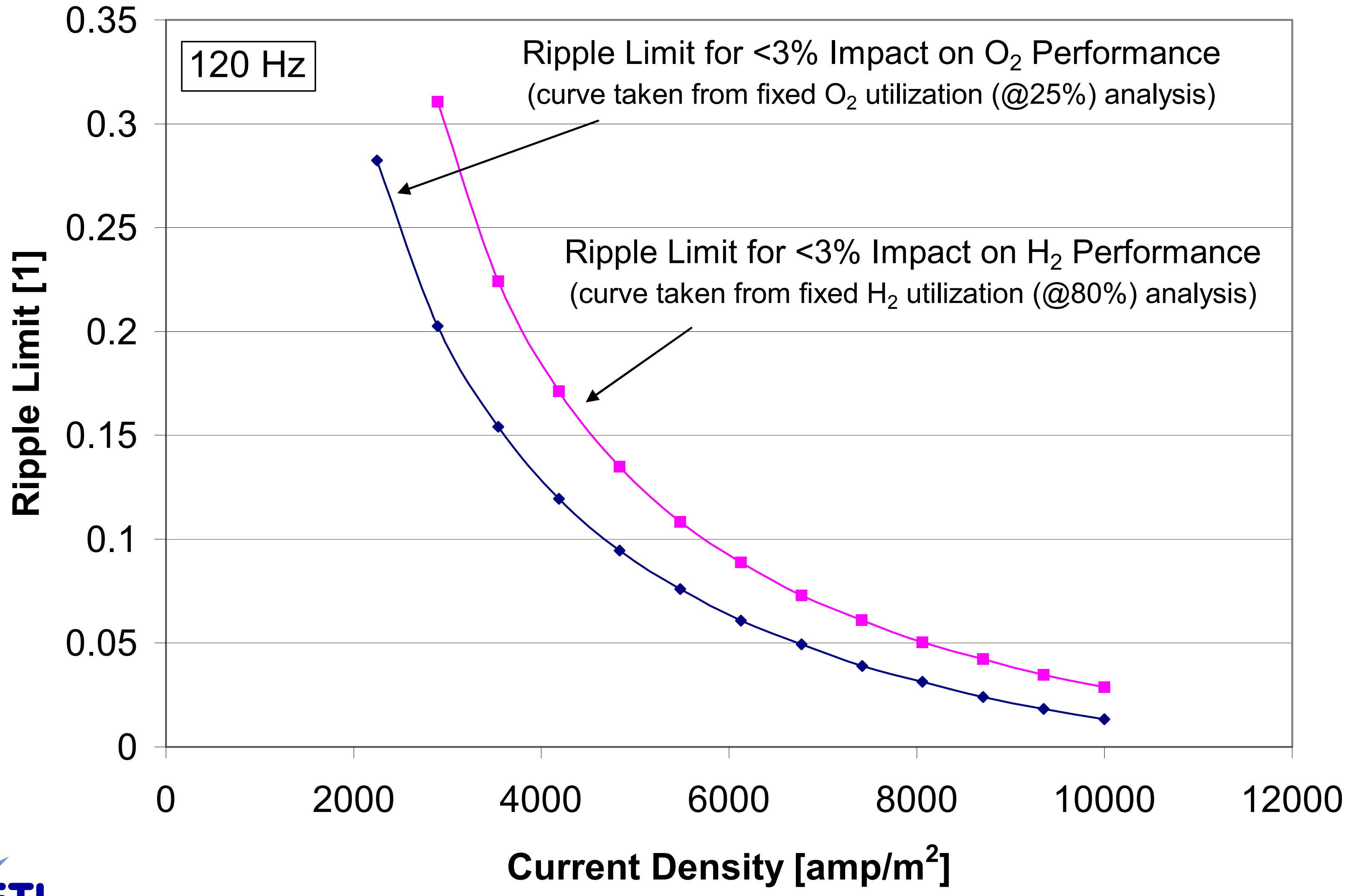


Impact of Inverter Dynamic Load

Cathode Electrode Model O2 Response (120 Hz fixed 0.25 utilization)



Ripple Limits – Anode & Cathode



Conclusion (Electrode Study)

- Unmitigated, inverter loads can significantly modify the conditions within and around the fuel cell electrodes as compared to *equivalent* steady loads.
- Both anode and cathode supported electrodes should be carefully examined…cathode supported electrodes are impacted more severely, however.
- To ensure minor impact to the fuel cell conditions, inverter ripple factors should be controlled to less than 6%-9%.
- Ripple frequencies above 400 Hz have minor effects.

Results (cont.)

- **Built & configured hardware needed to experimentally assess ripple and other dynamic issues for SOFC's.**
- **1st experimental ripple study now underway.**

Applicability to SOFC Commercialization

- **Providing basic understanding (engineering knowledge base) for how dynamic loads deviate from steady loads.**
- **Gained following understanding:**
  - Inverter loads can significantly modify the conditions within and around the fuel cell electrodes as compared to *equivalent* steady loads.
  - To ensure minor impact to the fuel cell conditions, inverter ripple factors should be controlled to less than 6%-9%.
  - Ripple frequencies above 400 Hz have minor effects.
  - For frequencies above 120Hz, response of fuel cell is mostly uniform over cell surface.
  - For frequencies below 120Hz, oxygen response begins to become ‘wave-like’, while hydrogen response remains mostly uniform over cell surface.
  - Current density response is mostly uniform for all cases studied (little frequency dependency).
  - Ripple induces a slightly modified time-average response to hydrogen (more H2 conc. at air inlet side, less at exit side).

FY04 Project Tasks

- **Task 1 – Obtain experimental data on cell degradation**
  - Obtain baseline steady load degradation rate using standard cells
  - Impose ripple (20-30% at simulated high utilization) to determine change in degradation rate
  - Acquire resistance data—impedance spectroscopy; potentiometric/galvanic interrupt studies
  - Run duplicate cases: 2^+ at steady load and 2^+ unsteady load
- **Task 2 – Evaluate material properties**
  - Evaluate material properties of both unsteady and steady cells to identify different or accelerated degradation behavior
    - SEM, XPS, EDS, XRD
- **Task 3 – Model experimental conditions**
  - Apply models to experimental cases
  - Provide detailed understanding of performance at the cell level
- **Task 4 – Journal publications and presentations**